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WHIZARD¹

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

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Abstract

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

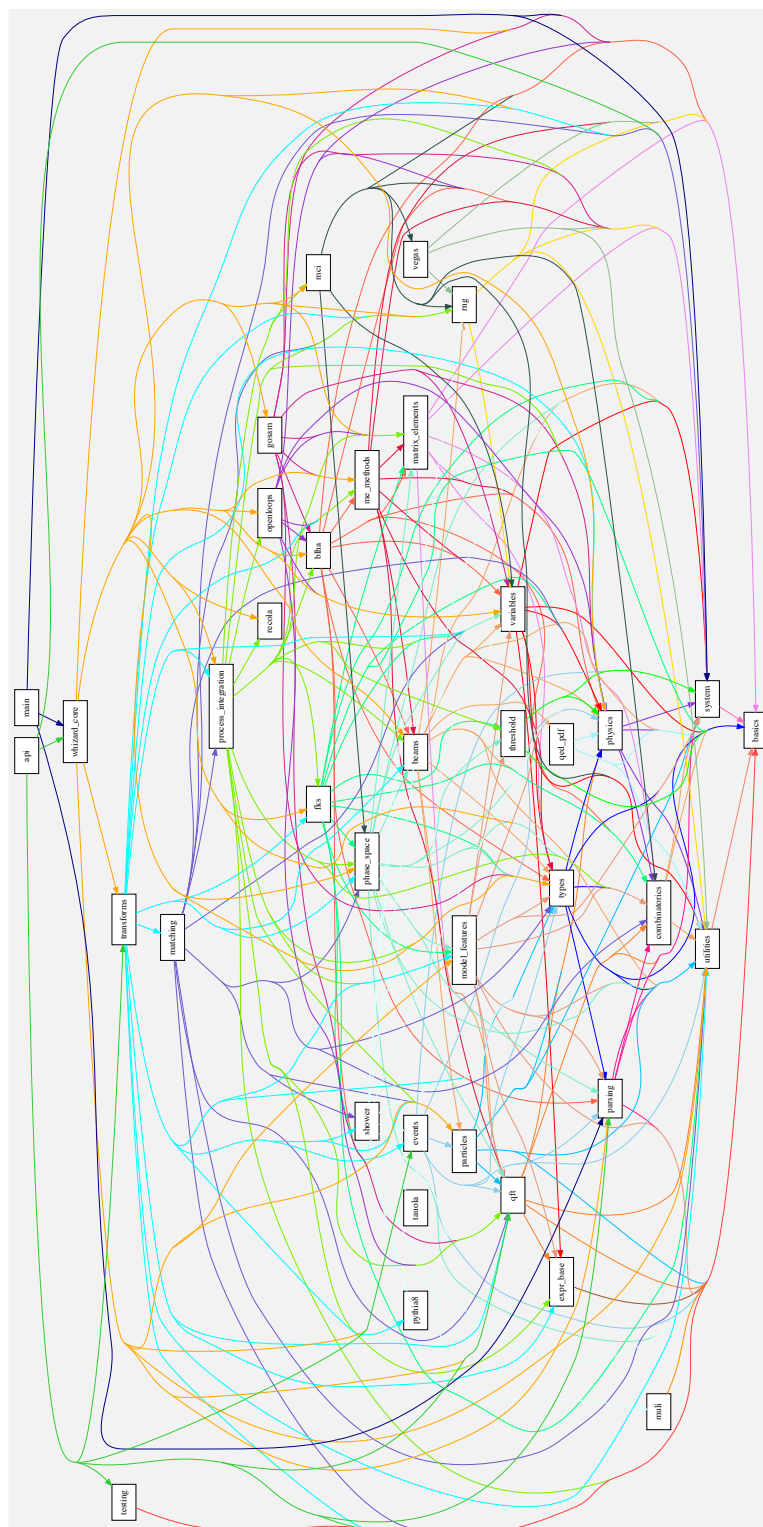


Figure 1: Overall folder structure

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Chapter 1

Changes

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

Chapter 2

Preliminaries

The WHIZARD file header:

```
<File header>≡
! WHIZARD <Version> <Date>
!
! Copyright (C) 1999-2021 by
!   Wolfgang Kilian <kilian@physik.uni-siegen.de>
!   Thorsten Ohl <ohl@physik.uni-wuerzburg.de>
!   Juergen Reuter <juergen.reuter@desy.de>
!
!   with contributions from
!   cf. main AUTHORS file
!
! WHIZARD is free software; you can redistribute it and/or modify it
! under the terms of the GNU General Public License as published by
! the Free Software Foundation; either version 2, or (at your option)
! any later version.
!
! WHIZARD is distributed in the hope that it will be useful, but
! WITHOUT ANY WARRANTY; without even the implied warranty of
! MERCHANTABILITY or FITNESS FOR A PARTICULAR PURPOSE. See the
! GNU General Public License for more details.
!
! You should have received a copy of the GNU General Public License
! along with this program; if not, write to the Free Software
! Foundation, Inc., 675 Mass Ave, Cambridge, MA 02139, USA.
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! This file has been stripped of most comments. For documentation, refer
! to the source 'whizard.nw'
```

We are strict with our names:

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

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

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


<Use kinds with double>≡

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

And we make heavy use of variable-length strings

<Use strings>≡

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

Access to the `debug_on` master switch

<Use debug>≡

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

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

<Use mpi f08>≡

<MPI: Use mpi f08>≡

```
use mpi_f08 !NODEP!
```

Chapter 3

Utilities

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

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

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

file_registries Manage files that are accessed by their name.

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

format_utils Utilities for pretty-printing.

format_defs Predefined format strings.

numeric_utils Utilities for comparing numerical values.

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

3.1 File Utilities

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

- Delete a named file

`<file_utils.f90>`≡

<File header>

`module file_utils`

`use io_units`

<Standard module head>

<File utils: public>

`contains`

No internal dependencies

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

⟨File utils: procedures⟩

```
end module file_utils
```

3.1.1 Deleting a file

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

⟨File utils: public⟩≡

```
public :: delete_file
```

⟨File utils: procedures⟩≡

```
subroutine delete_file (name)
  character(*), intent(in) :: name
  logical :: exist
  integer :: u
  inquire (file = name, exist = exist)
  if (exist) then
    u = free_unit ()
    open (unit = u, file = name)
    close (u, status = "delete")
  end if
end subroutine delete_file
```

3.2 File Registries

This module provides a file-registry facility. We can open and close files multiple times without inadvertently accessing a single file by two different I/O unit numbers. Opening a file the first time enters it into the registry. Opening again

just returns the associated I/O unit. The registry maintains a reference count, so closing a file does not actually complete until the last reference is released.

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

```

<file_registries.f90>≡
  <File header>

  module file_registries

    <Use strings>
      use io_units

    <Standard module head>

    <File registries: public>

    <File registries: types>

    contains

    <File registries: procedures>

  end module file_registries

```

3.2.1 File handle

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

```

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

```

Debugging output:

```

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

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

```

```

        write (u, "(3x,A,1x,'( ',IO,')')") &
            char (handle%file), handle%refcount
    end if
end subroutine file_handle_write

```

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

```

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

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

```

We check the `refcount` before actually opening the file.

```

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

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

```

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

```

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

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

```

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

```

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

```

```

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

```

Return the filename, so we can identify the entry.

```

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

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

```

For debugging, return the I/O unit number.

```

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

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

```

3.2.2 File handles registry

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

Extend the handle type to become a list entry:

```

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

```

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

```

<File registries: public>≡
public :: file_registry_t

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

```

Debugging output.

<File registries: file registry: TBP>≡

```
procedure :: write => file_registry_write
```

<File registries: procedures>+≡

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

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

<File registries: file registry: TBP>+≡

```
procedure :: open => file_registry_open
```

<File registries: procedures>+≡

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

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

```

<File registries: file_registry: TBP>+≡
    procedure :: close => file_registry_close

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

```

3.3 String Utilities

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

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

```

<string_utils.f90>≡
    <File header>

    module string_utils

        use, intrinsic :: iso_c_binding

        <Use kinds>
        <Use strings>

        <Standard module head>

        <String utils: public>

```


<String utils: interfaces>

contains

<String utils: procedures>

end module string_utils

3.3.1 Upper and Lower Case

These are, unfortunately, not part of Fortran.

<String utils: public>≡

```
public :: upper_case
public :: lower_case
```

<String utils: interfaces>≡

```
interface upper_case
  module procedure upper_case_char, upper_case_string
end interface
interface lower_case
  module procedure lower_case_char, lower_case_string
end interface
```

<String utils: procedures>≡

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

```
function lower_case_char (string) result (new_string)
  character(*), intent(in) :: string
  character(len(string)) :: new_string
  integer :: pos, code
  integer, parameter :: offset = ichar('a')-ichar('A')
  do pos = 1, len (string)
    code = ichar (string(pos:pos))
    select case (code)
      case (ichar('A'):ichar('Z'))
        new_string(pos:pos) = char (code + offset)
      case default
        new_string(pos:pos) = string(pos:pos)
    end select
  end do
end function lower_case_char
```

```

        end do
    end function lower_case_char

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

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

```

3.3.2 C-Fortran String Conversion

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

```

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

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

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

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

```

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

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

```

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

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

        integer :: i

```

```

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

end subroutine strcpy_f2c

```

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

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

```

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

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

        integer :: i, n

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

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

    end function string_c2f

```

3.3.3 Number Conversion

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

```

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

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

<String utils: procedures>+≡
    function str_log (l) result (s)
        logical, intent(in) :: l
        type(string_t) :: s
        if (l) then

```

```

        s = "True"
    else
        s = "False"
    end if
end function str_log

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

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

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

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

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

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

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

<concatenate strings>≡
type(string_t) :: s
integer :: i
s = '['
do i = 1, size(x) - 1
    s = s // str(x(i)) // ', '

```

```

end do
s = s // str(x(size(x))) // ']'

```

Auxiliary: Read real, integer, string value.

```

<String utils: public>+≡
  public :: read_rval
  public :: read_ival

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

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

```

3.3.4 String splitting

```

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

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

```

Create an array of strings using a separator.

```

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

<String utils: procedures>+≡
  pure subroutine split_string (str, separator, str_array)
    type(string_t), dimension(:), allocatable, intent(out) :: str_array
    type(string_t), intent(in) :: str, separator
    type(string_t) :: str_tmp, str_out

```

```

integer :: n_str
n_str = 0; str_tmp = str
do while (string_contains_word (str_tmp, separator))
    n_str = n_str + 1
    call split (str_tmp, str_out, separator)
end do
allocate (str_array (n_str))
n_str = 1; str_tmp = str
do while (string_contains_word (str_tmp, separator))
    call split (str_tmp, str_array (n_str), separator)
    n_str = n_str + 1
end do
end subroutine split_string

```

3.4 Format Utilities

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

- Horizontal separator lines in output
- Indenting an output line
- Formatting a number for T_EX output.
- Formatting a number for MetaPost output.
- Alternate numeric formats.

```

⟨format_utils.f90⟩≡
⟨File header⟩

module format_utils

  ⟨Use kinds⟩
  ⟨Use strings⟩
  use string_utils, only: lower_case
  use io_units, only: given_output_unit

  ⟨Standard module head⟩

  ⟨Format utils: public⟩

contains

  ⟨Format utils: procedures⟩

end module format_utils

```

3.4.1 Line Output

Write a separator line.

```

⟨Format utils: public⟩≡
public :: write_separator

```

```

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

```

Indent the line with given number of blanks.

```

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

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

```

3.4.2 Array Output

Write an array of integers.

```

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

<Format utils: procedures>+≡
subroutine write_integer_array (array, unit, n_max, no_skip)
  integer, intent(in), dimension(:) :: array
  integer, intent(in), optional :: unit
  integer, intent(in), optional :: n_max
  logical, intent(in), optional :: no_skip
  integer :: u, i, n
  logical :: yorn
  u = given_output_unit (unit)
  yorn = .false.; if (present (no_skip)) yorn = no_skip
  if (present (n_max)) then
    n = n_max
  else
    n = size (array)
  end if
  do i = 1, n
    if (i < n .or. yorn) then
      write (u, "(I0, A)", advance = "no") array(i), ", "
    end if
  end do
end subroutine write_integer_array

```

```

        else
            write (u, "(I0)") array(i)
        end if
    end do
end subroutine write_integer_array

```

3.4.3 T_EX-compatible Output

Quote underscore characters for use in T_EX output.

```

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

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

```

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

```

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

<Format utils: procedures>+≡
    function tex_format (rval, n_digits) result (string)
        type(string_t) :: string
        real(default), intent(in) :: rval
        integer, intent(in) :: n_digits
        integer :: e, n, w, d
        real(default) :: absval
        real(default) :: mantissa
        character :: sign
        character(20) :: format
        character(80) :: cstr
        n = min (abs (n_digits), 16)
        if (rval == 0) then
            string = "0"
        else
            absval = abs (rval)
            e = int (log10 (absval))
            if (rval < 0) then
                sign = "-"
            else
                sign = ""
            end if
        end if
    end function tex_format

```



```

end if
select case (e)
case (:-3)
  d = max (n - 1, 0)
  w = max (d + 2, 2)
  write (format, "(('F',IO,'.',IO,'A,IO,A)'))" w, d
  mantissa = absval * 10._default ** (1 - e)
  write (cstr, fmt=format) mantissa, "\times 10^{", e - 1, "}"
case (-2:0)
  d = max (n - e, 1 - e)
  w = max (d + e + 2, d + 2)
  write (format, "(('F',IO,'.',IO,''))" w, d
  write (cstr, fmt=format) absval
case (1:2)
  d = max (n - e - 1, -e, 0)
  w = max (d + e + 2, d + 2, e + 2)
  write (format, "(('F',IO,'.',IO,''))" w, d
  write (cstr, fmt=format) absval
case default
  d = max (n - 1, 0)
  w = max (d + 2, 2)
  write (format, "(('F',IO,'.',IO,'A,IO,A)'))" w, d
  mantissa = absval * 10._default ** (- e)
  write (cstr, fmt=format) mantissa, "\times 10^{", e, "}"
end select
string = sign // trim (cstr)
end if
end function tex_format

```

3.4.4 Metapost-compatible Output

Write a number for use in Metapost code:

```

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

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

```

3.4.5 Conditional Formatting

Conditional format string, intended for switchable numeric precision.

```

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

```

```

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

```

3.4.6 Guard tiny values

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

```

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

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

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

end function refmt_tiny

```

3.4.7 Compressed output of integer arrays

```

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

<Format utils: procedures>+≡
subroutine write_compressed_integer_array (chars, array)
  character(len=*), intent(out) :: chars

```

```

integer, intent(in), allocatable, dimension(:) :: array
logical, dimension(:), allocatable :: used
character(len=16) :: tmp
type(string_t) :: string
integer :: i, j, start_chain, end_chain
chars = '[none]'
string = ""
if (allocated (array)) then
  if (size (array) > 0) then
    allocate (used (size (array)))
    used = .false.
    do i = 1, size (array)
      if (.not. used(i)) then
        start_chain = array(i)
        end_chain = array(i)
        used(i) = .true.
        EXTEND: do
          do j = 1, size (array)
            if (array(j) == end_chain + 1) then
              end_chain = array(j)
              used(j) = .true.
              cycle EXTEND
            end if
            if (array(j) == start_chain - 1) then
              start_chain = array(j)
              used(j) = .true.
              cycle EXTEND
            end if
          end do
        end do
        exit
      end do EXTEND
    if (end_chain - start_chain > 0) then
      write (tmp, "(I0,A,I0)") start_chain, "-", end_chain
    else
      write (tmp, "(I0)") start_chain
    end if
    string = string // trim (tmp)
    if (any (.not. used)) then
      string = string // ', '
    end if
  end if
end if
chars = string
end if
chars = adjustl (chars)
end subroutine write_compressed_integer_array

```

3.5 Format Definitions

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

```

<format_defs.f90>≡
  <File header>

```

```

  module format_defs

```

```

    <Standard module head>

```

```

    <Format defs: public parameters>

```

```

  end module format_defs

```

We collect format strings for various numerical output formats here.

```

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

```

Fixed-point formats for better readability, where appropriate.

```

<Format defs: public parameters>+≡
  character(*), parameter, public :: FMT_12 = "F12.9"

```

3.6 Numeric Utilities

```

<numeric_utils.f90>≡
  <File header>

```

```

  module numeric_utils

```

```

    <Use kinds>

```

```

    <Use strings>

```

```

      use string_utils

```

```

      use constants

```

```

      use format_defs

```

```

    <Standard module head>

```

```

    <Numeric utils: public>

```

```

    <Numeric utils: parameters>

```

```

    <Numeric utils: types>

```

```

    <Numeric utils: interfaces>

```

```

  contains

```

<Numeric utils: procedures>

end module numeric_utils

<Numeric utils: public>≡

public :: assert

<Numeric utils: procedures>≡

```
subroutine assert (unit, ok, description, exit_on_fail)
  integer, intent(in) :: unit
  logical, intent(in) :: ok
  character(*), intent(in), optional :: description
  logical, intent(in), optional :: exit_on_fail
  logical :: ef
  ef = .false.; if (present (exit_on_fail)) ef = exit_on_fail
  if (.not. ok) then
    if (present(description)) then
      write (unit, "(A)") "* FAIL: " // description
    else
      write (unit, "(A)") "* FAIL: Assertion error"
    end if
    if (ef) stop 1
  end if
end subroutine assert
```

Compare numbers and output error message if not equal.

<Numeric utils: public>+≡

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

<Numeric utils: procedures>+≡

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

<Numeric utils: procedures>+≡

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

```

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

```

(Numeric utils: procedures)+≡

```

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

```

(Numeric utils: procedures)+≡

```

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

```

(Numeric utils: procedures)+≡

```

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

```

```

<Numeric utils: procedures>+=
  subroutine assert_equal_complexs (unit, lhs, rhs, description, &
                                   abs_smallness, rel_smallness, exit_on_fail)

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

```

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

```

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

```

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

```

<Numeric utils: public>+=
  public :: nearly_equal

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

```

```

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

```

```

        return
    end if
    abs_small = tiny_13; if (present (abs_smallness)) abs_small = abs_smallness
    rel_small = tiny_10; if (present (rel_smallness)) rel_small = rel_smallness
    if (abs_a < abs_small .and. abs_b < abs_small) then
        r = diff < abs_small
    else
        r = diff / max (abs_a, abs_b) < rel_small
    end if
end function nearly_equal_real

```

<Numeric utils: procedures>+≡

```

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

```

Often we will need to check whether floats vanish:

<Numeric utils: public>+≡

```

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

```

<Numeric utils: procedures>+≡

```

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

```

```

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

```

<Numeric utils: public>+≡

```

public :: expanded_amp2

```

<Numeric utils: procedures>+≡

```

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

```



```

<Numeric utils: public>+≡
  public :: abs2

<Numeric utils: procedures>+≡
  elemental function abs2 (c) result (c2)
    real(default) :: c2
    complex(default), intent(in) :: c
    c2 = real (c * conjg(c))
  end function abs2

```

Remove element with index from array

```

<Numeric utils: public>+≡
  public:: remove_array_element
  interface remove_array_element
    module procedure remove_array_element_logical
  end interface

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

```

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

```

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

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

```

```

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

```

```

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

```

```

<Numeric utils: public>+=
public :: crop_integer_array
<Numeric utils: procedures>+=
subroutine crop_integer_array (list, i_crop)
  integer, intent(inout), dimension(:), allocatable :: list
  integer, intent(in) :: i_crop
  integer, dimension(:), allocatable :: list_store
  allocate (list_store (i_crop))
  list_store = list(1:i_crop)
  deallocate (list)
  allocate (list (i_crop))
  list = list_store
  deallocate (list_store)
end subroutine crop_integer_array

```

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

```

<Numeric utils: public>+=
public :: log_prec
<Numeric utils: procedures>+=
function log_prec (x, xb) result (lx)
  real(default), intent(in) :: x, xb
  real(default) :: a1, a2, a3, lx
  a1 = xb
  a2 = a1 * xb / two
  a3 = a2 * xb * two / three
  if (abs (a3) < epsilon (a3)) then
    lx = - a1 - a2 - a3
  else
    lx = log (x)
  end if
end function log_prec

```

```

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

```

```

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

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

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

```

3.7 Binary Tree

```

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

    implicit none

    private

    type :: binary_tree_iterator_t
      integer, dimension(:), allocatable :: key
      integer :: current
      !! current \in {1, N}.
    contains
      procedure :: init => binary_tree_iterator_init
      procedure :: is_iterable => binary_tree_iterator_is_iterable
      procedure :: next => binary_tree_iterator_next
    end type binary_tree_iterator_t

```

```

type :: binary_tree_node_t
  integer :: height = 0
  type(binary_tree_node_t), pointer :: left => null ()
  type(binary_tree_node_t), pointer :: right => null ()
  !!
  integer :: key = 0
  class(*), pointer :: obj => null ()
contains
  procedure :: init => binary_tree_node_init
  procedure :: write => binary_tree_node_write
  procedure :: get_balance => binary_tree_node_get_balance
  procedure :: increment_height => binary_tree_node_increment_height
  final :: binary_tree_node_final
end type binary_tree_node_t

type :: binary_tree_t
  integer :: n_elements = 0
  type(binary_tree_node_t), pointer :: root => null ()
contains
  procedure :: write => binary_tree_write
  procedure :: get_n_elements => binary_tree_get_n_elements
  procedure :: insert => binary_tree_insert
  procedure, private :: insert_node => binary_tree_insert_node
  procedure, private :: balance => binary_tree_balance
  procedure :: search => binary_tree_search
  procedure :: has_key => binary_tree_has_key
  procedure, private :: rotate_left => binary_tree_rotate_left
  procedure, private :: rotate_right => binary_tree_rotate_right
  procedure :: clear => binary_tree_clear
  final :: binary_tree_final
end type binary_tree_t

public :: binary_tree_t, binary_tree_iterator_t
contains
  !! We store all keys of the binary tree in an index array.
  !! Flatten the tree  $O(\log n)$ , each access is then  $O(1)$ .
  !! However, accessing the corresponding object costs one  $O(\log n)$ .
  subroutine binary_tree_iterator_init (iterator, btree)
    class(binary_tree_iterator_t), intent(inout) :: iterator
    type(binary_tree_t), target :: btree
    type(binary_tree_node_t), pointer :: node
    integer :: idx
    iterator%current = 1
    allocate (iterator%key(btree%get_n_elements ()), source = 0)
    if (.not. btree%get_n_elements () > 0) return
    idx = 1; call fill_key (idx, iterator%key, btree%root)
contains
  recursive subroutine fill_key (idx, key, node)
    integer, intent(inout) :: idx
    integer, dimension(:), intent(inout) :: key
    type(binary_tree_node_t), pointer :: node
    if (associated (node%left)) &
      call fill_key (idx, key, node%left)
    key(idx) = node%key

```

```

        idx = idx + 1
        if (associated (node%right)) &
            call fill_key (idx, key, node%right)
        end subroutine fill_key
    end subroutine binary_tree_iterator_init

function binary_tree_iterator_is_iterable (iterator) result (flag)
    class(binary_tree_iterator_t), intent(in) :: iterator
    logical :: flag
    flag = iterator%current <= size (iterator%key)
end function binary_tree_iterator_is_iterable

subroutine binary_tree_iterator_next (iterator, key)
    class(binary_tree_iterator_t), intent(inout) :: iterator
    integer, intent(out) :: key
    if (.not. iterator%is_iterable ()) then
        key = 0
    else
        key = iterator%key(iterator%current)
        iterator%current = iterator%current + 1
    end if
end subroutine binary_tree_iterator_next

subroutine binary_tree_node_init (btree_node, key, obj)
    class(binary_tree_node_t), intent(inout) :: btree_node
    integer, intent(in) :: key
    class(*), pointer :: obj
    btree_node%height = 1
    btree_node%left => null ()
    btree_node%right => null ()
    btree_node%key = key
    btree_node%obj => obj
end subroutine binary_tree_node_init

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

integer function binary_tree_node_get_balance (btree_node) result (balance)

```

```

class(binary_tree_node_t), intent(in) :: btree_node
integer :: leftHeight, rightHeight
leftHeight = 0
rightHeight = 0
if (associated (btree_node%left)) leftHeight = btree_node%left%height
if (associated (btree_node%right)) rightHeight = btree_node%right%height
balance = leftHeight - rightHeight
end function binary_tree_node_get_balance

subroutine binary_tree_node_increment_height (btree_node)
class(binary_tree_node_t), intent(inout) :: btree_node
integer :: leftHeight, rightHeight
leftHeight = 0
rightHeight = 0
if (associated (btree_node%left)) leftHeight = btree_node%left%height
if (associated (btree_node%right)) rightHeight = btree_node%right%height
btree_node%height = max (leftHeight, rightHeight) + 1
end subroutine binary_tree_node_increment_height

recursive subroutine binary_tree_node_final (btree_node)
type(binary_tree_node_t), intent(inout) :: btree_node
if (associated (btree_node%left)) deallocate (btree_node%left)
if (associated (btree_node%right)) deallocate (btree_node%right)
deallocate (btree_node%obj)
end subroutine binary_tree_node_final

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

subroutine binary_tree_final (btree)
type(binary_tree_t), intent(inout) :: btree
btree%n_elements = 0
if (associated (btree%root)) then
deallocate (btree%root)
end if
end subroutine binary_tree_final

subroutine binary_tree_clear (btree)
class(binary_tree_t), intent(inout) :: btree
call binary_tree_final (btree)
end subroutine binary_tree_clear

integer function binary_tree_get_n_elements (btree) result (n)
class(binary_tree_t), intent(in) :: btree

```

```

    n = btree%n_elements
end function binary_tree_get_n_elements

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

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

!! Subtree: root of subtree (which is unbalance, refer to A in diagrams.)
subroutine binary_tree_balance (btree, subtree, key)
    class(binary_tree_t), intent(in) :: btree
    type(binary_tree_node_t), intent(inout), pointer :: subtree
    integer, intent(in) :: key
    type(binary_tree_node_t), pointer :: node, newNode
    integer :: balance
    balance = subtree%get_balance ()
    node => subtree
    newNode => null ()

```

```

!! balance := h_left - h_right.
!! Proof: balance > 0 => too many elements on the left side of the subtree.
!! Proof: balance < 0 => too many elements on the right side of the subtree.
if (balance > 1) then
  !! => left-side of subtree
  !!      A3(2)      B2(1)
  !!     /         /  \
  !!    B2(1)      C1(0) A1(0)
  !!   /
  !!  C1(0)
  !!
  !!      A3(3)      A1(2)      C2(1)
  !!     /         /         /  \
  !!    B1(1) LEFT C2(1) RIGHT B1(0) A3(0)
  !!   \         /
  !!    C2(0)    B1(0)
  if (subtree%left%key > key) then !! rotate right
    call btree%rotate_right (node, newNode)
  else !! subtree%left%key < key, rotate left, then right.
    call btree%rotate_left (node%left, newNode)
    node%left => newNode
    call btree%rotate_right (node, newNode)
  end if
else if (balance < -1) then
  !! => right-side of subtree
  !!      A0(2)      B1(1)
  !!     \         /  \
  !!    B1(1)      A1(0) C3(0)
  !!     \
  !!    C3(0)*
  !!
  !!      A1(2)      A1(2)      C2(1)
  !!     \         \         /  \
  !!    B3(1) RIGHT C2(1) LEFT A1(0) B3(0)
  !!     /         \
  !!    C2(0)      B3(0)
  if (subtree%right%key < key) then !! rotate left
    call btree%rotate_left (node, newNode)
  else !! subtree%right%key > key, rotate right, then left.
    call btree%rotate_right (node%right, newNode)
    node%right => newNode
    call btree%rotate_left (node, newNode)
  end if
end if
if (associated (newNode)) subtree => newNode
end subroutine binary_tree_balance

subroutine binary_tree_search (btree, key, obj)
  class(binary_tree_t), intent(in) :: btree
  integer, intent(in) :: key
  class(*), pointer, intent(out) :: obj
  type(binary_tree_node_t), pointer :: current
  current => btree%root
  obj => null ()

```



```

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

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

```

```

!!      A      Move B to A.
!!      / \
!!     B  E   1. Split B from A%left.
!!    / \    2. Temporarily pointer to D.
!!   C  D    3. Replace pointer to D by pointer to A - E.
!!           4. Set temporary pointer to D to A%left.
!!
!! 1.+2. B      T => D    A
!!      /        \
!!     C          E
!!
!! 3.    B      T => D
!!     / \
!!    C  A
!!       \
!!      E
!!

```

```

!! 4.      B
!!      / \
!!      C  A
!!      / \
!!      D  E
!!
!! \param[inout] root Root/parent root (A).
!! \param[out] new_root New root/parent root (B).
subroutine binary_tree_rotate_right (btree, root, new_root)
  class(binary_tree_t), intent(in) :: btree
  type(binary_tree_node_t), pointer, intent(inout) :: root
  type(binary_tree_node_t), pointer, intent(out) :: new_root
  type(binary_tree_node_t), pointer :: tmp
  new_root => root%left
  tmp => new_root%right
  new_root%right => root
  root%left => tmp
  call root%increment_height ()
  call new_root%increment_height ()
end subroutine binary_tree_rotate_right

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

```

```

        end subroutine binary_tree_rotate_left
    end module binary_tree

```

3.7.1 Unit tests

```

<binary_tree_ut.f90>≡
    <File header>

    module binary_tree_ut
        use unit_tests
        use binary_tree_util

    <Standard module head>

    <Binary tree: public test>

    contains

    <Binary tree: test driver>
    end module binary_tree_ut

<binary_tree_util.f90>≡
    <File header>

    module binary_tree_util

        use binary_tree

    <Standard module head>

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

    <Binary tree: test declarations>

    contains

    <Binary tree: tests>

    end module binary_tree_util

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

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

```

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

```

<Binary tree: execute tests>≡

```

```

call test (binary_tree_1, "binary_tree_1", &
  "check interface and implementation", &
  u, results)

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

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

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

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

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

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

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

    write (u, "(A)") "* Iterate over binary tree..."
    call iterator%init (btree)
    do while (iterator%is_iterable ())
      call iterator%next (key)
      call btree%search (key, obj)
      select type (obj)

```

```

        type is (btree_obj_t)
        write (u, "(2(A,1X,I3,1X))") "- KEY", key, "OBJ", obj%i
    end select
end do

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

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

```

3.8 Array List

```

(array_list.f90)≡
<File header>

module array_list
<Use kinds>
    use, intrinsic :: iso_fortran_env, only: ERROR_UNIT

    implicit none

    private

    integer, parameter :: ARRAY_LIST_START_SIZE = 10
    real(default), parameter :: ARRAY_LIST_GROW_FACTOR = 1.5_default, &
        ARRAY_LIST_SHRINK_THRESHOLD = 0.3_default

    type :: array_list_t
    private
        integer, dimension(:), allocatable :: array
        !! Track the index to *current* item, to be stored.
        !! Must fulfill: 0 <= count <= size.
        integer :: count = 0
        !! size \in N.
        integer :: size = 0
    contains
        procedure :: write => array_list_write
        procedure :: init => array_list_init
        procedure :: add => array_list_add

```

```

    procedure :: add_at => array_list_add_at
    procedure :: remove => array_list_remove
    procedure :: remove_at => array_list_remove_at
    procedure :: get => array_list_get
    procedure :: get_size => array_list_get_size
    procedure :: get_count => array_list_get_count
    procedure :: grow_size => array_list_grow_size
    procedure :: shrink_size => array_list_shrink_size
    procedure :: reverse_order => array_list_reverse_order
    procedure :: sort => array_list_sort
    procedure :: is_element => array_list_is_element
    procedure :: find => array_list_find
    procedure :: clear => array_list_clear
    procedure :: is_full => array_list_is_full
    procedure :: is_empty => array_list_is_empty
    procedure :: is_index => array_list_is_index
end type array_list_t

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

    subroutine array_list_init (list)
        class(array_list_t), intent(out) :: list
        allocate (list%array(ARRAY_LIST_START_SIZE), source = 0)
        list%count = 0
        list%size = ARRAY_LIST_START_SIZE
    end subroutine array_list_init

    elemental function array_list_get (list, index) result (data)
        class(array_list_t), intent(in) :: list
        integer, intent(in) :: index
        integer :: data
        if (list%is_index (index)) then
            data = list%array(index)
        else
            data = 0
        end if
    end function array_list_get

    pure function array_list_get_count (list) result (count)
        class(array_list_t), intent(in) :: list
        integer :: count
        count = list%count
    end function array_list_get_count

    pure function array_list_get_size (list) result (size)

```

```

        class(array_list_t), intent(in) :: list
        integer :: size
        size = list%size
    end function array_list_get_size

    pure function array_list_is_full (list) result (flag)
        class(array_list_t), intent(in) :: list
        logical :: flag
        flag = list%count >= list%size
    end function array_list_is_full

    pure function array_list_is_empty (list) result (flag)
        class(array_list_t), intent(in) :: list
        logical :: flag
        flag = .not. list%count > 0
    end function array_list_is_empty

    pure function array_list_is_index (list, index) result (flag)
        class(array_list_t), intent(in) :: list
        integer, intent(in) :: index
        logical :: flag
        flag = 0 < index .and. index <= list%count
    end function array_list_is_index

    subroutine array_list_clear (list)
        class(array_list_t), intent(inout) :: list
        list%array = 0
        list%count = 0
        call list%shrink_size ()
    end subroutine array_list_clear

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

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

    subroutine array_list_shrink_size (list)

```

```

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

subroutine array_list_reverse_order (list)
class(array_list_t), intent(inout) :: list
list%array(:list%count) = list%array(list%count:1:-1)
end subroutine array_list_reverse_order

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

pure function array_list_is_element (list, data) result (flag)

```



```

class(array_list_t), intent(in) :: list
integer, intent(in) :: data
logical :: flag
if (list%is_empty ()) then
    flag = .false.
else
    flag = any (data == list%array)
end if
end function array_list_is_element

function array_list_find (list, data) result (index)
class(array_list_t), intent(inout) :: list
integer, intent(in) :: data
integer :: index
if (list%is_empty () &
    .or. .not. list%is_element (data)) then
    index = 0
    return
end if
call list%sort () !! INTENT(INOUT)
index = binary_search_leftmost (list%array(:list%count), data)
contains
pure function binary_search_leftmost (array, data) result (index)
integer, dimension(:), intent(in) :: array
integer, intent(in) :: data
integer :: index
integer :: left, right
left = 1
right = size (array)
do while (left < right)
    index = floor ((left + right) / 2.)
    if (array(index) < data) then
        left = index + 1
    else
        right = index
    end if
end do
index = left
end function binary_search_leftmost
end function array_list_find

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

```

```

integer function array_list_remove (list) result (data)
  class(array_list_t), intent(inout) :: list
  if (list%is_empty ()) then
    data = 0
    return
  end if
  data = list%get (list%count)
  list%array(list%count) = 0
  list%count = list%count -1
end function array_list_remove

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

```

3.8.1 Unit tests

```

(array_list_ut.f90)≡
  <File header>

  module array_list_ut
    use unit_tests
    use array_list_util

    <Standard module head>

    <Array list: public test>

    contains

    <Array list: test driver>
  end module array_list_ut

(array_list_util.f90)≡
  <File header>

  module array_list_util

    use array_list

    <Standard module head>

    <Array list: test declarations>

```

```

contains

<Array list: tests>

end module array_list_util

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

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

```

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

```

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

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

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

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

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

```

```

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

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

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

subroutine test_sort (list)
  class(array_list_t), intent(inout) :: list
  call list%add (6)
  call list%add (2)
  call list%add (9)
  call list%add (4)
  call list%add (8)
  call list%add (7)
  call list%sort ()
end subroutine test_sort

```

```

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

```

3.9 Queue

<queue.f90>≡
 <File header>

```

module queue
  use, intrinsic :: iso_fortran_env, only: ERROR_UNIT

  implicit none

  private

  integer, parameter :: QUEUE_SIZE = 10, &
    QUEUE_START = 0, &
    QUEUE_END = QUEUE_SIZE

  type :: queue_t
    private
    integer, dimension(QUEUE_SIZE) :: item
    integer :: front = 0
    integer :: rear = 0
    contains
    procedure :: enqueue => queue_enqueue
    procedure :: dequeue => queue_dequeue
    procedure :: is_full => queue_is_full
    procedure :: is_empty => queue_is_empty
    procedure :: peek => queue_peek
    procedure :: write => queue_write
  end type queue_t

  public :: queue_t
contains
  elemental logical function queue_is_full (queue) result (flag)
    class(queue_t), intent(in) :: queue
    flag = queue%front == 1 .and. queue%rear == QUEUE_END
  end function queue_is_full

  elemental logical function queue_is_empty (queue) result (flag)
    class(queue_t), intent(in) :: queue
    flag = queue%front == QUEUE_START
  end function queue_is_empty

```

```

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

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

integer function queue_peek (queue) result (item)
  class(queue_t), intent(in) :: queue
  if (queue%is_empty ()) then
    item = 0
  else
    item = queue%item(queue%front)
  end if
end function queue_peek

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

```

```
end module queue
```

3.10 Iterator

```
<iterator.f90>≡
  <File header>
  module iterator
    use, intrinsic :: iso_fortran_env, only: ERROR_UNIT

    implicit none

    private

    !! Forward
    type :: iterator_t
      integer :: current = 0
      integer :: begin = 0
      integer :: end = 0
      integer :: step = 1
    contains
      procedure :: write => iterator_write
      procedure :: init => iterator_init
      procedure :: at_begin => iterator_at_begin
      procedure :: at_end => iterator_at_end
      procedure :: is_iterable => iterator_is_iterable
      procedure :: next => iterator_next
      procedure :: next_step => iterator_next_step
      procedure :: get_current => iterator_get_current
    end type iterator_t

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

    !! Proof: step > 0, begin < end.
    !! Proof: step < 0, begin > end.
    !! Proof: step /= 0.
    subroutine iterator_init (iter, begin, end, step)
      class(iterator_t), intent(inout) :: iter
      integer, intent(in) :: begin
      integer, intent(in) :: end
      integer, intent(in), optional :: step
      iter%begin = begin
      iter%end = end
      iter%step = 1; if (present (step)) iter%step = step
```

```

    if (abs (iter%step) > 0) then
        iter%current = iter%begin
    else
        write (ERROR_UNIT, "(A)") "ERROR: Step size MUST be unequal to zero."
        stop 1
    end if
end subroutine iterator_init

pure function iterator_at_begin (iter) result (flag)
    class(iterator_t), intent(in) :: iter
    logical :: flag
    flag = iter%current == iter%begin
end function iterator_at_begin

pure function iterator_at_end (iter) result (flag)
    class(iterator_t), intent(in) :: iter
    logical :: flag
    flag = iter%current == iter%end
end function iterator_at_end

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

subroutine iterator_next_step (iter)
    class(iterator_t), intent(inout) :: iter
    if (.not. iter%is_iterable ()) return
    iter%current = iter%current + iter%step
end subroutine iterator_next_step

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

pure function iterator_get_current (iter) result (ndx)
    class(iterator_t), intent(in) :: iter

```



```

integer :: ndx
if (.not. iter%is_iterable ()) then
    ndx = 0
    return
end if
ndx = iter%current
end function iterator_get_current
end module iterator

```

3.10.1 Unit tests

<iterator_ut.f90>≡
<File header>

```

module iterator_ut
    use unit_tests
    use iterator_uti

```

<Standard module head>

<Iterator: public test>

contains

<Iterator: test driver>

```
end module iterator_ut
```

<iterator_uti.f90>≡
<File header>

```

module iterator_uti

```

```
    use iterator

```

<Standard module head>

<Iterator: test declarations>

contains

<Iterator: tests>

```
end module iterator_uti
```

<Iterator: public test>≡
public :: iterator_test

<Iterator: test driver>≡

```

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

```

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

<Iterator: execute tests>≡

```
call test (iterator_1, "iterator_1", &
  "check interface and implementation", &
  u, results)
```

<Iterator: test declarations>≡

```
public :: iterator_1
```

<Iterator: tests>≡

```
subroutine iterator_1 (u)
  integer, intent(in) :: u
  type(iterator_t) :: iter
```

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

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

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

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

Chapter 4

Testing

This part contains tools for automatic testing.

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

4.1 Unit tests

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

```
<unit_tests.f90>≡  
  <File header>  
  
  module unit_tests  
  
    <Use strings>  
    use io_units  
  
    <Standard module head>  
  
    <Tests: public>  
  
    <Tests: parameters>  
  
    <Tests: types>  
  
    <Tests: interfaces>  
  
    contains  
  
    <Tests: procedures>  
  
  end module unit_tests
```

No internal dependencies

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

4.1.1 Parameters

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

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

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

4.1.2 Type for storing test results

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

```
<Tests: public>≡
  public :: test_results_t

<Tests: types>≡
  type :: test_result_t
    logical :: success = .false.
    type(string_t) :: name
    type(string_t) :: description
    type(test_result_t), pointer :: next => null ()
  end type test_result_t

  type :: test_results_t
    private
    type(test_result_t), pointer :: first => null ()
    type(test_result_t), pointer :: last => null ()
    integer :: n_success = 0
    integer :: n_failure = 0
  contains
```

```

    <Tests: test results: TBP>
end type test_results_t

```

Add a test result.

```

<Tests: test results: TBP>≡
    procedure :: add => test_results_add

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

```

Display the current state.

```

<Tests: test results: TBP>+≡
    procedure, private :: write => test_results_write

<Tests: procedures>+≡
    subroutine test_results_write (list, u)
        class(test_results_t), intent(in) :: list
        integer, intent(in) :: u
        type(test_result_t), pointer :: result
        write (u, "(A)") "*** Test Summary ***"
        if (list%n_success > 0) then
            write (u, "(2x,A)") "Success:"
            result => list%first
            do while (associated (result))
                if (result%success) write (u, "(4x,A,' : ',A)") &
                    char (result%name), char (result%description)
                result => result%next
            end do
        end if
        if (list%n_failure > 0) then
            write (u, "(2x,A)") "Failure:"
            result => list%first
            do while (associated (result))

```

```

        if (.not. result%success) write (u, "(4x,A,': ',A)") &
            char (result%name), char (result%description)
        result => result%next
    end do
end if
write (u, "(A,I0)") "Total    = ", list%n_success + list%n_failure
write (u, "(A,I0)") "Success = ", list%n_success
write (u, "(A,I0)") "Failure = ", list%n_failure
write (u, "(A)")   "*** End of test Summary ***"
end subroutine test_results_write

```

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

```

<Tests: test results: TBP>+≡
    procedure, private :: report => test_results_report

<Tests: procedures>+≡
    subroutine test_results_report (list, success)
        class(test_results_t), intent(in) :: list
        logical, intent(out) :: success
        success = list%n_failure == 0
    end subroutine test_results_report

```

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

```

<Tests: test results: TBP>+≡
    procedure :: get_n_pass => test_results_get_n_pass
    procedure :: get_n_fail => test_results_get_n_fail
    procedure :: get_n_total => test_results_get_n_total

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

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

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

```

Delete the list.

```

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

<Tests: procedures>+≡
    subroutine test_results_final (list)
        class(test_results_t), intent(inout) :: list

```

```

type(test_result_t), pointer :: result
do while (associated (list%first))
    result => list%first
    list%first => result%next
    deallocate (result)
end do
list%last => null ()
list%n_success = 0
list%n_failure = 0
end subroutine test_results_final

```

4.1.3 Wrapup

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

```

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

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

```

4.1.4 Tool for Unit Tests

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

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

```

<Tests: public>+≡
    public :: unit_test

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

```

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

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

```

<Tests: public>+≡
    public :: test

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

        call start_test (u_log, name)

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

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

    end subroutine test

```

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

```

<Tests: public>+≡
    public :: start_test

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

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

    end subroutine start_test

```

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

```

<Tests: public>+≡
    public :: compare_test_results

<Tests: procedures>+≡
    subroutine compare_test_results (u_test, u_log, name, success)
        integer, intent(in) :: u_test
        integer, intent(in) :: u_log

```



```

character(*), intent(in) :: name
logical, intent(out) :: success

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

inquire (file=ref_prefix//name//ref, exist=exist)
if (exist) then
    open (newunit = u_ref, file=ref_prefix//name//ref, &
          status="old", action="read")
    COMPARE_FILES: do
        read (u_test, "(A)", iostat=iostat1) buffer1
        read (u_ref, "(A)", iostat=iostat2) buffer2
        if (iostat1 /= iostat2) then
            success = .false.
            exit COMPARE_FILES
        else if (iostat1 < 0) then
            success = .true.
            exit COMPARE_FILES
        else if (buffer1 /= buffer2) then
            success = .false.
            exit COMPARE_FILES
        end if
    end do COMPARE_FILES
    close (u_ref)
else
    write (*, "(A)", advance="no") " ... no reference output available"
    write (u_log, "(A)") " No reference output available."
    success = .false.
end if
if (success) then
    write (*, "(A)") " ... success."
    write (u_log, "(A)") " Success."
else
    write (*, "(A)") " ... failure. See: " // err_prefix//name//err
    write (u_log, "(A)") " Failure."
    rewind (u_test)
    open (newunit = u_err, file=err_prefix//name//err, &
          action="write", status="replace")
    WRITE_OUTPUT: do
        read (u_test, "(A)", end=1) buffer1
        write (u_err, "(A)") trim (buffer1)
    end do WRITE_OUTPUT
1   close (u_err)
end if

end subroutine compare_test_results

```

Chapter 5

System: Interfaces and Handlers

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

system_defs Constants relevant for the modules in this set.

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

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

cputime Timer data type and methods, for measuring performance.

5.1 Constants

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

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

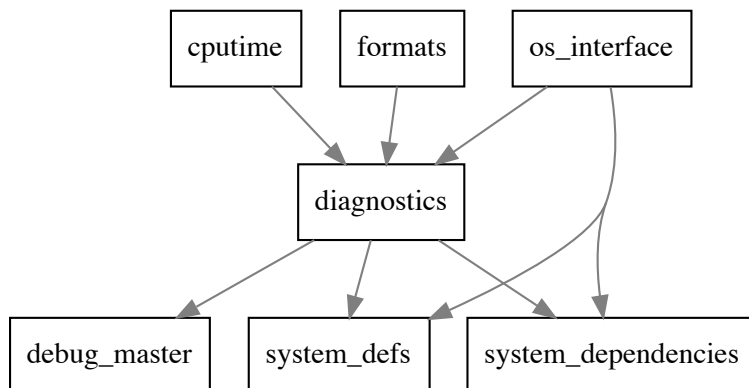


Figure 5.1: Module dependencies in `src/system`.

5.1.1 Version

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

```

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

```

5.1.2 Text Buffer

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

```

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

```

5.1.3 IOSTAT Codes

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

```

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

```

5.1.4 Character Codes

Single-character constants.

```

<System defs: public parameters>+≡

```

```

character, parameter, public :: BLANK = ' '
character, parameter, public :: TAB = achar(9)
character, parameter, public :: CR = achar(13)
character, parameter, public :: LF = achar(10)
character, parameter, public :: BACKSLASH = achar(92)

```

Character strings that indicate character classes.

```

⟨System defs: public parameters⟩+≡
  character(*), parameter, public :: WHITESPACE_CHARS = BLANK// TAB // CR // LF
  character(*), parameter, public :: LCLETTERS = "abcdefghijklmnopqrstuvwxyz"
  character(*), parameter, public :: UCLETTERS = "ABCDEFGHIJKLMNOPQRSTUVWXYZ"
  character(*), parameter, public :: DIGITS = "0123456789"

```

5.2 C wrapper for sigaction

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

```

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

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

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

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

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

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

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

```

```

    sa.sa_handler = wo_handler_sigint;
    return sigaction(SIGINT, &sa, NULL);
}

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

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

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

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

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

```

```

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

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

```

5.3 C wrapper for printf

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

This is used by the `formats` module.

```

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

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

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

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

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

⟨sprintf interfaces⟩≡
interface
    function sprintf_none (str, fmt) result (stat) bind(C)
        use iso_c_binding !NODEP!

```

```

        integer(c_int) :: stat
        character(c_char), dimension(*), intent(inout) :: str
        character(c_char), dimension(*), intent(in) :: fmt
    end function sprintf_none
end interface

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

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

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

```

5.4 Error, Message and Signal Handling

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

```

<diagnostics.f90>≡
    <File header>

```

```

module diagnostics

    use, intrinsic :: iso_c_binding !NODEP!

```

```

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

    <Use kinds>
    <Use strings>
    <Use debug>
    use string_utils, only: str
    use io_units

    use system_dependencies
    use system_defs, only: BUFFER_SIZE, MAX_ERRORS

    <Standard module head>

    <Diagnostics: public>

    <Diagnostics: parameters>

    <Diagnostics: types>

    <Diagnostics: variables>

    <Diagnostics: interfaces>

    contains

    <Diagnostics: procedures>

    end module diagnostics

    <Diagnostics: external procedures>
Diagnostics levels:
    <Diagnostics: public>≡
        public :: RESULT, DEBUG, DEBUG2
    <Diagnostics: parameters>≡
        integer, parameter :: TERMINATE=-2, BUG=-1, FATAL=1, &
            ERROR=2, WARNING=3, MESSAGE=4, RESULT=5, &
            DEBUG=6, DEBUG2=7
Diagnostics areas:
    <Diagnostics: public>+≡
        public :: d_area
    <Diagnostics: interfaces>≡
        interface d_area
            module procedure d_area_of_string
            module procedure d_area_to_string
        end interface
    <Diagnostics: procedures>≡
        function d_area_of_string (string) result (i)
            integer :: i
            type(string_t), intent(in) :: string
            select case (char (string))
            case ("particles")

```



```

        i = D_PARTICLES
    case ("events")
        i = D_EVENTS
    case ("shower")
        i = D_SHOWER
    case ("model_features")
        i = D_MODEL_F
    case ("matching")
        i = D_MATCHING
    case ("transforms")
        i = D_TRANSFORMS
    case ("subtraction")
        i = D_SUBTRACTION
    case ("virtual")
        i = D_VIRTUAL
    case ("threshold")
        i = D_THRESHOLD
    case ("phasespace")
        i = D_PHASESPACE
    case ("mismatch")
        i = D_MISMATCH
    case ("me_methods")
        i = D_ME_METHODS
    case ("process_integration")
        i = D_PROCESS_INTEGRATION
    case ("tauola")
        i = D_TAUOLA
    case ("core")
        i = D_CORE
    case ("vamp2")
        i = D_VAMP2
    case ("mpi")
        i = D_MPI
    case ("qft")
        i = D_QFT
    case ("beams")
        i = D_BEAMS
    case ("real")
        i = D_REAL
    case ("flavor")
        i = D_FLAVOR
    case ("all")
        i = D_ALL
    case default
        print "(A)", "Possible values for --debug are:"
        do i = 0, D_LAST
            print "(A)", char (' ' // d_area_to_string(i))
        end do
        call msg_fatal ("Please use one of the listed areas")
    end select
end function d_area_of_string

elemental function d_area_to_string (i) result (string)
    type(string_t) :: string

```

```

integer, intent(in) :: i
select case (i)
case (D_PARTICLES)
    string = "particles"
case (D_EVENTS)
    string = "events"
case (D_SHOWER)
    string = "shower"
case (D_MODEL_F)
    string = "model_features"
case (D_MATCHING)
    string = "matching"
case (D_TRANSFORMS)
    string = "transforms"
case (D_SUBTRACTION)
    string = "subtraction"
case (D_VIRTUAL)
    string = "virtual"
case (D_THRESHOLD)
    string = "threshold"
case (D_PHASESPACE)
    string = "phasespace"
case (D_MISMATCH)
    string = "mismatch"
case (D_ME_METHODS)
    string = "me_methods"
case (D_PROCESS_INTEGRATION)
    string = "process_integration"
case (D_TAUOLA)
    string = "tauola"
case (D_CORE)
    string = "core"
case (D_VAMP2)
    string = "vamp2"
case (D_MPI)
    string = "mpi"
case (D_QFT)
    string = "qft"
case (D_BEAMS)
    string = "beams"
case (D_REAL)
    string = "real"
case (D_FLAVOR)
    string = "flavor"
case (D_ALL)
    string = "all"
case default
    string = "undefined"
end select
end function d_area_to_string

```

(Diagnostics: public) +≡

```

public :: D_PARTICLES, D_EVENTS, D_SHOWER, D_MODEL_F, &
        D_MATCHING, D_TRANSFORMS, D_SUBTRACTION, D_VIRTUAL, D_THRESHOLD, &

```

```

        D_PHASESPACE, D_MISMATCH, D_ME_METHODS, D_PROCESS_INTEGRATION, &
        D_TAUOLA, D_CORE, D_VAMP2, D_MPI, D_QFT, D_BEAMS, D_REAL, D_FLAVOR

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

<Diagnostics: public>+≡
    public :: msg_level

<Diagnostics: variables>≡
    integer, save, dimension(D_ALL:D_LAST) :: msg_level = RESULT

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

<Diagnostics: public>+≡
    public :: set_debug_levels

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

<Diagnostics: public>+≡
    public :: set_debug2_levels

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

```

```

        msg_level(area) = DEBUG2
    end if
end subroutine set_debug2_levels

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

<Diagnostics: public>+≡
public :: term_col

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

<Diagnostics: procedures>+≡
function term_col_int (col_int) result (color)
    type(terminal_color_t) :: color
    integer, intent(in) :: col_int
    color%color = col_int
end function term_col_int

function term_col_char (col_char) result (color)
    type(terminal_color_t) :: color
    character(len=*), intent(in) :: col_char
    type(string_t) :: buf
    select case (col_char)
    case ('Grey')
        color%color = COL_GREY
    case ('Peach')
        color%color = COL_PEACH
    case ('Light Green')
        color%color = COL_LIGHT_GREEN
    case ('Light Yellow')
        color%color = COL_LIGHT_YELLOW
    case ('Light Blue')
        color%color = COL_LIGHT_BLUE
    case ('Pink')
        color%color = COL_PINK
    case ('Light Aqua')
        color%color = COL_LIGHT_AQUA
    case ('Pearl White')
        color%color = COL_PEARL_WHITE
    case ('Black')
        color%color = COL_BLACK
    case ('Red')
        color%color = COL_RED
    case ('Green')

```

```

        color%color = COL_GREEN
    case ('Yellow')
        color%color = COL_YELLOW
    case ('Blue')
        color%color = COL_BLUE
    case ('Purple')
        color%color = COL_PURPLE
    case ('Aqua')
        color%color = COL_AQUA
    case default
        buf = var_str ('Color ') // var_str (col_char) // var_str (' is not defined')
        call msg_warning (char (buf))
        color%color = COL_UNDEFINED
    end select
end function term_col_char

```

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

```

<Diagnostics: public>+≡
    public :: mask_fatal_errors

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

```

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

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

```

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

<Diagnostics: public>+≡
    public :: handle_fatal_errors

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

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

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

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

```

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

```

<Diagnostics: public>+≡
    public :: msg_count

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

```

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

```

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

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

```

Create a format string indicating color

Add the current message buffer contents to the internal list.

```

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

```

Initialization:

```

<Diagnostics: public>+≡
    public :: msg_list_clear

<Diagnostics: procedures>+≡
    subroutine msg_list_clear
        integer :: level
        type(string_list), pointer :: message
        do level = TERMINATE, WARNING
            do while (associated (msg_list(level)%first))

```

```

        message => msg_list(level)%first
        msg_list(level)%first => message%next
        deallocate (message)
    end do
    nullify (msg_list(level)%last)
end do
msg_count = 0
end subroutine msg_list_clear

```

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

```

<Diagnostics: public>+≡
    public :: msg_summary

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

```

Print the list of all messages of a given level.

```

<Diagnostics: public>+≡
    public :: msg_listing

<Diagnostics: procedures>+≡
    subroutine msg_listing (level, unit, prefix)
        integer, intent(in) :: level
        integer, intent(in), optional :: unit
        character(len=*), intent(in), optional :: prefix
        type(string_list), pointer :: message
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        if (present (unit)) u = unit
        message => msg_list(level)%first
        do while (associated (message))
            if (present (prefix)) then
                write (u, "(A)") prefix // trim (message%string)
            else
                write (u, "(A)") trim (message%string)
            end if
        end do
    end subroutine msg_listing

```

```

        message => message%/next
    end do
    flush (u)
end subroutine msg_listing

```

The message buffer:

```

<Diagnostics: public>+≡
    public :: msg_buffer

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

```

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

```

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

```

```

<Diagnostics: public>+≡
    public :: create_col_string

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

```

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

```

<Diagnostics: procedures>+≡
    subroutine message_print (level, string, str_arr, unit, logfile, area, color)
        integer, intent(in) :: level
        character(len=*), intent(in), optional :: string
        type(string_t), dimension(:), intent(in), optional :: str_arr
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: logfile
        integer, intent(in), optional :: area
        integer, intent(in), optional :: color
        type(string_t) :: col_string, prep_string, aux_string, head_footer, app_string
        integer :: lu, i, ar
        logical :: severe, is_error
        ar = D_ALL; if (present (area)) ar = area
        severe = .false.
        head_footer = "*****"
        aux_string = ""

```



```

is_error = .false.
app_string = ""
select case (level)
case (TERMINATE)
    prep_string = ""
case (BUG)
    prep_string = "*** WHIZARD BUG: "
    aux_string = "*** "
    severe = .true.
    is_error = .true.
case (FATAL)
    prep_string = "*** FATAL ERROR: "
    aux_string = "*** "
    severe = .true.
    is_error = .true.
case (ERROR)
    prep_string = "*** ERROR: "
    aux_string = "*** "
    is_error = .true.
case (WARNING)
    prep_string = "Warning: "
case (MESSAGE)
    prep_string = "| "
case (DEBUG, DEBUG2)
    prep_string = "D: "
case default
    prep_string = ""
end select
if (present (color)) then
    if (color > COL_UNDEFINED) then
        col_string = create_col_string (color)
        prep_string = achar(27) // col_string // prep_string
        app_string = app_string // achar(27) // "[0m"
    end if
end if
if (present(string)) msg_buffer = string
lu = log_unit
if (present(unit)) then
    if (unit /= output_unit) then
        if (severe) write (unit, "(A)") char(head_footer)
        if (is_error) write (unit, "(A)") char(head_footer)
        write (unit, "(A,A,A)") char(prepare_string), trim(msg_buffer), &
            char(app_string)
        if (present (str_arr)) then
            do i = 1, size(str_arr)
                write (unit, "(A,A)") char(aux_string), char(trim(str_arr(i)))
            end do
        end if
        if (is_error) write (unit, "(A)") char(head_footer)
        if (severe) write (unit, "(A)") char(head_footer)
        flush (unit)
        lu = -1
    else if (level <= msg_level(ar)) then
        if (severe) print "(A)", char(head_footer)
    end if
end if

```

```

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

```

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

<System defs: public parameters>+≡

integer, parameter, public :: MAX_ERRORS = 10

The specific handlers. In the case of fatal errors, bugs (failed assertions) and

normal termination execution is stopped. For non-fatal errors a message is printed to standard output if no unit is given. Only if the number of MAX_ERRORS errors is reached, we abort the program. There are no further actions in the other cases, but this may change.

<Diagnostics: public>+≡

```
public :: msg_terminate
public :: msg_bug, msg_fatal, msg_error, msg_warning
public :: msg_message, msg_result
```

<Diagnostics: procedures>+≡

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

subroutine msg_bug (string, arr, unit)
  integer, intent(in), optional :: unit
  character(len=*), intent(in), optional :: string
  type(string_t), dimension(:), intent(in), optional :: arr
  logical, pointer :: crash_ptr
  call message_print (BUG, string, arr, unit)
  call msg_summary (unit)
  select case (handle_fatal_errors)
```

```

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

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

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

subroutine msg_warning (string, arr, unit, color)
    integer, intent(in), optional :: unit
    character(len=*), intent(in), optional :: string
    type(string_t), dimension(:), intent(in), optional :: arr
    type(terminal_color_t), intent(in), optional :: color
    integer :: cl
    cl = COL_UNDEFINED; if (present (color)) cl = color%color

```

```

        call message_print (level = WARNING, string = string, &
            str_arr = arr, unit = unit, color = cl)
    end subroutine msg_warning

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

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

```

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

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

```

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

```

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

```

<Diagnostics: public>+≡
    public :: msg_debug

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

<Diagnostics: procedures>+≡
    subroutine msg_debug_none (area, string, color)

```

```

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

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

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

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

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

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

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

```

```

        color = color)
    else
        <debug guard>
    end if

<Diagnostics: public>+≡
    public :: msg_print_color

<Diagnostics: interfaces>+≡
    interface msg_print_color
        module procedure msg_print_color_none
        module procedure msg_print_color_logical
        module procedure msg_print_color_integer
        module procedure msg_print_color_real
    end interface

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

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

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

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

```

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

```

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

<Diagnostics: public>+≡
    public :: msg_debug2

```

```

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

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

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

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

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

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

subroutine msg_debug2_string (area, string, value, color)
  type(string_t), intent(in) :: value
  integer, intent(in) :: area
  character(len=*), intent(in) :: string
  type(terminal_color_t), intent(in), optional :: color
  if (debug2_active (area)) then
    call msg_debug2_none (area, string // " = " // char (value), &
      color = color)
  else
    <debug2 guard>
  end if
end subroutine msg_debug2_string

```



```

        end if
    end subroutine msg_debug2_string

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

<Diagnostics: public>+≡
    public :: debug_active

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

<Diagnostics: public>+≡
    public :: debug2_active

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

```

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

```

<Diagnostics: public>+≡
    public :: msg_show_progress

<Diagnostics: procedures>+≡
    subroutine msg_show_progress (i_call, n_calls)
        integer, intent(in) :: i_call, n_calls
        real(default) :: progress
        integer, save :: next_check
        if (i_call == 1) next_check = 10
        progress = (i_call * 100._default) / n_calls
        if (progress >= next_check) then
            write (msg_buffer, "(F5.1,A)") progress, "%"
            call msg_message ()
            next_check = next_check + 10
        end if
    end subroutine msg_show_progress

```

```

<Diagnostics: public>+≡
    public :: exit

<Diagnostics: interfaces>+≡
    interface
        subroutine exit (status) bind (C)
            use iso_c_binding !NODEP!
            integer(c_int), value :: status
        end subroutine exit
    end interface

```

$$\langle \textit{Diagnostics: public} \rangle + \equiv$$

$$\text{public} :: \text{msg_banner}$$

```

subroutine msg_banner (unit)
  integer, intent(in), optional :: unit
  call message_print (0, "|=====|")
  call message_print (0, "|
  call message_print (0, "|      WW      WW WW WW WW WWWWW      WW      WWWWW  WWWW
  call message_print (0, "|      WW      WW      WW WW WW WW      WW      WWWW  WW WW WW
  call message_print (0, "|      WW WW WW WW      WWWWWWW WW      WW      WW WW  WWWWW  WW
  call message_print (0, "|      WWWW  WWWW      WW WW WW      WW      WWWWWWWW  WW WW  WW
  call message_print (0, "|      WW      WW      WW WW WW WW WWWWWWW WW      WW  WW WW  WWWW
  call message_print (0, "|
  call message_print (0, "|
  call message_print (0, "|                                W
  call message_print (0, "|                                sW
  call message_print (0, "|                                WW
  call message_print (0, "|                                sWW
  call message_print (0, "|                                WWW
  call message_print (0, "|                                wWWW
  call message_print (0, "|                                wWWWw
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                wWW WW
  call message_print (0, "|                                wWW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|                                WW WW
  call message_print (0, "|      WWWWW      WW      WW
  call message_print (0, "|      WWWWWww      WW      WW
  call message_print (0, "|      WWWWWwwwww      WW      WW
  call message_print (0, "|      wWWWwwwwwwww      WW
  call message_print (0, "|      wWWWwwwwwwwwww      WW
  call message_print (0, "|      wWWW      wW      WWWWWWW
  call message_print (0, "|      WWWW      wW      WW wWWWwwwwwwww
  call message_print (0, "|      WWWW      WW      WWWWWWWWWWW
  call message_print (0, "|      WWWW      WWWW      WWw

```

```

call message_print (0, "|
call message_print (0, "|
call message_print (0, "|
call message_print (0, "|
call message_print (0, "|
call message_print (0, "|
call message_print (0, "|
call message_print (0, "| by: Wolfgang Kilian, Thorsten Ohl, Juergen Reuter
call message_print (0, "| with contributions from Christian Speckner
call message_print (0, "| Contact: <whizard@desy.de>
call message_print (0, "|
call message_print (0, "| if you use WHIZARD please cite:
call message_print (0, "| W. Kilian, T. Ohl, J. Reuter, Eur.Phys.J.C71 (2011) 1742
call message_print (0, "| [arXiv: 0708.4233 [hep-ph]]
call message_print (0, "| M. Moretti, T. Ohl, J. Reuter, arXiv: hep-ph/0102195
call message_print (0, "|=====
call message_print (0, "| WHIZARD " // WHIZARD_VERSION, unit=uni
call message_print (0, "|=====
end subroutine msg_banner

```

5.4.1 Logfile

All screen output should be duplicated in the logfile, unless requested otherwise.

```

<Diagnostics: public>+≡
public :: logging

<Diagnostics: variables>+≡
integer, save :: log_unit = -1
logical, target, save :: logging = .false.

<Diagnostics: public>+≡
public :: logfile_init

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

<Diagnostics: public>+≡
public :: logfile_final

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

```

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

```

<Diagnostics: public>+≡
    public :: logfile_unit

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

```

5.4.2 Checking values

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

```

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

<Diagnostics: public>+≡
    public :: expect_record

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

<Diagnostics: public>+≡
    public :: expect_clear

```

```

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

<Diagnostics: public>+≡
  public :: expect_summary

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

```

Helpers for converting integers into strings with minimal length.

```

<Diagnostics: public>+≡
  public :: int2string
  public :: int2char
  public :: int2fixed

<Diagnostics: procedures>+≡
  pure function int2fixed (i) result (c)
    integer, intent(in) :: i
    character(200) :: c
    c = ""
    write (c, *) i
    c = adjustl (c)
  end function int2fixed

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

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

```

Dito for reals.

```

<Diagnostics: public>+≡
  public :: real2string

```

```

public :: real2char
public :: real2fixed

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

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

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

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

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

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

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

```

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

```

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

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

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

```

5.4.3 Suppression of numerical noise

```

<Diagnostics: public>+≡
    public :: pacify

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

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

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

```

5.4.4 Signal handling

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

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

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

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

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

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

```
<Diagnostics: public>+≡
    public :: mask_term_signals

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


<Diagnostics: interfaces>+≡

```
interface
  integer(c_int) function wo_mask_sigint () bind(C)
  import
end function wo_mask_sigint
end interface
interface
  integer(c_int) function wo_mask_sigterm () bind(C)
  import
end function wo_mask_sigterm
end interface
interface
  integer(c_int) function wo_mask_sigxcpu () bind(C)
  import
end function wo_mask_sigxcpu
end interface
interface
  integer(c_int) function wo_mask_sigxfsz () bind(C)
  import
end function wo_mask_sigxfsz
end interface
```

<Diagnostics: public>+≡

```
public :: release_term_signals
```

<Diagnostics: procedures>+≡

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

<Diagnostics: interfaces>+≡

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

```

end interface
interface
    integer(c_int) function wo_release_sigxfsz () bind(C)
    import
    end function wo_release_sigxfsz
end interface

<Diagnostics: public>+≡
    public :: signal_is_pending

<Diagnostics: procedures>+≡
    function signal_is_pending () result (flag)
        logical :: flag
        flag = &
            wo_sigint /= 0 .or. &
            wo_sigterm /= 0 .or. &
            wo_sigxcpu /= 0 .or. &
            wo_sigxfsz /= 0
    end function signal_is_pending

<Diagnostics: public>+≡
    public :: terminate_now_if_signal

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

<Diagnostics: public>+≡
    public :: single_event

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

<Diagnostics: public>+≡
    public :: terminate_now_if_single_event

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

```

```

        end if
    end subroutine terminate_now_if_single_event

```

5.5 Operating-system interface

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

The current implementation lacks error handling.

```

<os_interface.f90>≡
  <File header>

  module os_interface

    use, intrinsic :: iso_c_binding !NODEP!

    <Use strings>
    use io_units
    use diagnostics
    use system_defs, only: DLERROR_LEN, ENVVAR_LEN
    use system_dependencies

    <Use mpi f08>

    <Standard module head>

    <OS interface: public>

    <OS interface: types>

    <OS interface: interfaces>

    contains

    <OS interface: procedures>

  end module os_interface

```

5.5.1 Path variables

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

```

<OS interface: public>≡
  public :: paths_t

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

```

```

        type(string_t) :: datarootdir
        type(string_t) :: localprefix
        type(string_t) :: libtool
        type(string_t) :: lhpdffdir
    end type paths_t

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

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

```

5.5.2 System dependencies

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

```

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

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

```

```

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

```

Since all are allocatable strings, explicit initialization is necessary.

```

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

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

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

```

```

os_data%makeflags      = DEFAULT_MAKEFLAGS
os_data%prefix         = PREFIX
os_data%exec_prefix    = EXEC_PREFIX
os_data%bindir         = BINDIR
os_data%libdir         = LIBDIR
os_data%includedir     = INCLUDEDIR
os_data%datarootdir    = DATAROOTDIR
if (present (paths)) then
  if (paths%prefix      /= "") os_data%prefix      = paths%prefix
  if (paths%exec_prefix /= "") os_data%exec_prefix = paths%exec_prefix
  if (paths%bindir      /= "") os_data%bindir      = paths%bindir
  if (paths%libdir      /= "") os_data%libdir      = paths%libdir
  if (paths%includedir  /= "") os_data%includedir  = paths%includedir
  if (paths%datarootdir /= "") os_data%datarootdir = paths%datarootdir
end if
if (os_data%use_testfiles) then
  os_data%whizard_omega_binpath = WHIZARD_TEST_OMEGA_BINPATH
  os_data%whizard_includes      = WHIZARD_TEST_INCLUDES
  os_data%whizard_ldflags       = WHIZARD_TEST_LDFLAGS
  os_data%whizard_libtool       = WHIZARD_LIBTOOL_TEST
  os_data%whizard_modelpath     = WHIZARD_TEST_MODELPATH
  os_data%whizard_modelpath_ufo = WHIZARD_TEST_MODELPATH_UFO
  os_data%whizard_models_libpath = WHIZARD_TEST_MODELS_LIBPATH
  os_data%whizard_susypath      = WHIZARD_TEST_SUSYPATH
  os_data%whizard_gmlpath      = WHIZARD_TEST_GMLPATH
  os_data%whizard_cutspath      = WHIZARD_TEST_CUTSPATH
  os_data%whizard_texpath       = WHIZARD_TEST_TEXPATH
  os_data%whizard_sharepath     = WHIZARD_TEST_SHAREPATH
  os_data%whizard_testdatapath  = WHIZARD_TEST_TESTDATAPATH
  os_data%whizard_circe2path    = WHIZARD_TEST_CIRCE2PATH
  os_data%whizard_beamsimp      = WHIZARD_TEST_BEAMSIMP
  os_data%whizard_mulipath      = WHIZARD_TEST_MULIPATH
  os_data%pdf_builtin_datapath  = PDF_BUILTIN_TEST_DATAPATH
else
  if (os_dir_exist (local_includes)) then
    os_data%whizard_includes = "-I" // local_includes // " //" &
      WHIZARD_INCLUDES
  else
    os_data%whizard_includes = WHIZARD_INCLUDES
  end if
  os_data%whizard_omega_binpath = WHIZARD_OMEGA_BINPATH
  os_data%whizard_ldflags       = WHIZARD_LDFLAGS
  os_data%whizard_libtool       = WHIZARD_LIBTOOL
  if (present(paths)) then
    if (paths%libtool /= "") os_data%whizard_libtool = paths%libtool
  end if
  os_data%whizard_modelpath     = WHIZARD_MODELPATH
  os_data%whizard_modelpath_ufo = WHIZARD_MODELPATH_UFO
  os_data%whizard_models_libpath = WHIZARD_MODELS_LIBPATH
  os_data%whizard_susypath      = WHIZARD_SUSYPATH
  os_data%whizard_gmlpath      = WHIZARD_GMLPATH
  os_data%whizard_cutspath      = WHIZARD_CUTSPATH
  os_data%whizard_texpath       = WHIZARD_TEXPATH
  os_data%whizard_sharepath     = WHIZARD_SHAREPATH

```

```

        os_data%whizard_testdatapath = WHIZARD_TESTDATAPATH
        os_data%whizard_circe2path   = WHIZARD_CIRCE2PATH
        os_data%whizard_beamsimpath  = WHIZARD_BEAMSIMPATH
        os_data%whizard_mulipath     = WHIZARD_MULIPATH
        os_data%pdf_builtin_datapath = PDF_BUILTIN_DATAPATH
    end if
    os_data%event_analysis    = EVENT_ANALYSIS    == "yes"
    os_data%event_analysis_ps = EVENT_ANALYSIS_PS == "yes"
    os_data%event_analysis_pdf = EVENT_ANALYSIS_PDF == "yes"
    os_data%latex = PRG_LATEX // " " // OPT_LATEX
    os_data%mpost = PRG_MPOST // " " // OPT_MPOST
    if (os_data%use_testfiles) then
        os_data%gml = os_data%whizard_gmlpath // "/whizard-gml" // " " // &
            OPT_MPOST // " " // "--gml" // os_data%whizard_gmlpath
    else
        os_data%gml = os_data%bindir // "/whizard-gml" // " " // OPT_MPOST &
            // " " // "--gml" // os_data%whizard_gmlpath
    end if
    os_data%dvips = PRG_DVIPS
    os_data%ps2pdf = PRG_PS2PDF
    call os_data_expand_paths (os_data)
    os_data%gosampath = GOSAM_DIR
    os_data%golempath = GOLEM_DIR
    os_data%formpath = FORM_DIR
    os_data%qgrafpath = QGRAF_DIR
    os_data%ninjabpath = NINJA_DIR
    os_data%samurairpath = SAMURAI_DIR
end subroutine os_data_init

```

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

(*OS interface: procedures*)+≡

```

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

```



```

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

```

Write contents

<OS interface: os data: TBP>+≡

```
procedure :: write => os_data_write
```

<OS interface: procedures>+≡

```

subroutine os_data_write (os_data, unit)
  class(os_data_t), intent(in) :: os_data
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(A)") "OS data:"
  write (u, *) "use_libtool      = ", os_data%use_libtool
  write (u, *) "use_testfiles   = ", os_data%use_testfiles
  write (u, *) "fc              = ", char (os_data%fc)
  write (u, *) "fcflags        = ", char (os_data%fcflags)
  write (u, *) "fcflags_pic     = ", char (os_data%fcflags_pic)
  write (u, *) "fclibs         = ", char (os_data%fclibs)
  write (u, *) "fc_src_ext      = ", char (os_data%fc_src_ext)
  write (u, *) "cc             = ", char (os_data%cc)
  write (u, *) "cflags         = ", char (os_data%cflags)
  write (u, *) "cflags_pic     = ", char (os_data%cflags_pic)
  write (u, *) "cxx            = ", char (os_data%cxx)
  write (u, *) "cxxflags       = ", char (os_data%cxxflags)
  write (u, *) "cxxlibs        = ", char (os_data%cxxlibs)
  write (u, *) "obj_ext        = ", char (os_data%obj_ext)
  write (u, *) "ld             = ", char (os_data%ld)
  write (u, *) "ldflags        = ", char (os_data%ldflags)
  write (u, *) "ldflags_so     = ", char (os_data%ldflags_so)
  write (u, *) "ldflags_static = ", char (os_data%ldflags_static)

```

```

write (u, *) "ldflags_hepmc = ", char (os_data%ldflags_hepmc)
write (u, *) "ldflags_lcio = ", char (os_data%ldflags_lcio)
write (u, *) "ldflags_hoppet = ", char (os_data%ldflags_hoppet)
write (u, *) "ldflags_looptools = ", char (os_data%ldflags_looptools)
write (u, *) "shrlib_ext = ", char (os_data%shrlib_ext)
write (u, *) "fc_shrlib_ext = ", char (os_data%fc_shrlib_ext)
write (u, *) "makeflags = ", char (os_data%makeflags)
write (u, *) "prefix = ", char (os_data%prefix)
write (u, *) "exec_prefix = ", char (os_data%exec_prefix)
write (u, *) "bindir = ", char (os_data%bindir)
write (u, *) "libdir = ", char (os_data%libdir)
write (u, *) "includedir = ", char (os_data%includedir)
write (u, *) "datarootdir = ", char (os_data%datarootdir)
write (u, *) "whizard_omega_binpath = ", &
char (os_data%whizard_omega_binpath)
write (u, *) "whizard_includes = ", char (os_data%whizard_includes)
write (u, *) "whizard_ldflags = ", char (os_data%whizard_ldflags)
write (u, *) "whizard_libtool = ", char (os_data%whizard_libtool)
write (u, *) "whizard_modelpath = ", &
char (os_data%whizard_modelpath)
write (u, *) "whizard_modelpath_ufo = ", &
char (os_data%whizard_modelpath_ufo)
write (u, *) "whizard_models_libpath = ", &
char (os_data%whizard_models_libpath)
write (u, *) "whizard_susypath = ", char (os_data%whizard_susypath)
write (u, *) "whizard_gmlpath = ", char (os_data%whizard_gmlpath)
write (u, *) "whizard_cutspath = ", char (os_data%whizard_cutspath)
write (u, *) "whizard_texpath = ", char (os_data%whizard_texpath)
write (u, *) "whizard_circe2path = ", char (os_data%whizard_circe2path)
write (u, *) "whizard_beamsimpath = ", char (os_data%whizard_beamsimpath)
write (u, *) "whizard_mulipath = ", char (os_data%whizard_mulipath)
write (u, *) "whizard_sharepath = ", &
char (os_data%whizard_sharepath)
write (u, *) "whizard_testdatapath = ", &
char (os_data%whizard_testdatapath)
write (u, *) "whizard_modelpath_local = ", &
char (os_data%whizard_modelpath_local)
write (u, *) "whizard_models_libpath_local = ", &
char (os_data%whizard_models_libpath_local)
write (u, *) "whizard_omega_binpath_local = ", &
char (os_data%whizard_omega_binpath_local)
write (u, *) "event_analysis = ", os_data%event_analysis
write (u, *) "event_analysis_ps = ", os_data%event_analysis_ps
write (u, *) "event_analysis_pdf = ", os_data%event_analysis_pdf
write (u, *) "latex = ", char (os_data%latex)
write (u, *) "mpost = ", char (os_data%mpost)
write (u, *) "gml = ", char (os_data%gml)
write (u, *) "dvips = ", char (os_data%dvips)
write (u, *) "ps2pdf = ", char (os_data%ps2pdf)
if (os_data%gosampath /= "") then
write (u, *) "gosam = ", char (os_data%gosampath)
write (u, *) "golem = ", char (os_data%golempath)
write (u, *) "form = ", char (os_data%formpath)
write (u, *) "qgraf = ", char (os_data%qgrafpath)

```

```

        write (u, *) "ninja   = ", char (os_data%ninjapath)
        write (u, *) "samurai = ", char (os_data%samuraipath)
    end if
end subroutine os_data_write

```

<OS interface: os data: TBP>+≡

```

    procedure :: build_latex_file => os_data_build_latex_file

```

<OS interface: procedures>+≡

```

subroutine os_data_build_latex_file (os_data, filename, stat_out)
    class(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: filename
    integer, intent(out), optional :: stat_out
    type(string_t) :: setenv_tex, pipe, pipe_dvi
    integer :: unit_dev, status
    status = -1
    if (os_data%event_analysis_ps) then
        !!! Check if our OS has a /dev/null
        unit_dev = free_unit ()
        open (file = "/dev/null", unit = unit_dev, &
             action = "write", iostat = status)
        close (unit_dev)
        if (status /= 0) then
            pipe = ""
            pipe_dvi = ""
        else
            pipe = " > /dev/null"
            pipe_dvi = " 2>/dev/null 1>/dev/null"
        end if
        if (os_data%whizard_texpath /= "") then
            setenv_tex = "TEXINPUTS=" // &
                os_data%whizard_texpath // ":$TEXINPUTS "
        else
            setenv_tex = ""
        end if
        call os_system_call (setenv_tex // &
            os_data%latex // " " // filename // ".tex " // pipe, &
            verbose = .true., status = status)
        call os_system_call (os_data%dvips // " -o " // filename // &
            ".ps " // filename // ".dvi" // pipe_dvi, verbose = .true., &
            status = status)
        call os_system_call (os_data%ps2pdf // " " // filename // ".ps", &
            verbose = .true., status = status)
    end if
    if (present (stat_out)) stat_out = status
end subroutine os_data_build_latex_file

```

5.5.3 Dynamic linking

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

access functions in this library.

```

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

```

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

```

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

```

The interface to the library functions:

```

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

  interface
    function dlclose (handle) result (status) bind(C)
      import
      type(c_ptr), value :: handle
      integer(c_int) :: status
    end function dlclose
  end interface

  interface
    function dlerror () result (str) bind(C)

```

```

import
type(c_ptr) :: str
end function dlerror
end interface

interface
function dlsym (handle, symbol) result (fptr) bind(C)
import
type(c_ptr), value :: handle
character(c_char), dimension(*) :: symbol
type(c_funptr) :: fptr
end function dlsym
end interface

```

This reads an error string and transforms it into a `string_t` object, if an error has occurred. If not, set the error flag to false and return an empty string.

```

<System defs: public parameters>+≡
integer, parameter, public :: DLERROR_LEN = 160

<OS interface: procedures>+≡
subroutine read_dlerror (has_error, error)
logical, intent(out) :: has_error
type(string_t), intent(out) :: error
type(c_ptr) :: err_cptr
character(len=DLERROR_LEN, kind=c_char), pointer :: err_fptr
integer :: str_end
err_cptr = dlerror ()
if (c_associated (err_cptr)) then
call c_f_pointer (err_cptr, err_fptr)
has_error = .true.
str_end = scan (err_fptr, c_null_char)
if (str_end > 0) then
error = err_fptr(1:str_end-1)
else
error = err_fptr
end if
else
has_error = .false.
error = ""
end if
end subroutine read_dlerror

```

This is the Fortran API. Init/final open and close the file, i.e., load and unload the library.

Note that a library can be opened more than once, and that for an ultimate close as many `dlclose` calls as `dlopen` calls are necessary. However, we assume that it is opened and closed only once.

```

<OS interface: public>+≡
public :: dlaccess_init
public :: dlaccess_final

<OS interface: dlaccess: TBP>+≡
procedure :: init => dlaccess_init
procedure :: final => dlaccess_final

```

```

<OS interface: procedures>+≡
subroutine dlaccess_init (dlaccess, prefix, libname, os_data)
  class(dlaccess_t), intent(out) :: dlaccess
  type(string_t), intent(in) :: prefix, libname
  type(os_data_t), intent(in), optional :: os_data
  type(string_t) :: filename
  logical :: exist
  dlaccess%filename = libname
  filename = prefix // "/" // libname
  inquire (file=char(filename), exist=exist)
  if (.not. exist) then
    filename = prefix // "/.libs/" // libname
    inquire (file=char(filename), exist=exist)
    if (.not. exist) then
      dlaccess%has_error = .true.
      dlaccess%error = "Library '" // filename // "' not found"
      return
    end if
  end if
  dlaccess%handle = dlopen (char (filename) // c_null_char, ior ( &
    RTLD_LAZY, RTLD_LOCAL))
  dlaccess%is_open = c_associated (dlaccess%handle)
  call read_dlerror (dlaccess%has_error, dlaccess%error)
end subroutine dlaccess_init

subroutine dlaccess_final (dlaccess)
  class(dlaccess_t), intent(inout) :: dlaccess
  integer(c_int) :: status
  if (dlaccess%is_open) then
    status = dlclose (dlaccess%handle)
    dlaccess%is_open = .false.
    call read_dlerror (dlaccess%has_error, dlaccess%error)
  end if
end subroutine dlaccess_final

```

Return true if an error has occurred.

```

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

<OS interface: procedures>+≡
function dlaccess_has_error (dlaccess) result (flag)
  logical :: flag
  type(dlaccess_t), intent(in) :: dlaccess
  flag = dlaccess%has_error
end function dlaccess_has_error

```

Return the error string currently stored in the dlaccess object.

```

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

<OS interface: procedures>+≡
function dlaccess_get_error (dlaccess) result (error)
  type(string_t) :: error
  type(dlaccess_t), intent(in) :: dlaccess

```

```

        error = dlaccess%error
    end function dlaccess_get_error

```

The symbol handler returns the C address of the function with the given string name. (It is a good idea to use `bind(C)` for all functions accessed by this, such that the name string is well-defined.) Call `c_f_procpointer` to cast this into a Fortran procedure pointer with an appropriate interface.

```

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

<OS interface: procedures>+≡
    function dlaccess_get_c_funptr (dlaccess, fname) result (fptr)
        type(c_funptr) :: fptr
        type(dlaccess_t), intent(inout) :: dlaccess
        type(string_t), intent(in) :: fname
        fptr = dlsym (dlaccess%handle, char (fname) // c_null_char)
        call read_dlerror (dlaccess%has_error, dlaccess%error)
    end function dlaccess_get_c_funptr

```

5.5.4 Predicates

Return true if the library is loaded. In particular, this is false if loading was unsuccessful.

```

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

<OS interface: procedures>+≡
    function dlaccess_is_open (dlaccess) result (flag)
        logical :: flag
        type(dlaccess_t), intent(in) :: dlaccess
        flag = dlaccess%is_open
    end function dlaccess_is_open

```

5.5.5 Shell access

This is the standard system call for executing a shell command, such as invoking a compiler.

In F2008 there will be the equivalent built-in command `execute_command_line`.

```

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

<OS interface: procedures>+≡
    subroutine os_system_call (command_string, status, verbose)
        type(string_t), intent(in) :: command_string
        integer, intent(out), optional :: status
        logical, intent(in), optional :: verbose
        logical :: verb
        integer :: stat
        verb = .false.; if (present (verbose)) verb = verbose
        if (verb) &
            call msg_message ("command: " // char (command_string))

```

```

stat = system (char (command_string) // c_null_char)
if (present (status)) then
  status = stat
else if (stat /= 0) then
  if (.not. verb) &
    call msg_message ("command: " // char (command_string))
  write (msg_buffer, "(A,I0)" "Return code = ", stat)
  call msg_message ()
  call msg_fatal ("System command returned with nonzero status code")
end if
end subroutine os_system_call

```

```

<OS interface: interfaces>+≡
interface
  function system (command) result (status) bind(C)
  import
  integer(c_int) :: status
  character(c_char), dimension(*) :: command
end function system
end interface

```

5.5.6 Querying for a directory

This queries for the existence of a directory. There is no standard way to achieve this in FORTRAN, and if we were to call into `libc`, we would need access to C macros for evaluating the result, so we resort to calling `test` as a system call.

```

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

<OS interface: procedures>+≡
function os_dir_exist (name) result (res)
  type(string_t), intent(in) :: name
  logical :: res
  integer :: status
  call os_system_call ('test -d "' // name // '"', status=status)
  res = status == 0
end function os_dir_exist

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

<OS interface: procedures>+≡
function os_file_exist (name) result (exist)
  type(string_t), intent(in) :: name
  logical :: exist
  inquire (file = char (name), exist=exist)
end function os_file_exist

```

5.5.7 Pack/unpack

The argument to `pack` may be a file or a directory. The name of the packed file will get the `pack_ext` extension appended. The argument to `unpack` must be a

file, with the extension already included in the file name.

```
<OS interface: public>+≡
  public :: os_pack_file
  public :: os_unpack_file

<OS interface: procedures>+≡
  subroutine os_pack_file (file, os_data, status)
    type(string_t), intent(in) :: file
    type(os_data_t), intent(in) :: os_data
    integer, intent(out), optional :: status
    type(string_t) :: command_string
    command_string = os_data%pack_cmd // " " &
      // file // os_data%pack_ext // " " // file
    call os_system_call (command_string, status)
  end subroutine os_pack_file

  subroutine os_unpack_file (file, os_data, status)
    type(string_t), intent(in) :: file
    type(os_data_t), intent(in) :: os_data
    integer, intent(out), optional :: status
    type(string_t) :: command_string
    command_string = os_data%unpack_cmd // " " // file
    call os_system_call (command_string, status)
  end subroutine os_unpack_file
```

5.5.8 Fortran compiler and linker

Compile a single module for use in a shared library, but without linking.

```
<OS interface: public>+≡
  public :: os_compile_shared

<OS interface: procedures>+≡
  subroutine os_compile_shared (src, os_data, status)
    type(string_t), intent(in) :: src
    type(os_data_t), intent(in) :: os_data
    integer, intent(out), optional :: status
    type(string_t) :: command_string
    if (os_data%use_libtool) then
      command_string = &
        os_data%whizard_libtool // " --mode=compile " // &
        os_data%fc // " " // &
        "-c " // &
        os_data%whizard_includes // " " // &
        os_data%fcflags // " " // &
        "" // src // os_data%fc_src_ext // ""
    else
      command_string = &
        os_data%fc // " " // &
        "-c " // &
        os_data%fcflags_pic // " " // &
        os_data%whizard_includes // " " // &
        os_data%fcflags // " " // &
        "" // src // os_data%fc_src_ext // ""
    end if
  end subroutine os_compile_shared
```

```

end if
call os_system_call (command_string, status)
end subroutine os_compile_shared

```

Link an array of object files to build a shared object library. In the libtool case, we have to specify a `-rpath`, otherwise only a static library can be built. However, since the library is never installed, this `rpath` is irrelevant.

```

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

<OS interface: procedures>+≡
subroutine os_link_shared (objlist, lib, os_data, status)
  type(string_t), intent(in) :: objlist, lib
  type(os_data_t), intent(in) :: os_data
  integer, intent(out), optional :: status
  type(string_t) :: command_string
  if (os_data%use_libtool) then
    command_string = &
      os_data%whizard_libtool // " --mode=link " // &
      os_data%fc // " " // &
      "-module " // &
      "-rpath /usr/local/lib" // " " // &
      os_data%fcflags // " " // &
      os_data%whizard_ldflags // " " // &
      os_data%ldflags // " " // &
      "-o '" // lib // ".la' " // &
      objlist
  else
    command_string = &
      os_data%ld // " " // &
      os_data%ldflags_so // " " // &
      os_data%fcflags // " " // &
      os_data%whizard_ldflags // " " // &
      os_data%ldflags // " " // &
      "-o '" // lib // "." // os_data%fc_shrlib_ext // "' " // &
      objlist
  end if
  call os_system_call (command_string, status)
end subroutine os_link_shared

```

Link an array of object files / libraries to build a static executable.

```

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

<OS interface: procedures>+≡
subroutine os_link_static (objlist, exec_name, os_data, status)
  type(string_t), intent(in) :: objlist, exec_name
  type(os_data_t), intent(in) :: os_data
  integer, intent(out), optional :: status
  type(string_t) :: command_string
  if (os_data%use_libtool) then
    command_string = &
      os_data%whizard_libtool // " --mode=link " // &
      os_data%fc // " " // &

```

```

        "-static " // &
        os_data%fcflags // " " // &
        os_data%whizard_ldflags // " " // &
        os_data%ldflags // " " // &
        os_data%ldflags_static // " " // &
        "-o '" // exec_name // "' " // &
        objlist // " " // &
        os_data%ldflags_hepmc // " " // &
        os_data%ldflags_lcio // " " // &
        os_data%ldflags_hoppet // " " // &
        os_data%ldflags_looptools
    else
        command_string = &
            os_data%ld // " " // &
            os_data%ldflags_so // " " // &
            os_data%fcflags // " " // &
            os_data%whizard_ldflags // " " // &
            os_data%ldflags // " " // &
            os_data%ldflags_static // " " // &
            "-o '" // exec_name // "' " // &
            objlist // " " // &
            os_data%ldflags_hepmc // " " // &
            os_data%ldflags_lcio // " " // &
            os_data%ldflags_hoppet // " " // &
            os_data%ldflags_looptools
    end if
    call os_system_call (command_string, status)
end subroutine os_link_static

```

Determine the name of the shared library to link. If libtool is used, this is encoded in the .la file which resides in place of the library itself.

```

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

<OS interface: procedures>+≡
    function os_get_dlname (lib, os_data, ignore, silent) result (dlname)
        type(string_t) :: dlname
        type(string_t), intent(in) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in), optional :: ignore, silent
        type(string_t) :: filename
        type(string_t) :: buffer
        logical :: exist, required, quiet
        integer :: u
        u = free_unit ()
        if (present (ignore)) then
            required = .not. ignore
        else
            required = .true.
        end if
        if (present (silent)) then
            quiet = silent
        else
            quiet = .false.
        end if
    end function

```

```

end if
if (os_data%use_libtool) then
  filename = lib // ".la"
  inquire (file=char(filename), exist=exist)
  if (exist) then
    open (unit=u, file=char(filename), action="read", status="old")
    SCAN_LTFILE: do
      call get (u, buffer)
      if (extract (buffer, 1, 7) == "dlname=") then
        dlname = extract (buffer, 9)
        dlname = remove (dlname, len (dlname))
        exit SCAN_LTFILE
      end if
    end do SCAN_LTFILE
    close (u)
  else if (required) then
    if (.not. quiet) call msg_fatal (" Library '" // char (lib) &
      // "': libtool archive not found")
    dlname = ""
  else
    if (.not. quiet) call msg_message ("[No compiled library '" &
      // char (lib) // "']")
    dlname = ""
  end if
else
  dlname = lib // "." // os_data%fc_shrlib_ext
  inquire (file=char(dlname), exist=exist)
  if (.not. exist) then
    if (required) then
      if (.not. quiet) call msg_fatal (" Library '" // char (lib) &
        // "' not found")
    else
      if (.not. quiet) call msg_message &
        ("[No compiled process library '" // char (lib) // "']")
      dlname = ""
    end if
  end if
end if
end function os_get_dlname

```

5.5.9 Controlling OpenMP

OpenMP is handled automatically by the library for the most part. Here is a convenience routine for setting the number of threads, with some diagnostics.

```

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

<OS interface: procedures>+≡
  subroutine openmp_set_num_threads_verbose (num_threads, openmp_logging)
    integer, intent(in) :: num_threads
    integer :: n_threads
    logical, intent(in), optional :: openmp_logging
    logical :: logging

```

```

if (present (openmp_logging)) then
  logging = openmp_logging
else
  logging = .true.
end if
n_threads = num_threads
if (openmp_is_active ()) then
  if (num_threads == 1) then
    if (logging) then
      write (msg_buffer, "(A,I0,A)") "OpenMP: Using ", num_threads, &
        " thread"
      call msg_message
    end if
    n_threads = num_threads
  else if (num_threads > 1) then
    if (logging) then
      write (msg_buffer, "(A,I0,A)") "OpenMP: Using ", num_threads, &
        " threads"
      call msg_message
    end if
    n_threads = num_threads
  else
    if (logging) then
      write (msg_buffer, "(A,I0,A)") "OpenMP: " &
        // "Illegal value of openmp_num_threads (", num_threads, &
        ") ignored"
      call msg_error
    end if
    n_threads = openmp_get_default_max_threads ()
    if (logging) then
      write (msg_buffer, "(A,I0,A)") "OpenMP: Using ", &
        n_threads, " threads"
      call msg_message
    end if
  end if
  if (n_threads > openmp_get_default_max_threads ()) then
    if (logging) then
      write (msg_buffer, "(A,I0)") "OpenMP: " &
        // "Number of threads is greater than library default of ", &
        openmp_get_default_max_threads ()
      call msg_warning
    end if
  end if
  call openmp_set_num_threads (n_threads)
else if (num_threads /= 1) then
  if (logging) then
    write (msg_buffer, "(A,I0,A)") "openmp_num_threads set to ", &
      num_threads, ", but OpenMP is not active: ignored"
    call msg_warning
  end if
end if
end if
end subroutine openmp_set_num_threads_verbose

```

5.5.10 Controlling MPI

The overall MPI handling has to be defined in a context specific way, but we can simplify things like logging or receiving `n_size` or `rank`.

```
<OS interface: public>+≡
    public :: mpi_set_logging

<OS interface: procedures>+≡
    subroutine mpi_set_logging (mpi_logging)
        logical, intent(in) :: mpi_logging
        integer :: n_size, rank
        call mpi_get_comm_id (n_size, rank)
        if (mpi_logging .and. n_size > 1) then
            write (msg_buffer, "(A,I0,A)") "MPI: Using ", n_size, " processes."
            call msg_message ()
            if (rank == 0) then
                call msg_message ("MPI: master worker")
            else
                write (msg_buffer, "(A,I0)") "MPI: slave worker #", rank
                call msg_message ()
            end if
        end if
    end subroutine mpi_set_logging
```

Receive communicator size and rank inside communicator. The subroutine is a stub, if not compiled with MPI.

```
<OS interface: public>+≡
    public :: mpi_get_comm_id

<OS interface: procedures>+≡
    subroutine mpi_get_comm_id (n_size, rank)
        integer, intent(out) :: n_size
        integer, intent(out) :: rank
        n_size = 1
        rank = 0
    <OS interface: mpi get comm id>
    end subroutine mpi_get_comm_id

<OS interface: mpi get comm id>≡

<MPI: OS interface: mpi get comm id>≡
    call MPI_Comm_size (MPI_COMM_WORLD, n_size)
    call MPI_Comm_rank (MPI_COMM_WORLD, rank)

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

<OS interface: procedures>+≡
    logical function mpi_is_comm_master () result (flag)
        integer :: n_size, rank
        call mpi_get_comm_id (n_size, rank)
        flag = (rank == 0)
    end function mpi_is_comm_master
```

5.5.11 Unit tests

Test module, followed by the corresponding implementation module.

```
<os_interface_ut.f90>≡  
  <File header>  
  
  module os_interface_ut  
    use unit_tests  
    use os_interface_utl  
  
    <Standard module head>  
  
    <OS interface: public test>  
  
    contains  
  
    <OS interface: test driver>  
  
  end module os_interface_ut  
  
<os_interface_uti.f90>≡  
  <File header>  
  
  module os_interface_uti  
  
    use, intrinsic :: iso_c_binding !NODEP!  
  
    <Use strings>  
    use io_units  
  
    use os_interface  
  
    <Standard module head>  
  
    <OS interface: test declarations>  
  
    contains  
  
    <OS interface: tests>  
  
  end module os_interface_uti  
API: driver for the unit tests below.  
<OS interface: public test>≡  
  public :: os_interface_test  
<OS interface: test driver>≡  
  subroutine os_interface_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <OS interface: execute tests>  
  end subroutine os_interface_test
```

Write a Fortran source file, compile it to a shared library, load it, and execute the contained function.

```

<OS interface: execute tests>≡
    call test (os_interface_1, "os_interface_1", &
        "check OS interface routines", &
        u, results)

<OS interface: test declarations>≡
    public :: os_interface_1

<OS interface: tests>≡
    subroutine os_interface_1 (u)
        integer, intent(in) :: u
        type(dlaccess_t) :: dlaccess
        type(string_t) :: fname, libname, ext
        type(os_data_t) :: os_data
        type(string_t) :: filename_src, filename_obj
        abstract interface
            function so_test_proc (i) result (j) bind(C)
                import c_int
                integer(c_int), intent(in) :: i
                integer(c_int) :: j
            end function so_test_proc
        end interface
        procedure(so_test_proc), pointer :: so_test => null ()
        type(c_funptr) :: c_fptr
        integer :: unit
        integer(c_int) :: i
        call os_data%init ()
        fname = "so_test"
        filename_src = fname // os_data%fc_src_ext
        if (os_data%use_libtool) then
            ext = ".lo"
        else
            ext = os_data%obj_ext
        end if
        filename_obj = fname // ext
        libname = fname // '.' // os_data%fc_shrlib_ext

        write (u, "(A)")  "* Test output: OS interface"
        write (u, "(A)")  "* Purpose: check os_interface routines"
        write (u, "(A)")

        write (u, "(A)")  "* write source file 'so_test.f90'"
        write (u, "(A)")
        unit = free_unit ()
        open (unit=unit, file=char(filename_src), action="write")
        write (unit, "(A)") "function so_test (i) result (j) bind(C)"
        write (unit, "(A)") " use iso_c_binding"
        write (unit, "(A)") " integer(c_int), intent(in) :: i"
        write (unit, "(A)") " integer(c_int) :: j"
        write (unit, "(A)") " j = 2 * i"
        write (unit, "(A)") "end function so_test"
        close (unit)
        write (u, "(A)")  "* compile and link as 'so_test.so/dylib'"
        write (u, "(A)")
        call os_compile_shared (fname, os_data)

```



```

call os_link_shared (filename_obj, fname, os_data)
write (u, "(A)")  "* load library 'so_test.so/dylib'"
write (u, "(A)")
call dlaccess_init (dlaccess, var_str (.), libname, os_data)
if (dlaccess_is_open (dlaccess)) then
  write (u, "(A)") "    success"
else
  write (u, "(A)") "    failure"
end if
write (u, "(A)")  "* load symbol 'so_test'"
write (u, "(A)")
c_fptr = dlaccess_get_c_funptr (dlaccess, fname)
if (c_associated (c_fptr)) then
  write (u, "(A)") "    success"
else
  write (u, "(A)") "    failure"
end if
call c_f_procpointer (c_fptr, so_test)
write (u, "(A)")  "* Execute function from 'so_test.so/dylib'"
i = 7
write (u, "(A,1x,I1)") "    input  = ", i
write (u, "(A,1x,I1)") "    result = ", so_test(i)
if (so_test(i) / i .ne. 2) then
  write (u, "(A)")  "* Compiling and linking ISO C functions failed."
else
  write (u, "(A)")  "* Successful."
end if
write (u, "(A)")
write (u, "(A)")  "* Cleanup"
call dlaccess_final (dlaccess)
end subroutine os_interface_1

```

5.6 Interface for formatted I/O

For access to formatted printing (possibly input), we interface the C `printf` family of functions. There are two important issues here:

1. `printf` takes an arbitrary number of arguments, relying on the C stack. This is not interoperable. We interface it with C wrappers that output a single integer, real or string and restrict the allowed formats accordingly.
2. Restricting format strings is essential also for preventing format string attacks. Allowing arbitrary format string would create a real security hole in a Fortran program.
3. The string returned by `sprintf` must be allocated to the right size.

```

<formats.f90>≡
  <File header>

```

```

module formats

```

```

    use, intrinsic :: iso_c_binding

    <Use kinds>
    <Use strings>
    use io_units
    use diagnostics

    <Standard module head>

    <Formats: public>

    <Formats: parameters>

    <Formats: types>

    <Formats: interfaces>

    contains

    <Formats: procedures>

    end module formats

```

5.6.1 Parsing a C format string

The C format string contains characters and format conversion specifications. The latter are initiated by a % sign. If the next letter is also a %, a percent sign is printed and no conversion is done. Otherwise, a conversion is done and applied to the next argument in the argument list. First comes an optional flag (#, 0, -, +, or space), an optional field width (decimal digits starting not with zero), an optional precision (period, then another decimal digit string), a length modifier (irrelevant for us, therefore not supported), and a conversion specifier: **d** or **i** for integer; **e**, **f**, **g** (also upper case) for double-precision real, **s** for a string.

We explicitly exclude all other conversion specifiers, and we check the specifiers against the actual arguments.

A type for passing arguments

This is a polymorphic type that can hold integer, real (double), and string arguments.

```

<Formats: parameters>≡
    integer, parameter, public :: ARGTYPE_NONE = 0
    integer, parameter, public :: ARGTYPE_LOG = 1
    integer, parameter, public :: ARGTYPE_INT = 2
    integer, parameter, public :: ARGTYPE_REAL = 3
    integer, parameter, public :: ARGTYPE_STR = 4

```

The integer and real entries are actually scalars, but we avoid relying on the allocatable-scalar feature and make them one-entry arrays. The character entry is a real array which is a copy of the string.

Logical values are mapped to strings (true or false), so this type parameter value is mostly unused.

```

<Formats: public>≡
    public :: sprintf_arg_t

<Formats: types>≡
    type :: sprintf_arg_t
    private
    integer :: type = ARGTYPE_NONE
    integer(c_int), dimension(:), allocatable :: ival
    real(c_double), dimension(:), allocatable :: rval
    character(c_char), dimension(:), allocatable :: sval
end type sprintf_arg_t

<Formats: public>+≡
    public :: sprintf_arg_init

<Formats: interfaces>≡
    interface sprintf_arg_init
        module procedure sprintf_arg_init_log
        module procedure sprintf_arg_init_int
        module procedure sprintf_arg_init_real
        module procedure sprintf_arg_init_str
    end interface

<Formats: procedures>≡
    subroutine sprintf_arg_init_log (arg, lval)
        type(sprintf_arg_t), intent(out) :: arg
        logical, intent(in) :: lval
        arg%type = ARGTYPE_STR
        if (lval) then
            allocate (arg%sval (5))
            arg%sval = ['t', 'r', 'u', 'e', c_null_char]
        else
            allocate (arg%sval (6))
            arg%sval = ['f', 'a', 'l', 's', 'e', c_null_char]
        end if
    end subroutine sprintf_arg_init_log

    subroutine sprintf_arg_init_int (arg, ival)
        type(sprintf_arg_t), intent(out) :: arg
        integer, intent(in) :: ival
        arg%type = ARGTYPE_INT
        allocate (arg%ival (1))
        arg%ival = ival
    end subroutine sprintf_arg_init_int

    subroutine sprintf_arg_init_real (arg, rval)
        type(sprintf_arg_t), intent(out) :: arg
        real(default), intent(in) :: rval
        arg%type = ARGTYPE_REAL
        allocate (arg%rval (1))
        arg%rval = rval
    end subroutine sprintf_arg_init_real

```

```

subroutine sprintf_arg_init_str (arg, sval)
  type(sprintf_arg_t), intent(out) :: arg
  type(string_t), intent(in) :: sval
  integer :: i
  arg%type = ARGTYPE_STR
  allocate (arg%sval (len (sval) + 1))
  do i = 1, len (sval)
    arg%sval(i) = extract (sval, i, i)
  end do
  arg%sval(len (sval) + 1) = c_null_char
end subroutine sprintf_arg_init_str

```

(Formats: procedures)+≡

```

subroutine sprintf_arg_write (arg, unit)
  type(sprintf_arg_t), intent(in) :: arg
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  select case (arg%type)
  case (ARGTYPE_NONE)
    write (u, *) "[none]"
  case (ARGTYPE_INT)
    write (u, "(1x,A,1x)", advance = "no") "[int]"
    write (u, *) arg%ival
  case (ARGTYPE_REAL)
    write (u, "(1x,A,1x)", advance = "no") "[real]"
    write (u, *) arg%rval
  case (ARGTYPE_STR)
    write (u, "(1x,A,1x,A)", advance = "no") "[string]", ''
    write (u, *) arg%rval, ''
  end select
end subroutine sprintf_arg_write

```

Return an upper bound for the length of the printed version; in case of strings the result is exact.

(Formats: procedures)+≡

```

elemental function sprintf_arg_get_length (arg) result (length)
  integer :: length
  type(sprintf_arg_t), intent(in) :: arg
  select case (arg%type)
  case (ARGTYPE_INT)
    length = log10 (real (huge (arg%ival(1)))) + 2
  case (ARGTYPE_REAL)
    length = log10 (real (radix (arg%rval(1))) ** digits (arg%rval(1))) + 8
  case (ARGTYPE_STR)
    length = size (arg%sval)
  case default
    length = 0
  end select
end function sprintf_arg_get_length

```

(Formats: procedures)+≡

```

subroutine sprintf_arg_apply_printf (arg, fmt, result, actual_length)
  type(sprintf_arg_t), intent(in) :: arg
  character(c_char), dimension(:), intent(in) :: fmt
  character(c_char), dimension(:), intent(inout) :: result
  integer, intent(out) :: actual_length
  integer(c_int) :: ival
  real(c_double) :: rval
  select case (arg%type)
  case (ARGTYPE_NONE)
    actual_length = sprintf_none (result, fmt)
  case (ARGTYPE_INT)
    ival = arg%ival(1)
    actual_length = sprintf_int (result, fmt, ival)
  case (ARGTYPE_REAL)
    rval = arg%rval(1)
    actual_length = sprintf_double (result, fmt, rval)
  case (ARGTYPE_STR)
    actual_length = sprintf_str (result, fmt, arg%sval)
  case default
    call msg_bug ("sprintf_arg_apply_printf called with illegal type")
  end select
  if (actual_length < 0) then
    write (msg_buffer, *) "Format: '", fmt, "'"
    call msg_message ()
    write (msg_buffer, *) "Output: '", result, "'"
    call msg_message ()
    call msg_error ("I/O error in sprintf call")
    actual_length = 0
  end if
end subroutine sprintf_arg_apply_printf

```

Container type for the output

There is a procedure which chops the format string into pieces that contain at most one conversion specifier. Pairing this with a `sprintf_arg` object, we get the actual input to the `sprintf` interface. The type below holds this input and can allocate the output string.

(Formats: types)+≡

```

type :: sprintf_interface_t
  private
  character(c_char), dimension(:), allocatable :: input_fmt
  type(sprintf_arg_t) :: arg
  character(c_char), dimension(:), allocatable :: output_str
  integer :: output_str_len = 0
end type sprintf_interface_t

```

(Formats: procedures)+≡

```

subroutine sprintf_interface_init (intf, fmt, arg)
  type(sprintf_interface_t), intent(out) :: intf
  type(string_t), intent(in) :: fmt
  type(sprintf_arg_t), intent(in) :: arg
  integer :: fmt_len, i

```

```

    fmt_len = len (fmt)
    allocate (intf%input_fmt (fmt_len + 1))
    do i = 1, fmt_len
        intf%input_fmt(i) = extract (fmt, i, i)
    end do
    intf%input_fmt(fmt_len+1) = c_null_char
    intf%arg = arg
    allocate (intf%output_str (len (fmt) + sprintf_arg_get_length (arg) + 1))
end subroutine sprintf_interface_init

```

<Formats: procedures>+≡

```

subroutine sprintf_interface_write (intf, unit)
    type(sprintf_interface_t), intent(in) :: intf
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, *) "Format string = ", "'", intf%input_fmt, "'"
    write (u, "(1x,A,1x)", advance = "no") "Argument = "
    call sprintf_arg_write (intf%arg, unit)
    if (intf%output_str_len > 0) then
        write (u, *) "Result string = ", &
            "'", intf%output_str (1:intf%output_str_len), "'"
    end if
end subroutine sprintf_interface_write

```

Return the output string:

<Formats: procedures>+≡

```

function sprintf_interface_get_result (intf) result (string)
    type(string_t) :: string
    type(sprintf_interface_t), intent(in) :: intf
    character(kind = c_char, len = max (intf%output_str_len, 0)) :: buffer
    integer :: i
    if (intf%output_str_len > 0) then
        do i = 1, intf%output_str_len
            buffer(i:i) = intf%output_str(i)
        end do
        string = buffer(1:intf%output_str_len)
    else
        string = ""
    end if
end function sprintf_interface_get_result

```

<Formats: procedures>+≡

```

subroutine sprintf_interface_apply_sprintf (intf)
    type(sprintf_interface_t), intent(inout) :: intf
    call sprintf_arg_apply_sprintf &
        (intf%arg, intf%input_fmt, intf%output_str, intf%output_str_len)
end subroutine sprintf_interface_apply_sprintf

```

Import the interfaces defined in the previous section:

<Formats: interfaces>+≡

<sprintf interfaces>

Scan the format string

Chop it into pieces that contain one conversion specifier each. The zero-th piece contains the part before the first specifier. Check the specifiers and allow only the subset that we support. Also check for an exact match between conversion specifiers and input arguments. The result is an allocated array of `sprintf_interface` object; each one contains a piece of the format string and the corresponding argument.

(Formats: procedures)+≡

```
subroutine chop_and_check_format_string (fmt, arg, intf)
  type(string_t), intent(in) :: fmt
  type(sprintf_arg_t), dimension(:), intent(in) :: arg
  type(sprintf_interface_t), dimension(:), intent(out), allocatable :: intf
  integer :: n_args, i
  type(string_t), dimension(:), allocatable :: split_fmt
  type(string_t) :: word, buffer, separator
  integer :: pos, length, l
  logical :: ok
  type(sprintf_arg_t) :: arg_null
  ok = .true.
  length = 0
  n_args = size (arg)
  allocate (split_fmt (0:n_args))
  split_fmt = ""
  buffer = fmt
  SCAN_ARGS: do i = 1, n_args
    FIND_CONVERSION: do
      call split (buffer, word, "%", separator=separator)
      if (separator == "") then
        call msg_message ('"' // char (fmt) // '"')
        call msg_error ("C-formatting string: " &
          // "too few conversion specifiers in format string")
        ok = .false.; exit SCAN_ARGS
      end if
      split_fmt(i-1) = split_fmt(i-1) // word
      if (extract (buffer, 1, 1) /= "%") then
        split_fmt(i) = "%"
        exit FIND_CONVERSION
      else
        split_fmt(i-1) = split_fmt(i-1) // "%"
      end if
    end do FIND_CONVERSION
    pos = verify (buffer, "#0-+ ") ! Flag characters (zero or more)
    split_fmt(i) = split_fmt(i) // extract (buffer, 1, pos-1)
    buffer = remove (buffer, 1, pos-1)
    pos = verify (buffer, "123456890") ! Field width
    word = extract (buffer, 1, pos-1)
    if (len (word) /= 0) then
      call read_int_from_string (word, len (word), 1)
      length = length + 1
    end if
  end do
```

```

split_fmt(i) = split_fmt(i) // word
buffer = remove (buffer, 1, pos-1)
if (extract (buffer, 1, 1) == ".") then
    buffer = remove (buffer, 1, 1)
    pos = verify (buffer, "1234567890")    ! Precision
    split_fmt(i) = split_fmt(i) // "." // extract (buffer, 1, pos-1)
    buffer = remove (buffer, 1, pos-1)
end if
! Length modifier would come here, but is not allowed
select case (char (extract (buffer, 1, 1))) ! conversion specifier
case ("d", "i")
    if (arg(i)%type /= ARGTYPE_INT) then
        call msg_message ('"' // char (fmt) // '"')
        call msg_error ("C-formatting string: " &
            // "argument type mismatch: integer value expected")
        ok = .false.; exit SCAN_ARGS
    end if
case ("e", "E", "f", "F", "g", "G")
    if (arg(i)%type /= ARGTYPE_REAL) then
        call msg_message ('"' // char (fmt) // '"')
        call msg_error ("C-formatting string: " &
            // "argument type mismatch: real value expected")
        ok = .false.; exit SCAN_ARGS
    end if
case ("s")
    if (arg(i)%type /= ARGTYPE_STR) then
        call msg_message ('"' // char (fmt) // '"')
        call msg_error ("C-formatting string: " &
            // "argument type mismatch: logical or string value expected")
        ok = .false.; exit SCAN_ARGS
    end if
case default
    call msg_message ('"' // char (fmt) // '"')
    call msg_error ("C-formatting string: " &
        // "illegal or incomprehensible conversion specifier")
    ok = .false.; exit SCAN_ARGS
end select
split_fmt(i) = split_fmt(i) // extract (buffer, 1, 1)
buffer = remove (buffer, 1, 1)
end do SCAN_ARGS
if (ok) then
    FIND_EXTRA_CONVERSION: do
        call split (buffer, word, "%", separator=separator)
        split_fmt(n_args) = split_fmt(n_args) // word // separator
        if (separator == "") exit FIND_EXTRA_CONVERSION
        if (extract (buffer, 1, 1) == "%") then
            split_fmt(n_args) = split_fmt(n_args) // "%"
            buffer = remove (buffer, 1, 1)
        else
            call msg_message ('"' // char (fmt) // '"')
            call msg_error ("C-formatting string: " &
                // "too many conversion specifiers in format string")
            ok = .false.; exit FIND_EXTRA_CONVERSION
        end if
    end do
end if

```



```

        end do FIND_EXTRA_CONVERSION
        split_fmt(n_args) = split_fmt(n_args) // buffer
        allocate (intf (0:n_args))
        call sprintf_interface_init (intf(0), split_fmt(0), arg_null)
        do i = 1, n_args
            call sprintf_interface_init (intf(i), split_fmt(i), arg(i))
        end do
    else
        allocate (intf (0))
    end if
contains
    subroutine read_int_from_string (word, length, l)
        type(string_t), intent(in) :: word
        integer, intent(in) :: length
        integer, intent(out) :: l
        character(len=length) :: buffer
        buffer = word
        read (buffer, *) l
    end subroutine read_int_from_string
end subroutine chop_and_check_format_string

```

5.6.2 API

<Formats: public>+≡

```
public :: sprintf
```

<Formats: procedures>+≡

```

function sprintf (fmt, arg) result (string)
    type(string_t) :: string
    type(string_t), intent(in) :: fmt
    type(sprintf_arg_t), dimension(:), intent(in) :: arg
    type(sprintf_interface_t), dimension(:), allocatable :: intf
    integer :: i
    string = ""
    call chop_and_check_format_string (fmt, arg, intf)
    if (size (intf) > 0) then
        do i = 0, ubound (intf, 1)
            call sprintf_interface_apply sprintf (intf(i))
            string = string // sprintf_interface_get_result (intf(i))
        end do
    end if
end function sprintf

```

5.6.3 Unit tests

Test module, followed by the corresponding implementation module.

<formats_ut.f90>≡

<File header>

```

module formats_ut
    use unit_tests

```

```

        use formats_uti

    <Standard module head>

    <Formats: public test>

contains

    <Formats: test driver>

end module formats_ut
<formats_uti.f90>≡
    <File header>

    module formats_uti

    <Use kinds>
    <Use strings>

        use formats

    <Standard module head>

    <Formats: test declarations>

    <Formats: test types>

contains

    <Formats: tests>

end module formats_uti
API: driver for the unit tests below.
<Formats: public test>≡
    public :: format_test
<Formats: test driver>≡
    subroutine format_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Formats: execute tests>
    end subroutine format_test

<Formats: execute tests>≡
    call test (format_1, "format_1", &
        "check formatting routines", &
        u, results)
<Formats: test declarations>≡
    public :: format_1
<Formats: tests>≡
    subroutine format_1 (u)
        integer, intent(in) :: u

```

```

write (u, "(A)")  "**** Test 1: a string ****"
write (u, "(A)")
call test_run (var_str("%s"), 1, [4], ['abcdefghij'], u)
write (u, "(A)")  "**** Test 2: two integers ****"
write (u, "(A)")
call test_run (var_str("%d,%d"), 2, [2, 2], ['42', '13'], u)
write (u, "(A)")  "**** Test 3: floating point number ****"
write (u, "(A)")
call test_run (var_str("%8.4f"), 1, [3], ['42567.12345'], u)
write (u, "(A)")  "**** Test 4: general expression ****"
call test_run (var_str("%g"), 1, [3], ['3.1415'], u)
contains
  subroutine test_run (fmt, n_args, type, buffer, unit)
    type(string_t), intent(in) :: fmt
    integer, intent(in) :: n_args, unit
    logical :: lval
    integer :: ival
    real(default) :: rval
    integer :: i
    type(string_t) :: string
    type(sprintf_arg_t), dimension(:), allocatable :: arg
    integer, dimension(n_args), intent(in) :: type
    character(*), dimension(n_args), intent(in) :: buffer
    write (unit, "(A,A)")  "Format string :", char(fmt)
    write (unit, "(A,I1)")  "Number of args:", n_args
    allocate (arg (n_args))
    do i = 1, n_args
      write (unit, "(A,I1)")  "Argument (type ) = ", type(i)
      select case (type(i))
      case (ARGTYPE_LOG)
        read (buffer(i), *) lval
        call sprintf_arg_init (arg(i), lval)
      case (ARGTYPE_INT)
        read (buffer(i), *) ival
        call sprintf_arg_init (arg(i), ival)
      case (ARGTYPE_REAL)
        read (buffer(i), *) rval
        call sprintf_arg_init (arg(i), rval)
      case (ARGTYPE_STR)
        call sprintf_arg_init (arg(i), var_str (trim (buffer(i))))
      end select
    end do
    string = sprintf (fmt, arg)
    write (unit, "(A,A,A)")  "Result: '", char (string), "'"
    deallocate (arg)
  end subroutine test_run
end subroutine format_1

```

5.7 CPU timing

The time is stored in a simple derived type which just holds a floating-point number.

```

<cpu_time.f90>≡
  <File header>

  module cpu_time

    <Use kinds>
    use io_units
    <Use strings>
    use diagnostics

    <Standard module head>

    <CPU time: public>

    <CPU time: types>

    <CPU time: interfaces>

    contains

    <CPU time: procedures>

  end module cpu_time

```

The CPU time is a floating-point number with an arbitrary reference time. It is single precision (default real, not `real(default)`). It is measured in seconds.

```

<CPU time: public>≡
  public :: time_t

<CPU time: types>≡
  type :: time_t
    private
    logical :: known = .false.
    real :: value = 0
    contains
    <CPU time: time: TBP>
  end type time_t

<CPU time: time: TBP>≡
  procedure :: write => time_write

<CPU time: procedures>≡
  subroutine time_write (object, unit)
    class(time_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "Time in seconds ="
    if (object%known) then
      write (u, "(1x,ES10.3)") object%value
    else
      write (u, "(1x,A)") "[unknown]"
    end if
  end subroutine time_write

```

Set the current time

```
<CPU time: time: TBP>+≡
  procedure :: set_current => time_set_current

<CPU time: procedures>+≡
  subroutine time_set_current (time)
    class(time_t), intent(out) :: time
    integer :: msec
    call system_clock (msec)
    time%value = real (msec) / 1000.
    time%known = time%value > 0
  end subroutine time_set_current
```

Assign to a real(default value. If the time is undefined, return zero.

```
<CPU time: public>+≡
  public :: assignment(=)

<CPU time: interfaces>≡
  interface assignment(=)
    module procedure real_assign_time
    module procedure real_default_assign_time
  end interface

<CPU time: procedures>+≡
  pure subroutine real_assign_time (r, time)
    real, intent(out) :: r
    class(time_t), intent(in) :: time
    if (time%known) then
      r = time%value
    else
      r = 0
    end if
  end subroutine real_assign_time

  pure subroutine real_default_assign_time (r, time)
    real(default), intent(out) :: r
    class(time_t), intent(in) :: time
    if (time%known) then
      r = time%value
    else
      r = 0
    end if
  end subroutine real_default_assign_time
```

Assign an integer or (single precision) real value to the time object.

```
<CPU time: time: TBP>+≡
  generic :: assignment(=) => time_assign_from_integer, time_assign_from_real
  procedure, private :: time_assign_from_integer
  procedure, private :: time_assign_from_real

<CPU time: procedures>+≡
  subroutine time_assign_from_integer (time, ival)
    class(time_t), intent(out) :: time
    integer, intent(in) :: ival
```

```

        time%value = ival
        time%known = .true.
    end subroutine time_assign_from_integer

    subroutine time_assign_from_real (time, rval)
        class(time_t), intent(out) :: time
        real, intent(in) :: rval
        time%value = rval
        time%known = .true.
    end subroutine time_assign_from_real

```

Add times and compute time differences. If any input value is undefined, the result is undefined.

```

<CPU time: time: TBP>+≡
    generic :: operator(-) => subtract_times
    generic :: operator(+) => add_times
    procedure, private :: subtract_times
    procedure, private :: add_times

<CPU time: procedures>+≡
    pure function subtract_times (t_end, t_begin) result (time)
        type(time_t) :: time
        class(time_t), intent(in) :: t_end, t_begin
        if (t_end%known .and. t_begin%known) then
            time%known = .true.
            time%value = t_end%value - t_begin%value
        end if
    end function subtract_times

    pure function add_times (t1, t2) result (time)
        type(time_t) :: time
        class(time_t), intent(in) :: t1, t2
        if (t1%known .and. t2%known) then
            time%known = .true.
            time%value = t1%value + t2%value
        end if
    end function add_times

```

Check if a time is known, so we can use it:

```

<CPU time: time: TBP>+≡
    procedure :: is_known => time_is_known

<CPU time: procedures>+≡
    function time_is_known (time) result (flag)
        class(time_t), intent(in) :: time
        logical :: flag
        flag = time%known
    end function time_is_known

```

We define functions for converting the time into ss / mm:ss / hh:mm:ss / dd:mm:hh:ss.

```

<CPU time: time: TBP>+≡
    generic :: expand => time_expand_s, time_expand_ms, &

```

```

        time_expand_hms, time_expand_dhms
procedure, private :: time_expand_s
procedure, private :: time_expand_ms
procedure, private :: time_expand_hms
procedure, private :: time_expand_dhms
<CPU time: procedures>+≡
subroutine time_expand_s (time, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: sec
    if (time%known) then
        sec = time%value
    else
        call msg_bug ("Time: attempt to expand undefined value")
    end if
end subroutine time_expand_s

subroutine time_expand_ms (time, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: min, sec
    if (time%known) then
        if (time%value >= 0) then
            sec = mod (int (time%value), 60)
        else
            sec = - mod (int (- time%value), 60)
        end if
        min = time%value / 60
    else
        call msg_bug ("Time: attempt to expand undefined value")
    end if
end subroutine time_expand_ms

subroutine time_expand_hms (time, hour, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: hour, min, sec
    call time%expand (min, sec)
    hour = min / 60
    if (min >= 0) then
        min = mod (min, 60)
    else
        min = - mod (-min, 60)
    end if
end subroutine time_expand_hms

subroutine time_expand_dhms (time, day, hour, min, sec)
    class(time_t), intent(in) :: time
    integer, intent(out) :: day, hour, min, sec
    call time%expand (hour, min, sec)
    day = hour / 24
    if (hour >= 0) then
        hour = mod (hour, 24)
    else
        hour = - mod (- hour, 24)
    end if
end subroutine time_expand_dhms

```

Use the above expansions to generate a time string.

```

(CPU time: time: TBP)+≡
  procedure :: to_string_s => time_to_string_s
  procedure :: to_string_ms => time_to_string_ms
  procedure :: to_string_hms => time_to_string_hms
  procedure :: to_string_dhms => time_to_string_dhms

(CPU time: procedures)+≡
  function time_to_string_s (time) result (str)
    class(time_t), intent(in) :: time
    type(string_t) :: str
    character(256) :: buffer
    integer :: s
    call time%expand (s)
    write (buffer, "(I0,'s')") s
    str = trim (buffer)
  end function time_to_string_s

  function time_to_string_ms (time, blank) result (str)
    class(time_t), intent(in) :: time
    logical, intent(in), optional :: blank
    type(string_t) :: str
    character(256) :: buffer
    integer :: s, m
    logical :: x_out
    x_out = .false.
    if (present (blank)) x_out = blank
    call time%expand (m, s)
    write (buffer, "(I0,'m:',I2.2,'s')") m, abs (s)
    str = trim (buffer)
    if (x_out) then
      str = replace (str, len(str)-1, "X")
    end if
  end function time_to_string_ms

  function time_to_string_hms (time) result (str)
    class(time_t), intent(in) :: time
    type(string_t) :: str
    character(256) :: buffer
    integer :: s, m, h
    call time%expand (h, m, s)
    write (buffer, "(I0,'h:',I2.2,'m:',I2.2,'s')") h, abs (m), abs (s)
    str = trim (buffer)
  end function time_to_string_hms

  function time_to_string_dhms (time) result (str)
    class(time_t), intent(in) :: time
    type(string_t) :: str
    character(256) :: buffer
    integer :: s, m, h, d
    call time%expand (d, h, m, s)
    write (buffer, "(I0,'d:',I2.2,'h:',I2.2,'m:',I2.2,'s')") &
      d, abs (h), abs (m), abs (s)

```



```

    str = trim (buffer)
end function time_to_string_dhms

```

5.7.1 Timer

A timer can measure real (wallclock) time differences. The base type corresponds to the result, i.e., time difference. The object contains two further times for start and stop time.

```

⟨CPU time: public⟩+≡
    public :: timer_t

⟨CPU time: types⟩+≡
    type, extends (time_t) :: timer_t
    private
        logical :: running = .false.
        type(time_t) :: t1, t2
    contains
        ⟨CPU time: timer: TBP⟩
    end type timer_t

```

Output. If the timer is running, we indicate this, otherwise write just the result.

```

⟨CPU time: timer: TBP⟩≡
    procedure :: write => timer_write

⟨CPU time: procedures⟩+≡
    subroutine timer_write (object, unit)
        class(timer_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (object%running) then
            write (u, "(1x,A)") "Time in seconds = [running]"
        else
            call object%time_t%write (u)
        end if
    end subroutine timer_write

```

Start the timer: store the current time in the first entry and adapt the status. We forget any previous values.

```

⟨CPU time: timer: TBP⟩+≡
    procedure :: start => timer_start

⟨CPU time: procedures⟩+≡
    subroutine timer_start (timer)
        class(timer_t), intent(out) :: timer
        call timer%t1%set_current ()
        timer%running = .true.
    end subroutine timer_start

```

Restart the timer: simply adapt the status, keeping the start time.

```

⟨CPU time: timer: TBP⟩+≡
    procedure :: restart => timer_restart

```

```

<CPU time: procedures>+≡
subroutine timer_restart (timer)
  class(timer_t), intent(inout) :: timer
  if (timer%t1%known .and. .not. timer%running) then
    timer%running = .true.
  else
    call msg_bug ("Timer: restart attempt from wrong status")
  end if
end subroutine timer_restart

```

Stop the timer: store the current time in the second entry, adapt the status, and compute the elapsed time.

```

<CPU time: timer: TBP>+≡
  procedure :: stop => timer_stop

<CPU time: procedures>+≡
subroutine timer_stop (timer)
  class(timer_t), intent(inout) :: timer
  call timer%t2%set_current ()
  timer%running = .false.
  call timer%evaluate ()
end subroutine timer_stop

```

Manually set the time (for unit test)

```

<CPU time: timer: TBP>+≡
  procedure :: set_test_time1 => timer_set_test_time1
  procedure :: set_test_time2 => timer_set_test_time2

<CPU time: procedures>+≡
subroutine timer_set_test_time1 (timer, t)
  class(timer_t), intent(inout) :: timer
  integer, intent(in) :: t
  timer%t1 = t
end subroutine timer_set_test_time1

subroutine timer_set_test_time2 (timer, t)
  class(timer_t), intent(inout) :: timer
  integer, intent(in) :: t
  timer%t2 = t
end subroutine timer_set_test_time2

```

This is separate, available for the unit test.

```

<CPU time: timer: TBP>+≡
  procedure :: evaluate => timer_evaluate

<CPU time: procedures>+≡
subroutine timer_evaluate (timer)
  class(timer_t), intent(inout) :: timer
  timer%time_t = timer%t2 - timer%t1
end subroutine timer_evaluate

```

5.7.2 Unit tests

Test module, followed by the corresponding implementation module.

`<ctime_ut.f90>`≡
<File header>

```
module cptime_ut
  use unit_tests
  use cptime_uti
```

<Standard module head>

<CPU time: public test>

contains

<CPU time: test driver>

```
end module cptime_ut
```

`<ctime_uti.f90>`≡
<File header>

```
module cptime_uti
```

<Use strings>

```
  use cptime
```

<Standard module head>

<CPU time: test declarations>

contains

<CPU time: tests>

```
end module cptime_uti
```

API: driver for the unit tests below.

<CPU time: public test>≡
public :: cptime_test

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

Basic tests

Check basic functions of the time object. The part which we can't check is getting the actual time from the system clock, since the output will not be

reproducible. However, we can check time formats and operations.

```

<CPU time: execute tests>≡
    call test (cputime_1, "cputime_1", &
               "time operations", &
               u, results)

<CPU time: test declarations>≡
    public :: cputime_1

<CPU time: tests>≡
    subroutine cputime_1 (u)
        integer, intent(in) :: u
        type(time_t) :: time, time1, time2
        real :: t
        integer :: d, h, m, s

        write (u, "(A)")  "* Test output: cputime_1"
        write (u, "(A)")  "* Purpose: check time operations"
        write (u, "(A)")

        write (u, "(A)")  "* Undefined time"
        write (u, *)

        call time%write (u)

        write (u, *)
        write (u, "(A)")  "* Set time to zero"
        write (u, *)

        time = 0
        call time%write (u)

        write (u, *)
        write (u, "(A)")  "* Set time to 1.234 s"
        write (u, *)

        time = 1.234
        call time%write (u)

        t = time
        write (u, "(1x,A,F6.3)")  "Time as real =", t

        write (u, *)
        write (u, "(A)")  "* Compute time difference"
        write (u, *)

        time1 = 5.33
        time2 = 7.55
        time = time2 - time1

        call time1%write (u)
        call time2%write (u)
        call time%write (u)

        write (u, *)

```

```

write (u, "(A)") "* Compute time sum"
write (u, *)

time = time2 + time1

call time1%write (u)
call time2%write (u)
call time%write (u)

write (u, *)
write (u, "(A)") "* Expand time"
write (u, *)

time1 = ((24 + 1) * 60 + 1) * 60 + 1
time2 = ((3 * 24 + 23) * 60 + 59) * 60 + 59

call time1%expand (s)
write (u, 1) "s =", s
call time1%expand (m,s)
write (u, 1) "ms =", m, s
call time1%expand (h,m,s)
write (u, 1) "hms =", h, m, s
call time1%expand (d,h,m,s)
write (u, 1) "dhms =", d, h, m, s

call time2%expand (s)
write (u, 1) "s =", s
call time2%expand (m,s)
write (u, 1) "ms =", m, s
call time2%expand (h,m,s)
write (u, 1) "hms =", h, m, s
call time2%expand (d,h,m,s)
write (u, 1) "dhms =", d, h, m, s

write (u, *)
write (u, "(A)") "* Expand negative time"
write (u, *)

time1 = - (((24 + 1) * 60 + 1) * 60 + 1)
time2 = - (((3 * 24 + 23) * 60 + 59) * 60 + 59)

call time1%expand (s)
write (u, 1) "s =", s
call time1%expand (m,s)
write (u, 1) "ms =", m, s
call time1%expand (h,m,s)
write (u, 1) "hms =", h, m, s
call time1%expand (d,h,m,s)
write (u, 1) "dhms =", d, h, m, s

call time2%expand (s)
write (u, 1) "s =", s
call time2%expand (m,s)
write (u, 1) "ms =", m, s

```

```

call time2%expand (h,m,s)
write (u, 1) "hms =", h, m, s
call time2%expand (d,h,m,s)
write (u, 1) "dhms =", d, h, m, s

1  format (1x,A,1x,4(I0,:',':'))

write (u, *)
write (u, "(A)") "* String from time"
write (u, *)

time1 = ((24 + 1) * 60 + 1) * 60 + 1
time2 = ((3 * 24 + 23) * 60 + 59) * 60 + 59

write (u, "(A)") char (time1%to_string_s ())
write (u, "(A)") char (time1%to_string_ms ())
write (u, "(A)") char (time1%to_string_hms ())
write (u, "(A)") char (time1%to_string_dhms ())

write (u, "(A)") char (time2%to_string_s ())
write (u, "(A)") char (time2%to_string_ms ())
write (u, "(A)") char (time2%to_string_hms ())
write (u, "(A)") char (time2%to_string_dhms ())

write (u, "(A)")
write (u, "(A)") "* Blanking out the last second entry"
write (u, "(A)")

write (u, "(A)") char (time1%to_string_ms ())
write (u, "(A)") char (time1%to_string_ms (.true.))

write (u, *)
write (u, "(A)") "* String from negative time"
write (u, *)

time1 = -(((24 + 1) * 60 + 1) * 60 + 1)
time2 = -(((3 * 24 + 23) * 60 + 59) * 60 + 59)

write (u, "(A)") char (time1%to_string_s ())
write (u, "(A)") char (time1%to_string_ms ())
write (u, "(A)") char (time1%to_string_hms ())
write (u, "(A)") char (time1%to_string_dhms ())

write (u, "(A)") char (time2%to_string_s ())
write (u, "(A)") char (time2%to_string_ms ())
write (u, "(A)") char (time2%to_string_hms ())
write (u, "(A)") char (time2%to_string_dhms ())

write (u, "(A)")
write (u, "(A)") "* Test output end: cputime_1"

end subroutine cputime_1

```

Timer tests

Check a timer object.

```
<CPU time: execute tests>+≡
    call test (cputime_2, "cputime_2", &
               "timer", &
               u, results)

<CPU time: test declarations>+≡
    public :: cputime_2

<CPU time: tests>+≡
    subroutine cputime_2 (u)
        integer, intent(in) :: u
        type(timer_t) :: timer

        write (u, "(A)")  "* Test output: cputime_2"
        write (u, "(A)")  "* Purpose: check timer"
        write (u, "(A)")

        write (u, "(A)")  "* Undefined timer"
        write (u, *)

        call timer%write (u)

        write (u, *)
        write (u, "(A)")  "* Start timer"
        write (u, *)

        call timer%start ()
        call timer%write (u)

        write (u, *)
        write (u, "(A)")  "* Stop timer (injecting fake timings)"
        write (u, *)

        call timer%stop ()
        call timer%set_test_time1 (2)
        call timer%set_test_time2 (5)
        call timer%evaluate ()
        call timer%write (u)

        write (u, *)
        write (u, "(A)")  "* Restart timer"
        write (u, *)

        call timer%restart ()
        call timer%write (u)

        write (u, *)
        write (u, "(A)")  "* Stop timer again (injecting fake timing)"
        write (u, *)

        call timer%stop ()
        call timer%set_test_time2 (10)
```

```
call timer%evaluate ()
call timer%write (u)

write (u, *)
write (u, "(A)")  "* Test output end: cputime_2"

end subroutine cputime_2
```


Chapter 6

Combinatorics

These modules implement standard algorithms (sorting, hashing, etc.) that are not available in Fortran.

Fortran doesn't support generic programming, therefore the algorithms are implemented only for specific data types.

bytes Derived types for bytes and words.

hashes Types and tools for setting up hashtables.

md5 The MD5 algorithm for message digest.

permutations Permuting an array of integers.

sorting Sorting integer and real values.

grids d -dimensional grids can be saved to disk and used for interpolation, maximum finding, etc.

6.1 Bytes and such

In a few instances we will need the notion of a byte (8-bit) and a word (32 bit), even a 64-bit word. A block of 512 bit is also needed (for MD5).

We rely on integers up to 64 bit being supported by the processor. The main difference to standard integers is the interpretation as unsigned integers.

`<bytes.f90>` \equiv
<File header>

```
module bytes
```

```
    use kinds, only: i8, i32, i64
    use io_units
```

<Standard module head>

<Bytes: public>

<Bytes: types>

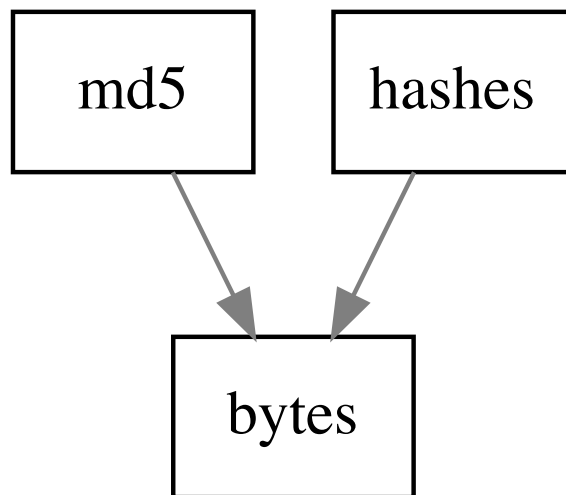


Figure 6.1: Module dependencies in `src/combinatorics`.

⟨Bytes: parameters⟩

⟨Bytes: interfaces⟩

contains

⟨Bytes: procedures⟩

end module bytes

6.1.1 8-bit words: bytes

This is essentially a wrapper around 8-bit integers. The wrapper emphasises their special interpretation as a sequence of bits. However, we interpret bytes as unsigned integers.

⟨Bytes: public⟩≡

public :: byte_t

⟨Bytes: types⟩≡

type :: byte_t

private

integer(i8) :: i

end type byte_t

⟨Bytes: public⟩+≡

public :: byte_zero

⟨Bytes: parameters⟩≡

type(byte_t), parameter :: byte_zero = byte_t (0_i8)

Set a byte from 8-bit integer:

⟨Bytes: public⟩+≡

public :: assignment(=)

⟨Bytes: interfaces⟩≡

interface assignment(=)

module procedure set_byte_from_i8

end interface

⟨Bytes: procedures⟩≡

subroutine set_byte_from_i8 (b, i)

type(byte_t), intent(out) :: b

integer(i8), intent(in) :: i

b%i = i

end subroutine set_byte_from_i8

Write a byte in one of two formats: either as a hexadecimal number (two digits, default) or as a decimal number (one to three digits). The decimal version is nontrivial because bytes are unsigned integers. Optionally append a newline.

⟨Bytes: public⟩+≡

public :: byte_write

```

<Bytes: interfaces>+≡
    interface byte_write
        module procedure byte_write_unit, byte_write_string
    end interface

<Bytes: procedures>+≡
    subroutine byte_write_unit (b, unit, decimal, newline)
        type(byte_t), intent(in), optional :: b
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: decimal, newline
        logical :: dc, nl
        type(word32_t) :: w
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        dc = .false.; if (present (decimal)) dc = decimal
        nl = .false.; if (present (newline)) nl = newline
        if (dc) then
            w = b
            write (u, '(I3)', advance='no') w%i
        else
            write (u, '(z2.2)', advance='no') b%i
        end if
        if (nl) write (u, *)
    end subroutine byte_write_unit

```

The string version is hex-only

```

<Bytes: procedures>+≡
    subroutine byte_write_string (b, s)
        type(byte_t), intent(in) :: b
        character(len=2), intent(inout) :: s
        write (s, '(z2.2)') b%i
    end subroutine byte_write_string

```

6.1.2 32-bit words

This is not exactly a 32-bit integer. A word is to be filled with bytes, and it may be partially filled. The filling is done lowest-byte first, highest-byte last. We count the bits, so fill should be either 0, 8, 16, 24, or 32. In printing words, we correspondingly distinguish between printing zeros and printing blanks.

```

<Bytes: public>+≡
    public :: word32_t

<Bytes: types>+≡
    type :: word32_t
        private
        integer(i32) :: i
        integer :: fill = 0
    end type word32_t

```

Assignment: the word is filled by inserting a 32-bit integer

```

<Bytes: interfaces>+≡
    interface assignment(=)

```

```

        module procedure word32_set_from_i32
        module procedure word32_set_from_byte
    end interface
<Bytes: procedures>+≡
    subroutine word32_set_from_i32 (w, i)
        type(word32_t), intent(out) :: w
        integer(i32), intent(in) :: i
        w%i = i
        w%fill = 32
    end subroutine word32_set_from_i32

```

Reverse assignment to a 32-bit integer. We do not check the fill status.

```

<Bytes: interfaces>+≡
    interface assignment(=)
        module procedure i32_from_word32
    end interface
<Bytes: procedures>+≡
    subroutine i32_from_word32 (i, w)
        integer(i32), intent(out) :: i
        type(word32_t), intent(in) :: w
        i = w%i
    end subroutine i32_from_word32

```

Filling with a 8-bit integer is slightly tricky, because in this interpretation integers are unsigned.

```

<Bytes: procedures>+≡
    subroutine word32_set_from_byte (w, b)
        type(word32_t), intent(out) :: w
        type(byte_t), intent(in) :: b
        if (b%i >= 0_i8) then
            w%i = b%i
        else
            w%i = 2_i32*(huge(0_i8)+1_i32) + b%i
        end if
        w%fill = 32
    end subroutine word32_set_from_byte

```

Check the fill status

```

<Bytes: public>+≡
    public :: word32_empty, word32_filled, word32_fill
<Bytes: procedures>+≡
    function word32_empty (w)
        type(word32_t), intent(in) :: w
        logical :: word32_empty
        word32_empty = (w%fill == 0)
    end function word32_empty

    function word32_filled (w)
        type(word32_t), intent(in) :: w
        logical :: word32_filled
        word32_filled = (w%fill == 32)
    end function word32_filled

```

```

end function word32_filled

function word32_fill (w)
    type(word32_t), intent(in) :: w
    integer :: word32_fill
    word32_fill = w%fill
end function word32_fill

```

Partial assignment: append a byte to a partially filled word. (Note: no assignment if the word is filled, so check this before if necessary.)

```

<Bytes: public>+≡
    public :: word32_append_byte

<Bytes: procedures>+≡
    subroutine word32_append_byte (w, b)
        type(word32_t), intent(inout) :: w
        type(byte_t), intent(in) :: b
        type(word32_t) :: w1
        if (.not. word32_filled (w)) then
            w1 = b
            call mvbits (w1%i, 0, 8, w%i, w%fill)
            w%fill = w%fill + 8
        end if
    end subroutine word32_append_byte

```

Extract a byte from a word. The argument *i* is the position, which may be 0, 1, 2, or 3.

For the final assignment, we set the highest bit separately. Otherwise, we might trigger an overflow condition for a compiler with strict checking turned on.

```

<Bytes: public>+≡
    public :: byte_from_word32

<Bytes: procedures>+≡
    function byte_from_word32 (w, i) result (b)
        type(word32_t), intent(in) :: w
        integer, intent(in) :: i
        type(byte_t) :: b
        integer(i32) :: j
        j = 0
        if (i >= 0 .and. i*8 < w%fill) then
            call mvbits (w%i, i*8, 8, j, 0)
        end if
        b%i = int (ibclr (j, 7), kind=i8)
        if (btest (j, 7)) b%i = ibset (b%i, 7)
    end function byte_from_word32

```

Write a word to file or STDOUT. We understand words as unsigned integers, therefore we cannot use the built-in routine unchanged. However, we can make use of the existence of 64-bit integers and their output routine.

In hexadecimal format, the default version prints eight hex characters, highest-first. The `bytes` version prints four bytes (two-hex characters), lowest first, with

spaces in-between. The decimal bytes version is analogous. In the `bytes` version, missing bytes are printed as whitespace.

```

<Bytes: public>+≡
    public :: word32_write

<Bytes: interfaces>+≡
    interface word32_write
        module procedure word32_write_unit
    end interface

<Bytes: procedures>+≡
    subroutine word32_write_unit (w, unit, bytes, decimal, newline)
        type(word32_t), intent(in) :: w
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: bytes, decimal, newline
        logical :: dc, by, nl
        type(word64_t) :: ww
        integer :: i, u
        u = given_output_unit (unit); if (u < 0) return
        by = .false.; if (present (bytes)) by = bytes
        dc = .false.; if (present (decimal)) dc = decimal
        nl = .false.; if (present (newline)) nl = newline
        if (by) then
            do i = 0, 3
                if (i>0) write (u, '(1x)', advance='no')
                if (8*i < w%fill) then
                    call byte_write (byte_from_word32 (w, i), unit, decimal=decimal)
                else if (dc) then
                    write (u, '(3x)', advance='no')
                else
                    write (u, '(2x)', advance='no')
                end if
            end do
        else if (dc) then
            ww = w
            write (u, '(I10)', advance='no') ww%i
        else
            select case (w%fill)
            case ( 0)
            case ( 8); write (6, '(1x,z8.2)', advance='no') ibits (w%i, 0, 8)
            case (16); write (6, '(1x,z8.4)', advance='no') ibits (w%i, 0,16)
            case (24); write (6, '(1x,z8.6)', advance='no') ibits (w%i, 0,24)
            case (32); write (6, '(1x,z8.8)', advance='no') ibits (w%i, 0,32)
            end select
        end if
        if (nl) write (u, *)
    end subroutine word32_write_unit

```

6.1.3 Operations on 32-bit words

Define the usual logical operations, as well as addition (mod 2^{32}). We assume that all operands are completely filled.

```

<Bytes: public>+≡

```

```

    public :: not, ior, ieor, iand, ishft, ishftc
<Bytes: interfaces>+≡
    interface not
        module procedure word_not
    end interface
    interface ior
        module procedure word_or
    end interface
    interface ieor
        module procedure word_eor
    end interface
    interface iand
        module procedure word_and
    end interface
    interface ishft
        module procedure word_shft
    end interface
    interface ishftc
        module procedure word_shftc
    end interface
<Bytes: procedures>+≡
    function word_not (w1) result (w2)
        type(word32_t), intent(in) :: w1
        type(word32_t) :: w2
        w2 = not (w1%i)
    end function word_not

    function word_or (w1, w2) result (w3)
        type(word32_t), intent(in) :: w1, w2
        type(word32_t) :: w3
        w3 = ior (w1%i, w2%i)
    end function word_or

    function word_eor (w1, w2) result (w3)
        type(word32_t), intent(in) :: w1, w2
        type(word32_t) :: w3
        w3 = ieor (w1%i, w2%i)
    end function word_eor

    function word_and (w1, w2) result (w3)
        type(word32_t), intent(in) :: w1, w2
        type(word32_t) :: w3
        w3 = iand (w1%i, w2%i)
    end function word_and

    function word_shft (w1, s) result (w2)
        type(word32_t), intent(in) :: w1
        integer, intent(in) :: s
        type(word32_t) :: w2
        w2 = ishft (w1%i, s)
    end function word_shft

    function word_shftc (w1, s) result (w2)

```



```

    type(word32_t), intent(in) :: w1
    integer, intent(in) :: s
    type(word32_t) :: w2
    w2 = ishftc (w1%i, s, 32)
end function word_shftc

```

Addition is defined mod 2^{32} , i.e., without overflow checking. This means that we have to work around a possible overflow check enforced by the compiler.

```

<Bytes: public>+≡
    public :: operator(+)

<Bytes: interfaces>+≡
    interface operator(+)
        module procedure word_add
        module procedure word_add_i8
        module procedure word_add_i32
    end interface

<Bytes: procedures>+≡
    function word_add (w1, w2) result (w3)
        type(word32_t), intent(in) :: w1, w2
        type(word32_t) :: w3
        integer(i64) :: j
        j = int (ibclr (w1%i, 31), i64) + int (ibclr (w2%i, 31), i64)
        w3 = int (ibclr (j, 31), kind=i32)
        if (btest (j, 31)) then
            if (btest (w1%i, 31) .eqv. btest (w2%i, 31)) w3 = ibset (w3%i, 31)
        else
            if (btest (w1%i, 31) .neqv. btest (w2%i, 31)) w3 = ibset (w3%i, 31)
        end if
    end function word_add

    function word_add_i8 (w1, i) result (w3)
        type(word32_t), intent(in) :: w1
        integer(i8), intent(in) :: i
        type(word32_t) :: w3
        integer(i64) :: j
        j = int (ibclr (w1%i, 31), i64) + int (ibclr (i, 7), i64)
        if (btest (i, 7)) j = j + 128
        w3 = int (ibclr (j, 31), kind=i32)
        if (btest (j, 31) .neqv. btest (w1%i, 31)) w3 = ibset (w3%i, 31)
    end function word_add_i8

    function word_add_i32 (w1, i) result (w3)
        type(word32_t), intent(in) :: w1
        integer(i32), intent(in) :: i
        type(word32_t) :: w3
        integer(i64) :: j
        j = int (ibclr (w1%i, 31), i64) + int (ibclr (i, 31), i64)
        w3 = int (ibclr (j, 31), kind=i32)
        if (btest (j, 31)) then
            if (btest (w1%i, 31) .eqv. btest (i, 31)) w3 = ibset (w3%i, 31)
        else
            if (btest (w1%i, 31) .neqv. btest (i, 31)) w3 = ibset (w3%i, 31)
        end if
    end function word_add_i32

```

```

        end if
    end function word_add_i32

```

6.1.4 64-bit words

These objects consist of two 32-bit words. They thus can hold integer numbers larger than 2^{32} (to be exact, 2^{31} since FORTRAN integers are signed). The order is low-word, high-word.

```

<Bytes: public>+≡
    public :: word64_t

<Bytes: types>+≡
    type :: word64_t
        private
        integer(i64) :: i
    end type word64_t

```

Set a 64 bit word:

```

<Bytes: interfaces>+≡
    interface assignment(=)
        module procedure word64_set_from_i64
        module procedure word64_set_from_word32
    end interface

<Bytes: procedures>+≡
    subroutine word64_set_from_i64 (ww, i)
        type(word64_t), intent(out) :: ww
        integer(i64), intent(in) :: i
        ww%i = i
    end subroutine word64_set_from_i64

```

Filling with a 32-bit word:

```

<Bytes: procedures>+≡
    subroutine word64_set_from_word32 (ww, w)
        type(word64_t), intent(out) :: ww
        type(word32_t), intent(in) :: w
        if (w%i >= 0_i32) then
            ww%i = w%i
        else
            ww%i = 2_i64*(huge(0_i32)+1_i64) + w%i
        end if
    end subroutine word64_set_from_word32

```

Extract a byte from a word. The argument *i* is the position, which may be between 0 and 7.

For the final assignment, we set the highest bit separately. Otherwise, we might trigger an overflow condition for a compiler with strict checking turned on.

```

<Bytes: public>+≡
    public :: byte_from_word64, word32_from_word64

```

```

<Bytes: procedures>+≡
function byte_from_word64 (ww, i) result (b)
  type(word64_t), intent(in) :: ww
  integer, intent(in) :: i
  type(byte_t) :: b
  integer(i64) :: j
  j = 0
  if (i >= 0 .and. i*8 < 64) then
    call mvbits (ww%i, i*8, 8, j, 0)
  end if
  b%i = int (ibclr (j, 7), kind=i8)
  if (btest (j, 7)) b%i = ibset (b%i, 7)
end function byte_from_word64

```

Extract a 32-bit word from a 64-bit word. The position is either 0 or 1.

```

<Bytes: procedures>+≡
function word32_from_word64 (ww, i) result (w)
  type(word64_t), intent(in) :: ww
  integer, intent(in) :: i
  type(word32_t) :: w
  integer(i64) :: j
  j = 0
  select case (i)
    case (0); call mvbits (ww%i, 0, 32, j, 0)
    case (1); call mvbits (ww%i, 32, 32, j, 0)
  end select
  w = int (ibclr (j, 31), kind=i32)
  if (btest (j, 31)) w = ibset (w%i, 31)
end function word32_from_word64

```

Print a 64-bit word. Decimal version works up to 2^{63} . The `words` version uses the 'word32' printout, separated by two spaces. The low-word is printed first. The `bytes` version also uses the 'word32' printout. This implies that the lowest byte is first. The default version prints a hexadecimal number without spaces, highest byte first.

```

<Bytes: public>+≡
public :: word64_write

<Bytes: interfaces>+≡
interface word64_write
  module procedure word64_write_unit
end interface

<Bytes: procedures>+≡
subroutine word64_write_unit (ww, unit, words, bytes, decimal, newline)
  type(word64_t), intent(in) :: ww
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: words, bytes, decimal, newline
  logical :: wo, by, dc, nl
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  wo = .false.; if (present (words)) wo = words
  by = .false.; if (present (bytes)) by = bytes
  dc = .false.; if (present (decimal)) dc = decimal

```

```

nl = .false.; if (present (newline)) nl = newline
if (wo .or. by) then
  call word32_write_unit (word32_from_word64 (ww, 0), unit, by, dc)
  write (u, '(2x)', advance='no')
  call word32_write_unit (word32_from_word64 (ww, 1), unit, by, dc)
else if (dc) then
  write (u, '(I19)', advance='no') ww%i
else
  write (u, '(Z16)', advance='no') ww%i
end if
if (nl) write (u, *)
end subroutine word64_write_unit

```

6.2 Hashtables

Hash tables, like lists, are not part of Fortran and must be defined on a per-case basis. In this section we define a module that contains a hash function.

Furthermore, for reference there is a complete framework of hashtable type definitions and access functions. This code is to be replicated where hash tables are used, mutatis mutandis.

```

<hashes.f90>≡
  <File header>

  module hashes

    use kinds, only: i8, i32
    use bytes

    <Standard module head>

    <Hashes: public>

    contains

    <Hashes: procedures>

  end module hashes

```

6.2.1 The hash function

This is the one-at-a-time hash function by Bob Jenkins (from Wikipedia), re-implemented in Fortran. The function works on an array of bytes (8-bit integers), as could be produced by, e.g., the `transfer` function, and returns a single 32-bit integer. For determining the position in a hashtable, one can pick the lower bits of the result as appropriate to the hashtable size (which should be a power of 2). Note that we are working on signed integers, so the interpretation of values differs from the C version. This should not matter in practice, however.

```

<Hashes: public>≡
  public :: hash

```

```

<Hashes: procedures>≡
function hash (key) result (hashval)
  integer(i32) :: hashval
  integer(i8), dimension(:), intent(in) :: key
  type(word32_t) :: w
  integer :: i
  w = 0_i32
  do i = 1, size (key)
    w = w + key(i)
    w = w + ishft (w, 10)
    w = ieor (w, ishft (w, -6))
  end do
  w = w + ishft (w, 3)
  w = ieor (w, ishft (w, -11))
  w = w + ishft (w, 15)
  hashval = w
end function hash

```

6.2.2 The hash table

We define a generic hashtable type (that depends on the `hash_data_t` type) together with associated methods.

This is a template:

```

<Hashtables: types>≡
type :: hash_data_t
  integer :: i
end type hash_data_t

```

Associated methods:

```

<Hashtables: procedures>≡
subroutine hash_data_final (data)
  type(hash_data_t), intent(inout) :: data
end subroutine hash_data_final

subroutine hash_data_write (data, unit)
  type(hash_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, *) data%i
end subroutine hash_data_write

```

Each hash entry stores the unmasked hash value, the key, and points to actual data if present. Note that this could be an allocatable scalar in principle, but making it a pointer avoids deep copy when expanding the hashtable.

```

<Hashtables: types>+≡
type :: hash_entry_t
  integer(i32) :: hashval = 0
  integer(i8), dimension(:), allocatable :: key
  type(hash_data_t), pointer :: data => null ()
end type hash_entry_t

```

The hashtable object holds the actual table, the number of filled entries and the number of entries after which the size should be doubled. The mask is equal to the table size minus one and thus coincides with the upper bound of the table index, which starts at zero.

```

<Hashtables: types>+≡
type :: hashtable_t
  integer :: n_entries = 0
  real :: fill_ratio = 0
  integer :: n_entries_max = 0
  integer(i32) :: mask = 0
  type(hash_entry_t), dimension(:), allocatable :: entry
end type hashtable_t

```

Initializer: The size has to be a power of two, the fill ratio is a real (machine-default!) number between 0 and 1.

```

<Hashtables: procedures>+≡
subroutine hashtable_init (hashtable, size, fill_ratio)
  type(hashtable_t), intent(out) :: hashtable
  integer, intent(in) :: size
  real, intent(in) :: fill_ratio
  hashtable%fill_ratio = fill_ratio
  hashtable%n_entries_max = size * fill_ratio
  hashtable%mask = size - 1
  allocate (hashtable%entry (0:hashtable%mask))
end subroutine hashtable_init

```

Finalizer: This calls a `hash_data_final` subroutine which must exist.

```

<Hashtables: procedures>+≡
subroutine hashtable_final (hashtable)
  type(hashtable_t), intent(inout) :: hashtable
  integer :: i
  do i = 0, hashtable%mask
    if (associated (hashtable%entry(i)%data)) then
      call hash_data_final (hashtable%entry(i)%data)
      deallocate (hashtable%entry(i)%data)
    end if
  end do
  deallocate (hashtable%entry)
end subroutine hashtable_final

```

Output. Here, we refer to a `hash_data_write` subroutine.

```

<Hashtables: procedures>+≡
subroutine hashtable_write (hashtable, unit)
  type(hashtable_t), intent(in) :: hashtable
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  do i = 0, hashtable%mask
    if (associated (hashtable%entry(i)%data)) then
      write (u, *) i, "(hash =", hashtable%entry(i)%hashval, ")", &

```

```

        hashtable%entry(i)%key
        call hash_data_write (hashtable%entry(i)%data, unit)
    end if
end do
end subroutine hashtable_write

```

6.2.3 Hashtable insertion

Insert a single entry with the hash value as trial place. If the table is filled, first expand it.

```

(Hashtables: procedures) +=
subroutine hashtable_insert (hashtable, key, data)
    type(hashtable_t), intent(inout) :: hashtable
    integer(i8), dimension(:), intent(in) :: key
    type(hash_data_t), intent(in), target :: data
    integer(i32) :: h
    if (hashtable%n_entries >= hashtable%n_entries_max) &
        call hashtable_expand (hashtable)
    h = hash (key)
    call hashtable_insert_rec (hashtable, h, h, key, data)
end subroutine hashtable_insert

```

We need this auxiliary routine for doubling the size of the hashtable. We rely on the fact that default assignment copies the data pointer, not the data themselves. The temporary array must not be finalized; it is deallocated automatically together with its allocatable components.

```

(Hashtables: procedures) +=
subroutine hashtable_expand (hashtable)
    type(hashtable_t), intent(inout) :: hashtable
    type(hash_entry_t), dimension(:), allocatable :: table_tmp
    integer :: i, s
    allocate (table_tmp (0:hashtable%mask))
    table_tmp = hashtable%entry
    deallocate (hashtable%entry)
    s = 2 * size (table_tmp)
    hashtable%n_entries = 0
    hashtable%n_entries_max = s * hashtable%fill_ratio
    hashtable%mask = s - 1
    allocate (hashtable%entry (0:hashtable%mask))
    do i = 0, ubound (table_tmp, 1)
        if (associated (table_tmp(i)%data)) then
            call hashtable_insert_rec (hashtable, table_tmp(i)%hashval, &
                table_tmp(i)%hashval, table_tmp(i)%key, table_tmp(i)%data)
        end if
    end do
end subroutine hashtable_expand

```

Insert a single entry at a trial place `h`, reduced to the table size. Collision resolution is done simply by choosing the next element, recursively until the place is empty. For bookkeeping, we preserve the original hash value. For a good hash function, there should be no clustering.

Note that if the new key exactly matches an existing key, nothing is done.

```

<Hashtables: procedures>+=
recursive subroutine hashtable_insert_rec (hashtable, h, hashval, key, data)
  type(hashtable_t), intent(inout) :: hashtable
  integer(i32), intent(in) :: h, hashval
  integer(i8), dimension(:), intent(in) :: key
  type(hash_data_t), intent(in), target :: data
  integer(i32) :: i
  i = iand (h, hashtable%mask)
  if (associated (hashtable%entry(i)%data)) then
    if (size (hashtable%entry(i)%key) /= size (key)) then
      call hashtable_insert_rec (hashtable, h + 1, hashval, key, data)
    else if (any (hashtable%entry(i)%key /= key)) then
      call hashtable_insert_rec (hashtable, h + 1, hashval, key, data)
    end if
  else
    hashtable%entry(i)%hashval = hashval
    allocate (hashtable%entry(i)%key (size (key)))
    hashtable%entry(i)%key = key
    hashtable%entry(i)%data => data
    hashtable%n_entries = hashtable%n_entries + 1
  end if
end subroutine hashtable_insert_rec

```

6.2.4 Hashtable lookup

The lookup function has to parallel the insert function. If the place is filled, check if the key matches. Yes: return the pointer; no: increment the hash value and check again.

```

<Hashtables: procedures>+=
function hashtable_lookup (hashtable, key) result (ptr)
  type(hash_data_t), pointer :: ptr
  type(hashtable_t), intent(in) :: hashtable
  integer(i8), dimension(:), intent(in) :: key
  ptr => hashtable_lookup_rec (hashtable, hash (key), key)
end function hashtable_lookup

<Hashtables: procedures>+=
recursive function hashtable_lookup_rec (hashtable, h, key) result (ptr)
  type(hash_data_t), pointer :: ptr
  type(hashtable_t), intent(in) :: hashtable
  integer(i32), intent(in) :: h
  integer(i8), dimension(:), intent(in) :: key
  integer(i32) :: i
  i = iand (h, hashtable%mask)
  if (associated (hashtable%entry(i)%data)) then
    if (size (hashtable%entry(i)%key) == size (key)) then
      if (all (hashtable%entry(i)%key == key)) then
        ptr => hashtable%entry(i)%data
      else
        ptr => hashtable_lookup_rec (hashtable, h + 1, key)
      end if
    end if
  end if
end function hashtable_lookup_rec

```



```

        else
            ptr => hashtable_lookup_rec (hashtable, h + 1, key)
        end if
    else
        ptr => null ()
    end if
end function hashtable_lookup_rec

```

<Hashtables: public>≡

```

    public :: hashtable_test

```

<Hashtables: procedures>+≡

```

subroutine hashtable_test ()
    type(hash_data_t), pointer :: data
    type(hashtable_t) :: hashtable
    integer(i8) :: i
    call hashtable_init (hashtable, 16, 0.25)
    do i = 1, 10
        allocate (data)
        data%i = i*i
        call hashtable_insert (hashtable, [i, i+i], data)
    end do
    call hashtable_insert (hashtable, [2_i8, 4_i8], data)
    call hashtable_write (hashtable)
    data => hashtable_lookup (hashtable, [5_i8, 10_i8])
    if (associated (data)) then
        print *, "lookup:", data%i
    else
        print *, "lookup: --"
    end if
    data => hashtable_lookup (hashtable, [6_i8, 12_i8])
    if (associated (data)) then
        print *, "lookup:", data%i
    else
        print *, "lookup: --"
    end if
    data => hashtable_lookup (hashtable, [4_i8, 9_i8])
    if (associated (data)) then
        print *, "lookup:", data%i
    else
        print *, "lookup: --"
    end if
    call hashtable_final (hashtable)
end subroutine hashtable_test

```

6.3 MD5 Checksums

Implementing MD5 checksums allows us to check input/file integrity on the basis of a well-known standard. The building blocks have been introduced in the `bytes` module.

<md5.f90>≡

⟨File header⟩

```
module md5

    use kinds, only: i8, i32, i64
    use io_units
    use system_defs, only: BUFFER_SIZE
    use system_defs, only: LF, EOR, EOF
    use diagnostics
    use bytes
```

⟨Standard module head⟩

⟨MD5: public⟩

⟨MD5: types⟩

⟨MD5: variables⟩

⟨MD5: interfaces⟩

contains

⟨MD5: procedures⟩

```
end module md5
```

6.3.1 Blocks

A block is a sequence of 16 words (64 bytes or 512 bits). We anticipate that blocks will be linked, so include a pointer to the next block. There is a fill status (word counter), as there is one for each word. The fill status is equal to the number of bytes that are in, so it may be between 0 and 64.

```
⟨MD5: types⟩≡
    type :: block_t
    private
        type(word32_t), dimension(0:15) :: w
        type(block_t), pointer :: next => null ()
        integer :: fill = 0
    end type block_t
```

Check if a block is completely filled or empty:

```
⟨MD5: procedures⟩≡
    function block_is_empty (b)
        type(block_t), intent(in) :: b
        logical :: block_is_empty
        block_is_empty = (b%fill == 0 .and. word32_empty (b%w(0)))
    end function block_is_empty

    function block_is_filled (b)
        type(block_t), intent(in) :: b
        logical :: block_is_filled
        block_is_filled = (b%fill == 64)
```

```
end function block_is_filled
```

Append a single byte to a block. Works only if the block is not yet filled.

(MD5: procedures)+≡

```
subroutine block_append_byte (bl, by)
  type(block_t), intent(inout) :: bl
  type(byte_t), intent(in) :: by
  if (.not. block_is_filled (bl)) then
    call word32_append_byte (bl%w(bl%fill/4), by)
    bl%fill = bl%fill + 1
  end if
end subroutine block_append_byte
```

The printing routine allows for printing as sequences of words or bytes, decimal or hex.

(MD5: interfaces)≡

```
interface block_write
  module procedure block_write_unit
end interface
```

(MD5: procedures)+≡

```
subroutine block_write_unit (b, unit, bytes, decimal)
  type(block_t), intent(in) :: b
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: bytes, decimal
  logical :: by, dc
  integer :: i, u
  u = given_output_unit (unit); if (u < 0) return
  by = .false.; if (present (bytes)) by = bytes
  dc = .false.; if (present (decimal)) dc = decimal
  do i = 0, b%fill/4 - 1
    call newline_or_blank (u, i, by, dc)
    call word32_write (b%w(i), unit, bytes, decimal)
  end do
  if (.not. block_is_filled (b)) then
    i = b%fill/4
    if (.not. word32_empty (b%w(i))) then
      call newline_or_blank (u, i, by, dc)
      call word32_write (b%w(i), unit, bytes, decimal)
    end if
  end if
  write (u, *)
contains
  subroutine newline_or_blank (u, i, bytes, decimal)
    integer, intent(in) :: u, i
    logical, intent(in) :: bytes, decimal
    if (decimal) then
      select case (i)
        case (0)
        case (2,4,6,8,10,12,14); write (u, *)
        case default
          write (u, '(2x)', advance='no')
        end select
    end if
  end subroutine
end subroutine
```

```

        else if (bytes) then
            select case (i)
            case (0)
            case (4,8,12); write (u, *)
            case default
                write (u, '(2x)', advance='no')
            end select
        else
            if (i == 8) write (u, *)
        end if
    end subroutine newline_or_blank
end subroutine block_write_unit

```

6.3.2 Messages

A message (within this module) is a linked list of blocks.

(MD5: types)+≡

```

type :: message_t
private
type(block_t), pointer :: first => null ()
type(block_t), pointer :: last => null ()
integer :: n_blocks = 0
end type message_t

```

Clear the message list

(MD5: procedures)+≡

```

subroutine message_clear (m)
type(message_t), intent(inout) :: m
type(block_t), pointer :: b
nullify (m%last)
do
    b => m%first
    if (.not.(associated (b))) exit
    m%first => b%next
    deallocate (b)
end do
m%n_blocks = 0
end subroutine message_clear

```

Append an empty block to the message list

(MD5: procedures)+≡

```

subroutine message_append_new_block (m)
type(message_t), intent(inout) :: m
if (associated (m%last)) then
    allocate (m%last%next)
    m%last => m%last%next
    m%n_blocks = m%n_blocks + 1
else
    allocate (m%first)
    m%last => m%first
    m%n_blocks = 1
end if

```

```

        end if
    end subroutine message_append_new_block

```

Initialize: clear and allocate the first (empty) block.

(MD5: procedures)+≡

```

subroutine message_init (m)
    type(message_t), intent(inout) :: m
    call message_clear (m)
    call message_append_new_block (m)
end subroutine message_init

```

Append a single byte to a message. If necessary, allocate a new block. If the message is empty, initialize it.

(MD5: procedures)+≡

```

subroutine message_append_byte (m, b)
    type(message_t), intent(inout) :: m
    type(byte_t), intent(in) :: b
    if (.not. associated (m%last)) then
        call message_init (m)
    else if (block_is_filled (m%last)) then
        call message_append_new_block (m)
    end if
    call block_append_byte (m%last, b)
end subroutine message_append_byte

```

Append zero bytes until the current block is filled up to the required position. If we are already beyond that, append a new block and fill that one.

(MD5: procedures)+≡

```

subroutine message_pad_zero (m, i)
    type(message_t), intent(inout) :: m
    integer, intent(in) :: i
    type(block_t), pointer :: b
    integer :: j
    if (associated (m%last)) then
        b => m%last
        if (b%fill > i) then
            do j = b%fill + 1, 64 + i
                call message_append_byte (m, byte_zero)
            end do
        else
            do j = b%fill + 1, i
                call message_append_byte (m, byte_zero)
            end do
        end if
    end if
end subroutine message_pad_zero

```

This returns the number of bits within a message. We need a 64-bit word for the result since it may be more than 2^{31} . This is also required by the MD5 standard.

(MD5: procedures)+≡

```

function message_bits (m) result (length)
  type(message_t), intent(in) :: m
  type(word64_t) :: length
  type(block_t), pointer :: b
  integer(i64) :: n_blocks_filled, n_bytes_extra
  if (m%n_blocks > 0) then
    b => m%last
    if (block_is_filled (b)) then
      n_blocks_filled = m%n_blocks
      n_bytes_extra = 0
    else
      n_blocks_filled = m%n_blocks - 1
      n_bytes_extra = b%fill
    end if
    length = n_blocks_filled * 512 + n_bytes_extra * 8
  else
    length = 0_i64
  end if
end function message_bits

```

6.3.3 Message I/O

Append the contents of a string to a message. We first cast the character string into a 8-bit integer array and then append this byte by byte.

(MD5: procedures)+≡

```

subroutine message_append_string (m, s)
  type(message_t), intent(inout) :: m
  character(len=*), intent(in) :: s
  integer(i64) :: i, n_bytes
  integer(i8), dimension(:), allocatable :: buffer
  integer(i8), dimension(1) :: mold
  type(byte_t) :: b
  n_bytes = size (transfer (s, mold))
  allocate (buffer (n_bytes))
  buffer = transfer (s, mold)
  do i = 1, size (buffer)
    b = buffer(i)
    call message_append_byte (m, b)
  end do
  deallocate (buffer)
end subroutine message_append_string

```

Append the contents of a 32-bit integer to a message. We first cast the 32-bit integer into a 8-bit integer array and then append this byte by byte.

(MD5: procedures)+≡

```

subroutine message_append_i32 (m, x)
  type(message_t), intent(inout) :: m
  integer(i32), intent(in) :: x
  integer(i8), dimension(4) :: buffer
  type(byte_t) :: b
  integer :: i
  buffer = transfer (x, buffer, size(buffer))

```

```

do i = 1, size (buffer)
  b = buffer(i)
  call message_append_byte (m, b)
end do
end subroutine message_append_i32

```

Append one line from file to a message. Include the newline character.

<MD5: procedures>+≡

```

subroutine message_append_from_unit (m, u, iostat)
  type(message_t), intent(inout) :: m
  integer, intent(in) :: u
  integer, intent(out) :: iostat
  character(len=BUFFER_SIZE) :: buffer
  read (u, *, iostat=iostat) buffer
  call message_append_string (m, trim (buffer))
  call message_append_string (m, LF)
end subroutine message_append_from_unit

```

Fill a message from file. (Each line counts as a string.)

<MD5: procedures>+≡

```

subroutine message_read_from_file (m, f)
  type(message_t), intent(inout) :: m
  character(len=*), intent(in) :: f
  integer :: u, iostat
  u = free_unit ()
  open (file=f, unit=u, action='read')
  do
    call message_append_from_unit (m, u, iostat=iostat)
    if (iostat < 0) exit
  end do
  close (u)
end subroutine message_read_from_file

```

Write a message. After each block, insert an empty line.

<MD5: interfaces>+≡

```

interface message_write
  module procedure message_write_unit
end interface

```

<MD5: procedures>+≡

```

subroutine message_write_unit (m, unit, bytes, decimal)
  type(message_t), intent(in) :: m
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: bytes, decimal
  type(block_t), pointer :: b
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  b => m%first
  if (associated (b)) then
    do
      call block_write_unit (b, unit, bytes, decimal)
      b => b%next
    if (.not. associated (b)) exit
  end if
end subroutine message_write_unit

```

```

        write (u, *)
    end do
end if
end subroutine message_write_unit

```

6.3.4 Auxiliary functions

These four functions on three words are defined in the MD5 standard:

```

⟨MD5: procedures⟩+≡
function ff (x, y, z)
    type(word32_t), intent(in) :: x, y, z
    type(word32_t) :: ff
    ff = ior (iand (x, y), iand (not (x), z))
end function ff

function fg (x, y, z)
    type(word32_t), intent(in) :: x, y, z
    type(word32_t) :: fg
    fg = ior (iand (x, z), iand (y, not (z)))
end function fg

function fh (x, y, z)
    type(word32_t), intent(in) :: x, y, z
    type(word32_t) :: fh
    fh = ieor (ieor (x, y), z)
end function fh

function fi (x, y, z)
    type(word32_t), intent(in) :: x, y, z
    type(word32_t) :: fi
    fi = ieor (y, ior (x, not (z)))
end function fi

```

6.3.5 Auxiliary stuff

This defines and initializes the table of transformation constants:

```

⟨MD5: variables⟩≡
type(word32_t), dimension(64), save :: t
logical, save :: table_initialized = .false.

⟨MD5: procedures⟩+≡
subroutine table_init
    type(word64_t) :: ww
    integer :: i
    if (.not.table_initialized) then
        do i = 1, 64
            ww = int (4294967296d0 * abs (sin (i * 1d0)), kind=i64)
            t(i) = word32_from_word64 (ww, 0)
        end do
        table_initialized = .true.
    end if
end subroutine table_init

```



```
end subroutine table_init
```

This encodes the message digest (4 words) into a 32-character string.

(MD5: procedures)+≡

```
function digest_string (aa) result (s)
  type(word32_t), dimension (0:3), intent(in) :: aa
  character(len=32) :: s
  integer :: i, j
  do i = 0, 3
    do j = 0, 3
      call byte_write (byte_from_word32 (aa(i), j), s(i*8+j*2+1:i*8+j*2+2))
    end do
  end do
end function digest_string
```

6.3.6 MD5 algorithm

Pad the message with a byte x80 and then pad zeros up to a full block minus two words; in these words, insert the message length (before padding) as a 64-bit word, low-word first.

(MD5: procedures)+≡

```
subroutine message_pad (m)
  type(message_t), intent(inout) :: m
  type(word64_t) :: length
  integer(i8), parameter :: ipad = -128 ! z'80'
  type(byte_t) :: b
  integer :: i
  length = message_bits (m)
  b = ipad
  call message_append_byte (m, b)
  call message_pad_zero (m, 56)
  do i = 0, 7
    call message_append_byte (m, byte_from_word64 (length, i))
  end do
end subroutine message_pad
```

Apply a series of transformations onto a state a,b,c,d, where the transform function uses each word of the message together with the predefined words. Finally, encode the state as a 32-character string.

(MD5: procedures)+≡

```
subroutine message_digest (m, s)
  type(message_t), intent(in) :: m
  character(len=32), intent(out) :: s
  integer(i32), parameter :: ia = 1732584193 ! z'67452301'
  integer(i32), parameter :: ib = -271733879 ! z'efcdab89'
  integer(i32), parameter :: ic = -1732584194 ! z'98badcfe'
  integer(i32), parameter :: id = 271733878 ! z'10325476'
  type(word32_t) :: a, b, c, d
  type(word32_t) :: aa, bb, cc, dd
  type(word32_t), dimension(0:15) :: x
  type(block_t), pointer :: bl
```

```

call table_init
a = ia; b = ib; c = ic; d = id
bl => m%first
do
  if (.not.associated (bl)) exit
  x = bl%w
  aa = a; bb = b; cc = c; dd = d
  call transform (ff, a, b, c, d, 0, 7, 1)
  call transform (ff, d, a, b, c, 1, 12, 2)
  call transform (ff, c, d, a, b, 2, 17, 3)
  call transform (ff, b, c, d, a, 3, 22, 4)
  call transform (ff, a, b, c, d, 4, 7, 5)
  call transform (ff, d, a, b, c, 5, 12, 6)
  call transform (ff, c, d, a, b, 6, 17, 7)
  call transform (ff, b, c, d, a, 7, 22, 8)
  call transform (ff, a, b, c, d, 8, 7, 9)
  call transform (ff, d, a, b, c, 9, 12, 10)
  call transform (ff, c, d, a, b, 10, 17, 11)
  call transform (ff, b, c, d, a, 11, 22, 12)
  call transform (ff, a, b, c, d, 12, 7, 13)
  call transform (ff, d, a, b, c, 13, 12, 14)
  call transform (ff, c, d, a, b, 14, 17, 15)
  call transform (ff, b, c, d, a, 15, 22, 16)
  call transform (fg, a, b, c, d, 1, 5, 17)
  call transform (fg, d, a, b, c, 6, 9, 18)
  call transform (fg, c, d, a, b, 11, 14, 19)
  call transform (fg, b, c, d, a, 0, 20, 20)
  call transform (fg, a, b, c, d, 5, 5, 21)
  call transform (fg, d, a, b, c, 10, 9, 22)
  call transform (fg, c, d, a, b, 15, 14, 23)
  call transform (fg, b, c, d, a, 4, 20, 24)
  call transform (fg, a, b, c, d, 9, 5, 25)
  call transform (fg, d, a, b, c, 14, 9, 26)
  call transform (fg, c, d, a, b, 3, 14, 27)
  call transform (fg, b, c, d, a, 8, 20, 28)
  call transform (fg, a, b, c, d, 13, 5, 29)
  call transform (fg, d, a, b, c, 2, 9, 30)
  call transform (fg, c, d, a, b, 7, 14, 31)
  call transform (fg, b, c, d, a, 12, 20, 32)
  call transform (fh, a, b, c, d, 5, 4, 33)
  call transform (fh, d, a, b, c, 8, 11, 34)
  call transform (fh, c, d, a, b, 11, 16, 35)
  call transform (fh, b, c, d, a, 14, 23, 36)
  call transform (fh, a, b, c, d, 1, 4, 37)
  call transform (fh, d, a, b, c, 4, 11, 38)
  call transform (fh, c, d, a, b, 7, 16, 39)
  call transform (fh, b, c, d, a, 10, 23, 40)
  call transform (fh, a, b, c, d, 13, 4, 41)
  call transform (fh, d, a, b, c, 0, 11, 42)
  call transform (fh, c, d, a, b, 3, 16, 43)
  call transform (fh, b, c, d, a, 6, 23, 44)
  call transform (fh, a, b, c, d, 9, 4, 45)
  call transform (fh, d, a, b, c, 12, 11, 46)
  call transform (fh, c, d, a, b, 15, 16, 47)

```

```

        call transform (fh, b, c, d, a, 2, 23, 48)
        call transform (fi, a, b, c, d, 0, 6, 49)
        call transform (fi, d, a, b, c, 7, 10, 50)
        call transform (fi, c, d, a, b, 14, 15, 51)
        call transform (fi, b, c, d, a, 5, 21, 52)
        call transform (fi, a, b, c, d, 12, 6, 53)
        call transform (fi, d, a, b, c, 3, 10, 54)
        call transform (fi, c, d, a, b, 10, 15, 55)
        call transform (fi, b, c, d, a, 1, 21, 56)
        call transform (fi, a, b, c, d, 8, 6, 57)
        call transform (fi, d, a, b, c, 15, 10, 58)
        call transform (fi, c, d, a, b, 6, 15, 59)
        call transform (fi, b, c, d, a, 13, 21, 60)
        call transform (fi, a, b, c, d, 4, 6, 61)
        call transform (fi, d, a, b, c, 11, 10, 62)
        call transform (fi, c, d, a, b, 2, 15, 63)
        call transform (fi, b, c, d, a, 9, 21, 64)
        a = a + aa
        b = b + bb
        c = c + cc
        d = d + dd
        bl => bl%next
    end do
    s = digest_string ([a, b, c, d])
contains
    <MD5: Internal subroutine transform>
end subroutine message_digest

```

And this is the actual transformation that depends on one of the previous functions, four words, and three integers. The implicit arguments are *x*, the word from the message to digest, and *t*, the entry in the predefined table.

```

<MD5: Internal subroutine transform>≡
    subroutine transform (f, a, b, c, d, k, s, i)
        interface
            function f (x, y, z)
                import word32_t
                type(word32_t), intent(in) :: x, y, z
                type(word32_t) :: f
            end function f
        end interface
        type(word32_t), intent(inout) :: a
        type(word32_t), intent(in) :: b, c, d
        integer, intent(in) :: k, s, i
        a = b + ishftc (a + f(b, c, d) + x(k) + t(i), s)
    end subroutine transform

```

6.3.7 User interface

```

<MD5: public>≡
    public :: md5sum
<MD5: interfaces>+≡
    interface md5sum

```

```

        module procedure md5sum_from_string
        module procedure md5sum_from_unit
    end interface

```

This function computes the MD5 sum of the input string and returns it as a 32-character string

(MD5: procedures)+≡

```

function md5sum_from_string (s) result (digest)
    character(len=*), intent(in) :: s
    character(len=32) :: digest
    type(message_t) :: m
    call message_append_string (m, s)
    call message_pad (m)
    call message_digest (m, digest)
    call message_clear (m)
end function md5sum_from_string

```

This funct. reads from unit u (an unformatted sequence of integers) and computes the MD5 sum.

(MD5: procedures)+≡

```

function md5sum_from_unit (u) result (digest)
    integer, intent(in) :: u
    character(len=32) :: digest
    type(message_t) :: m
    character :: char
    integer :: iostat
    READ_CHARS: do
        read (u, "(A)", advance="no", iostat=iostat) char
        select case (iostat)
            case (0)
                call message_append_string (m, char)
            case (EOR)
                call message_append_string (m, LF)
            case (EOF)
                exit READ_CHARS
            case default
                call msg_fatal &
                    ("Computing MD5 sum: I/O error while reading from scratch file")
        end select
    end do READ_CHARS
    call message_pad (m)
    call message_digest (m, digest)
    call message_clear (m)
end function md5sum_from_unit

```

6.3.8 Unit tests

Test module, followed by the corresponding implementation module.

(md5_ut.f90)≡

(File header)

```

module md5_ut

```

```

        use unit_tests
        use md5_util

    <Standard module head>

    <MD5: public test>

contains

    <MD5: test driver>

end module md5_util
<md5_util.f90>≡
    <File header>

```

```

module md5_util

    use diagnostics

    use md5

    <Standard module head>

    <MD5: test declarations>

contains

    <MD5: tests>

end module md5_util

```

API: driver for the unit tests below.

```

<MD5: public test>≡
    public :: md5_test

<MD5: test driver>≡
    subroutine md5_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <MD5: execute tests>
    end subroutine md5_test

```

This function checks the implementation by computing the checksum of certain strings and comparing them with the known values.

```

<MD5: execute tests>≡
    call test (md5_1, "md5_1", &
        "check MD5 sums", &
        u, results)

<MD5: test declarations>≡
    public :: md5_1

<MD5: tests>≡
    subroutine md5_1 (u)
        integer, intent(in) :: u

```

[illegible]

6.4 Permutations

Permute arrays of integers (of specific kind).

$$\langle \text{permutations.f90} \rangle \equiv \langle \text{File header} \rangle$$

```
module permutations
```

```
use kinds, only: TC
```

 $\langle Standard\ module\ head \rangle$

```

    <Permutations: public>

    <Permutations: types>

    <Permutations: interfaces>

contains

    <Permutations: procedures>

end module permutations

```

6.4.1 Permutations

A permutation is an array of integers. Each integer between one and `size` should occur exactly once.

```

<Permutations: public>≡
    public :: permutation_t

<Permutations: types>≡
    type :: permutation_t
    private
        integer, dimension(:), allocatable :: p
    end type permutation_t

```

Initialize with the identity permutation.

```

<Permutations: public>+=
    public :: permutation_init
    public :: permutation_final

<Permutations: procedures>≡
    elemental subroutine permutation_init (p, size)
        type(permutation_t), intent(inout) :: p
        integer, intent(in) :: size
        integer :: i
        allocate (p%p (size))
        forall (i = 1:size)
            p%p(i) = i
        end forall
    end subroutine permutation_init

    elemental subroutine permutation_final (p)
        type(permutation_t), intent(inout) :: p
        deallocate (p%p)
    end subroutine permutation_final

```

I/O:

```

<Permutations: public>+=
    public :: permutation_write

<Permutations: procedures>+=
    subroutine permutation_write (p, u)
        type(permutation_t), intent (in) :: p

```

```

integer, intent(in) :: u
integer :: i
do i = 1, size (p%p)
  if (size (p%p) < 10) then
    write (u,"(1x,I1)", advance="no") p%p(i)
  else
    write (u,"(1x,I3)", advance="no") p%p(i)
  end if
end do
write (u, *)
end subroutine permutation_write

```

Administration:

```

⟨Permutations: public⟩+≡
  public :: permutation_size

⟨Permutations: procedures⟩+≡
  elemental function permutation_size (perm) result (s)
    type(permutation_t), intent(in) :: perm
    integer :: s
    s = size (perm%p)
  end function permutation_size

```

Extract an entry in a permutation.

```

⟨Permutations: public⟩+≡
  public :: permute

⟨Permutations: procedures⟩+≡
  elemental function permute (i, p) result (j)
    integer, intent(in) :: i
    type(permutation_t), intent(in) :: p
    integer :: j
    if (i > 0 .and. i <= size (p%p)) then
      j = p%p(i)
    else
      j = 0
    end if
  end function permute

```

Check whether a permutation is valid: Each integer in the range occurs exactly once.

```

⟨Permutations: public⟩+≡
  public :: permutation_ok

⟨Permutations: procedures⟩+≡
  elemental function permutation_ok (perm) result (ok)
    type(permutation_t), intent(in) :: perm
    logical :: ok
    integer :: i
    logical, dimension(:), allocatable :: set
    ok = .true.
    allocate (set (size (perm%p)))
    set = .false.

```



```

do i = 1, size (perm%p)
  ok = (perm%p(i) > 0 .and. perm%p(i) <= size (perm%p))
  if (.not.ok) return
  set(perm%p(i)) = .true.
end do
ok = all (set)
end function permutation_ok

```

Find the permutation that transforms the second array into the first one. We assume that this is possible and unique and all bounds are set correctly.

This cannot be elemental.

```

<Permutations: public>+≡
  public :: permutation_find

<Permutations: procedures>+≡
  subroutine permutation_find (perm, a1, a2)
    type(permutation_t), intent(inout) :: perm
    integer, dimension(:), intent(in) :: a1, a2
    integer :: i, j
    if (allocated (perm%p)) deallocate (perm%p)
    allocate (perm%p (size (a1)))
    do i = 1, size (a1)
      do j = 1, size (a2)
        if (a1(i) == a2(j)) then
          perm%p(i) = j
          exit
        end if
      perm%p(i) = 0
      end do
    end do
  end subroutine permutation_find

```

Find all permutations that transform an array of integers into itself. The resulting permutation list is allocated with the correct length and filled.

The first step is to count the number of different entries in `code`. Next, we scan `code` again and assign a mask to each different entry, true for all identical entries. Finally, we recursively permute the identity for each possible mask.

The permutation is done as follows: A list of all permutations of the initial one with respect to the current mask is generated, then the permutations are generated in turn for each permutation in this list with the next mask. The result is always stored back into the main list, starting from the end of the current list.

```

<Permutations: public>+≡
  public :: permutation_array_make

<Permutations: procedures>+≡
  subroutine permutation_array_make (pa, code)
    type(permutation_t), dimension(:), allocatable, intent(out) :: pa
    integer, dimension(:), intent(in) :: code
    logical, dimension(size(code)) :: mask
    logical, dimension(:,:), allocatable :: imask
    integer, dimension(:), allocatable :: n_i
    type(permutation_t) :: p_init

```

```

type(permutation_t), dimension(:), allocatable :: p_tmp
integer :: psize, i, j, k, n_different, n, nn_k
psize = size (code)
mask = .true.
n_different = 0
do i=1, psize
  if (mask(i)) then
    n_different = n_different + 1
    mask = mask .and. (code /= code(i))
  end if
end do
allocate (imask(psize, n_different), n_i(n_different))
mask = .true.
k = 0
do i=1, psize
  if (mask(i)) then
    k = k + 1
    imask(:,k) = (code == code(i))
    n_i(k) = factorial (count(imask(:,k)))
    mask = mask .and. (code /= code(i))
  end if
end do
n = product (n_i)
allocate (pa (n))
call permutation_init (p_init, psize)
pa(1) = p_init
nn_k = 1
do k = 1, n_different
  allocate (p_tmp (n_i(k)))
  do i = nn_k, 1, -1
    call permutation_array_with_mask (p_tmp, imask(:,k), pa(i))
    do j = n_i(k), 1, -1
      pa((i-1)*n_i(k) + j) = p_tmp(j)
    end do
  end do
  deallocate (p_tmp)
  nn_k = nn_k * n_i(k)
end do
call permutation_final (p_init)
deallocate (imask, n_i)
end subroutine permutation_array_make

```

Make a list of permutations of the elements marked true in the `mask` array. The final permutation list must be allocated with the correct length ($n!$). The third argument is the initial permutation to start with, which must have the same length as the `mask` array (this is not checked).

(Permutations: procedures)+≡

```

subroutine permutation_array_with_mask (pa, mask, p_init)
  type(permutation_t), dimension(:), intent(inout) :: pa
  logical, dimension(:), intent(in) :: mask
  type(permutation_t), intent(in) :: p_init
  integer :: plen
  integer :: i, ii, j, fac_i, k, x

```

```

integer, dimension(:), allocatable :: index
plen = size (pa)
allocate (index(count(mask)))
ii = 0
do i = 1, size (mask)
  if (mask(i)) then
    ii = ii + 1
    index(ii) = i
  end if
end do
pa = p_init
ii = 0
fac_i = 1
do i = 1, size (mask)
  if (mask(i)) then
    ii = ii + 1
    fac_i = fac_i * ii
    x = permute (i, p_init)
    do j = 1, plen
      k = ii - mod (((j-1)*fac_i)/plen, ii)
      call insert (pa(j), x, k, ii, index)
    end do
  end if
end do
deallocate (index)
contains
subroutine insert (p, x, k, n, index)
  type(permutation_t), intent(inout) :: p
  integer, intent(in) :: x, k, n
  integer, dimension(:), intent(in) :: index
  integer :: i
  do i = n, k+1, -1
    p%p(index(i)) = p%p(index(i-1))
  end do
  p%p(index(k)) = x
end subroutine insert
end subroutine permutation_array_with_mask

```

The factorial function is needed for pre-determining the number of permutations that will be generated:

```

<Permutations: public>+=
  public :: factorial

<Permutations: procedures>+=
  function factorial (n) result (f)
    integer, intent(in) :: n
    integer :: f
    integer :: i
    f = 1
    do i=2, abs(n)
      f = f*i
    end do
  end function factorial

```

6.4.2 Operations on binary codes

Binary codes are needed for phase-space trees. Since the permutation function uses permutations, and no other special type is involved, we put the functions here.

This is needed for phase space trees: permute bits in a tree binary code. If no permutation is given, leave as is. (We may want to access the permutation directly here if this is efficiency-critical.)

```

⟨Permutations: public⟩+=
    public :: tc_permute

⟨Permutations: procedures⟩+=
    function tc_permute (k, perm, mask_in) result (pk)
        integer(TC), intent(in) :: k, mask_in
        type(permutation_t), intent(in) :: perm
        integer(TC) :: pk
        integer :: i
        pk = iand (k, mask_in)
        do i = 1, size (perm%p)
            if (btest(k,i-1)) pk = ibset (pk, perm%p(i)-1)
        end do
    end function tc_permute

```

This routine returns the number of set bits in the tree code value **k**. Hence, it is the number of externals connected to the current line. If **mask** is present, the complement of the tree code is also considered, and the smaller number is returned. This gives the true distance from the external states, taking into account the initial particles. The complement number is increased by one, since for a scattering diagram the vertex with the sum of all final-state codes is still one point apart from the initial particles.

```

⟨Permutations: public⟩+=
    public :: tc_decay_level

⟨Permutations: interfaces⟩=
    interface tc_decay_level
        module procedure decay_level_simple
        module procedure decay_level_complement
    end interface

⟨Permutations: procedures⟩+=
    function decay_level_complement (k, mask) result (l)
        integer(TC), intent(in) :: k, mask
        integer :: l
        l = min (decay_level_simple (k), &
            & decay_level_simple (ieor (k, mask)) + 1)
    end function decay_level_complement

    function decay_level_simple (k) result(l)
        integer(TC), intent(in) :: k
        integer :: l
        integer :: i
        l = 0
        do i=0, bit_size(k)-1
            if (btest(k,i)) l = l+1
        end do
    end function decay_level_simple

```

```

        end do
    end function decay_level_simple

```

6.5 Sorting

This small module provides functions for sorting integer or real arrays.

```

<sorting.f90>≡
  <File header>

  module sorting

    <Use kinds>
    use diagnostics

    <Standard module head>

    <Sorting: public>

    <Sorting: interfaces>

    contains

    <Sorting: procedures>

  end module sorting

```

6.5.1 Implementation

The `sort` function returns, for a given integer or real array, the array sorted by increasing value. The current implementation is *mergesort*, which has $O(n \ln n)$ behavior in all cases, and is stable for elements of equal value.

The `sort_abs` variant sorts by increasing absolute value, where for identical absolute value, the positive number comes first.

```

<Sorting: public>≡
  public :: sort
  public :: sort_abs

<Sorting: interfaces>≡
  interface sort
    module procedure sort_int
    module procedure sort_real
  end interface

  interface sort_abs
    module procedure sort_int_abs
  end interface

```

This variant of integer sort returns The body is identical, just the interface differs.

```

<Sorting: procedures>≡

```

```

function sort_int (val_in) result (val)
  integer, dimension(:), intent(in) :: val_in
  integer, dimension(size(val_in)) :: val
  <Sorting: sort>
end function sort_int

function sort_real (val_in) result (val)
  real(default), dimension(:), intent(in) :: val_in
  real(default), dimension(size(val_in)) :: val
  <Sorting: sort>
end function sort_real

function sort_int_abs (val_in) result (val)
  integer, dimension(:), intent(in) :: val_in
  integer, dimension(size(val_in)) :: val
  <Sorting: sort abs>
end function sort_int_abs

```

```

<Sorting: sort>≡
  val = val_in( order (val_in) )

<Sorting: sort abs>≡
  val = val_in( order_abs (val_in) )

```

The `order` function returns, for a given integer or real array, the array of indices of the elements sorted by increasing value.

```

<Sorting: public>+≡
  public :: order
  public :: order_abs

<Sorting: interfaces>+≡
  interface order
    module procedure order_int
    module procedure order_real
  end interface

  interface order_abs
    module procedure order_int_abs
  end interface

```

```

<Sorting: procedures>+≡
  function order_int (val) result (idx)
    integer, dimension(:), intent(in) :: val
    integer, dimension(size(val)) :: idx
    <Sorting: order>
  end function order_int

  function order_real (val) result (idx)
    real(default), dimension(:), intent(in) :: val
    integer, dimension(size(val)) :: idx
    <Sorting: order>
  end function order_real

  function order_int_abs (val) result (idx)
    integer, dimension(:), intent(in) :: val

```

```

integer, dimension(size(val)) :: idx
<Sorting: order abs>
end function order_int_abs

```

We start by individual elements, merge them to pairs, merge those to four-element subarrays, and so on. The last subarray can extend only up to the original array bound, of course, and the second of the subarrays to merge should contain at least one element.

```

<Sorting: order>≡
  <Sorting: order1>
    call merge (idx(b1:e2), idx(b1:e1), idx(b2:e2), val)
  <Sorting: order2>

<Sorting: order abs>≡
  <Sorting: order1>
    call merge_abs (idx(b1:e2), idx(b1:e1), idx(b2:e2), val)
  <Sorting: order2>

<Sorting: order1>≡
  integer :: n, i, s, b1, b2, e1, e2
  n = size (idx)
  do i = 1, n
    idx(i) = i
  end do
  s = 1
  do while (s < n)
    do b1 = 1, n-s, 2*s
      b2 = b1 + s
      e1 = b2 - 1
      e2 = min (e1 + s, n)
    end do
    s = 2 * s
  end do
end do

```

The merging step does the actual sorting. We take two sorted array sections and merge them to a sorted result array. We are working on the indices, and comparing is done by taking the associated `val` which is real or integer.

```

<Sorting: interfaces>+≡
  interface merge
    module procedure merge_int
    module procedure merge_real
  end interface

  interface merge_abs
    module procedure merge_int_abs
  end interface

<Sorting: procedures>+≡
  subroutine merge_int (res, src1, src2, val)
    integer, dimension(:), intent(out) :: res
    integer, dimension(:), intent(in) :: src1, src2
    integer, dimension(:), intent(in) :: val
  end subroutine

```

```

    integer, dimension(size(res)) :: tmp
    <Sorting: merge>
end subroutine merge_int

subroutine merge_real (res, src1, src2, val)
    integer, dimension(:), intent(out) :: res
    integer, dimension(:), intent(in) :: src1, src2
    real(default), dimension(:), intent(in) :: val
    integer, dimension(size(res)) :: tmp
    <Sorting: merge>
end subroutine merge_real

subroutine merge_int_abs (res, src1, src2, val)
    integer, dimension(:), intent(out) :: res
    integer, dimension(:), intent(in) :: src1, src2
    integer, dimension(:), intent(in) :: val
    integer, dimension(size(res)) :: tmp
    <Sorting: merge abs>
end subroutine merge_int_abs

<Sorting: merge>≡
    <Sorting: merge1>
        if (val(src1(i1)) <= val(src2(i2))) then
    <Sorting: merge2>

We keep the elements if the absolute values are strictly ordered. If they are
equal in magnitude, we keep them if the larger value comes first, or if they are
equal.

<Sorting: merge abs>≡
    <Sorting: merge1>
        if (abs (val(src1(i1))) < abs (val(src2(i2))) .or. &
            (abs (val(src1(i1))) == abs (val(src2(i2))) .and. &
            val(src1(i1)) >= val(src2(i2)))) then
    <Sorting: merge2>

<Sorting: merge1>≡
    integer :: i1, i2, i
    i1 = 1
    i2 = 1
    do i = 1, size (tmp)
    <Sorting: merge2>≡
        tmp(i) = src1(i1); i1 = i1 + 1
        if (i1 > size (src1)) then
            tmp(i+1:) = src2(i2:)
            exit
        end if
    else
        tmp(i) = src2(i2); i2 = i2 + 1
        if (i2 > size (src2)) then
            tmp(i+1:) = src1(i1:)
            exit
        end if
    end if
end do

```



```
res = tmp
```

6.5.2 Unit tests

Test module, followed by the corresponding implementation module.

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

```
module sorting_ut  
  use unit_tests  
  use sorting_uti
```

```
  <Standard module head>
```

```
  <Sorting: public test>
```

```
contains
```

```
  <Sorting: test driver>
```

```
end module sorting_ut
```

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

```
module sorting_uti
```

```
  <Use kinds>
```

```
  use sorting
```

```
  <Standard module head>
```

```
  <Sorting: test declarations>
```

```
contains
```

```
  <Sorting: tests>
```

```
end module sorting_uti
```

API: driver for the unit tests below.

```
<Sorting: public test>≡  
  public :: sorting_test
```

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

This checks whether the sorting routine works correctly.

<Sorting: execute tests>≡

```
call test (sorting_1, "sorting_1", &
           "check sorting routines", &
           u, results)
```

<Sorting: test declarations>≡

```
public :: sorting_1
```

<Sorting: tests>≡

```
subroutine sorting_1 (u)
  integer, intent(in) :: u
  integer, parameter :: NMAX = 10
  real(default), dimension(NMAX) :: rval
  integer, dimension(NMAX) :: ival
  real, dimension(NMAX,NMAX) :: harvest_r
  integer, dimension(NMAX,NMAX) :: harvest_i
  integer, dimension(NMAX,NMAX) :: harvest_a
  integer :: i, j
  harvest_r(:, 1) = [0.9976, 0., 0., 0., 0., 0., 0., 0., 0., 0.]
  harvest_r(:, 2) = [0.5668, 0.9659, 0., 0., 0., 0., 0., 0., 0., 0.]
  harvest_r(:, 3) = [0.7479, 0.3674, 0.4806, 0., 0., 0., 0., 0., 0., &
                    0.]
  harvest_r(:, 4) = [0.0738, 0.0054, 0.3471, 0.3422, 0., 0., 0., 0., &
                    0., 0.]
  harvest_r(:, 5) = [0.2180, 0.1332, 0.9005, 0.3868, 0.4455, 0., 0., &
                    0., 0., 0.]
  harvest_r(:, 6) = [0.6619, 0.0161, 0.6509, 0.6464, 0.3230, &
                    0.8557, 0., 0., 0., 0.]
  harvest_r(:, 7) = [0.4013, 0.2069, 0.9685, 0.5984, 0.6730, &
                    0.4569, 0.3300, 0., 0., 0.]
  harvest_r(:, 8) = [0.1004, 0.7555, 0.6057, 0.7190, 0.8973, &
                    0.6582, 0.1507, 0.6123, 0., 0.]
  harvest_r(:, 9) = [0.9787, 0.9991, 0.2568, 0.5509, 0.6590, &
                    0.5540, 0.9778, 0.9019, 0.6579, 0.]
  harvest_r(:,10) = [0.7289, 0.4025, 0.9286, 0.1478, 0.6745, &
                    0.7696, 0.3393, 0.1158, 0.6144, 0.8206]

  harvest_i(:, 1) = [18, 0, 0, 0, 0, 0, 0, 0, 0, 0]
  harvest_i(:, 2) = [14, 9, 0, 0, 0, 0, 0, 0, 0, 0]
  harvest_i(:, 3) = [ 7, 8,11, 0, 0, 0, 0, 0, 0, 0]
  harvest_i(:, 4) = [19,19,14,19, 0, 0, 0, 0, 0, 0]
  harvest_i(:, 5) = [ 1,14,15,18,14, 0, 0, 0, 0, 0]
  harvest_i(:, 6) = [16,11, 1, 9,11, 2, 0, 0, 0, 0]
  harvest_i(:, 7) = [11,10,17, 6,13,13,10, 0, 0, 0]
  harvest_i(:, 8) = [ 5, 1, 2,10, 7, 0,15,12, 0, 0]
  harvest_i(:, 9) = [15,19, 2, 6,11, 0, 2, 4, 2, 0]
  harvest_i(:,10) = [ 1, 4, 8, 4,11, 0, 8, 7,19,13]

  harvest_a(:, 1) = [-6,  0,  0,  0,  0,  0,  0,  0,  0,  0]
  harvest_a(:, 2) = [-8, -9,  0,  0,  0,  0,  0,  0,  0,  0]
  harvest_a(:, 3) = [ 4, -3,  3,  0,  0,  0,  0,  0,  0,  0]
  harvest_a(:, 4) = [-6,  6,  2, -2,  0,  0,  0,  0,  0,  0]
  harvest_a(:, 5) = [ 1, -2,  0, -6,  8,  0,  0,  0,  0,  0]
  harvest_a(:, 6) = [-2, -1, -8, -5,  8, -5,  0,  0,  0,  0]
```

```

harvest_a(:, 7) = [-9, 0, -6, 2, 5, 3, 2, 0, 0, 0]
harvest_a(:, 8) = [-5, -7, 6, 7, -3, 0, -7, 4, 0, 0]
harvest_a(:, 9) = [ 5, 0, -1, -7, 5, 2, 7, -3, 3, 0]
harvest_a(:,10) = [-9, 2, -6, 3, -9, 5, 5, 7, 5, -9]

write (u, "(A)")  "* Test output: Sorting"
write (u, "(A)")  "* Purpose: test sorting routines"
write (u, "(A)")

write (u, "(A)")  "* Sorting real values:"

do i = 1, NMAX
  write (u, "(A)")
  rval(:i) = harvest_r(:,i)
  write (u, "(10(1x,F7.4))") rval(:i)
  rval(:i) = sort (rval(:i))
  write (u, "(10(1x,F7.4))") rval(:i)
  do j = i, 2, -1
    if (rval(j)-rval(j-1) < 0) &
      write (u, "(A)") "*** Sorting failure. ***"
  end do
end do

write (u, "(A)")
write (u, "(A)")  "* Sorting integer values:"

do i = 1, NMAX
  write (u, "(A)")
  ival(:i) = harvest_i(:,i)
  write (u, "(10(1x,I2))") ival(:i)
  ival(:i) = sort (ival(:i))
  write (u, "(10(1x,I2))") ival(:i)
  do j = i, 2, -1
    if (ival(j)-ival(j-1) < 0) &
      write (u, "(A)") "*** Sorting failure. ***"
  end do
end do

write (u, "(A)")
write (u, "(A)")  "* Sorting integer values by absolute value:"

do i = 1, NMAX
  write (u, "(A)")
  ival(:i) = harvest_a(:,i)
  write (u, "(10(1x,I2))") ival(:i)
  ival(:i) = sort_abs (ival(:i))
  write (u, "(10(1x,I2))") ival(:i)
  do j = i, 2, -1
    if (abs(ival(j))-abs(ival(j-1)) < 0 .or. &
        (abs(ival(j))==abs(ival(j-1))) .and. ival(j)>ival(j-1)) &
      write (u, "(A)") "*** Sorting failure. ***"
  end do
end do

```

```

write (u, "(A)")
write (u, "(A)")  "** Test output end: sorting_1"

end subroutine sorting_1

```

6.6 Grids

This is not really a combinatorics module but this directory is the closest I could find. Maybe this will be moved to a seperate directory or combined with related stuff.

```

⟨grids.f90⟩≡
⟨File header⟩

module grids

  ⟨Use kinds⟩
  use constants, only: zero, one, tiny_07
  use io_units
  use format_defs, only: FMT_16
  use diagnostics
  ⟨Use mpi f08⟩

  ⟨Standard module head⟩

  ⟨Grids: public⟩

  ⟨Grids: parameters⟩

  ⟨Grids: types⟩

  contains

  ⟨Grids: procedures⟩

end module grids

```

Grids are used in many applications and a general implementation seems useful. The relevant properties implemented so far are

- Segments of the hypercube are represented by an integer array with size d corresponding to the dimension.
- There is a mapping from the indices to the location in the continuous memory block of values.
- Given a point in the hypercube, find the corresponding segment and the value of the grid therein.
- Update the grid sequentially to represent the maximum of a function over the unit hypercube.
- The grid can be saved to and recovered from disk.

The following might be implemented in the future

- Generate a random point in the hypercube by interpreting the grid as probability distribution.

This would most likely be solved by using projections and the `selector_t`, which would make a move of this module higher up in the dependency tree necessary.

- Update the grid sequentially to represent the *minimum* of a function over the unit hypercube.

```

<Grids: public>≡
  public :: grid_t

<Grids: types>≡
  type :: grid_t
    private
      real(default), dimension(:), allocatable :: values
      integer, dimension(:), allocatable :: points
    contains
      <Grids: grid: TBP>
    end type grid_t

```

6.6.1 Initializer and finalizer

For initialization, we expect the number of points for each dimension as an array or the the number of dimensions as a scalar whereby the default number of points is used then for each dimension.

```

<Grids: grid: TBP>≡
  generic :: init => init_base, init_simple
  procedure :: init_base => grid_init_base
  procedure :: init_simple => grid_init_simple

<Grids: procedures>≡
  pure subroutine grid_init_base (grid, points)
    class(grid_t), intent(inout) :: grid
    integer, dimension(:), intent(in) :: points
    allocate (grid%points (size (points)))
    allocate (grid%values (product (points)))
    grid%points = points
    grid%values = zero
  end subroutine grid_init_base

<Grids: procedures>+≡
  pure subroutine grid_init_simple (grid, dimensions)
    class(grid_t), intent(inout) :: grid
    integer, intent(in) :: dimensions
    allocate (grid%points (dimensions))
    allocate (grid%values (DEFAULT_POINTS_PER_DIMENSION ** dimensions))
    grid%points = DEFAULT_POINTS_PER_DIMENSION
    grid%values = zero
  end subroutine grid_init_simple

```

Manual assignment (tests)

```
<Grids: grid: TBP>+≡
  procedure :: set_values => grid_set_values

<Grids: procedures>+≡
  subroutine grid_set_values (grid, values)
    class(grid_t), intent(inout) :: grid
    real(default), dimension(:), intent(in) :: values
    grid%values = values
  end subroutine grid_set_values
```

A reasonable default

```
<Grids: parameters>≡
  integer, parameter :: DEFAULT_POINTS_PER_DIMENSION = 100
```

Calling this is not mandatory, when an instance of `grid_t` goes out of scope as it will be done by Fortran automatically.

```
<Grids: grid: TBP>+≡
  procedure :: final => grid_final

<Grids: procedures>+≡
  pure subroutine grid_final (grid)
    class(grid_t), intent(inout) :: grid
    if (allocated (grid%values)) then
      deallocate (grid%values)
    end if
    if (allocated (grid%points)) then
      deallocate (grid%points)
    end if
  end subroutine grid_final
```

6.6.2 Segment finding and memory mapping

The `indices` array is expected to go from 1 to d whereby the entries for the different dims are from 1 to $n_{\text{points}}(\text{dim})$.

We get the value of the grid either from given `indices` or from a point `x` in the hypercube. In the latter case, we have to find the segment first.

```
<Grids: grid: TBP>+≡
  generic :: get_value => get_value_from_x, get_value_from_indices
  procedure :: get_value_from_x => grid_get_value_from_x
  procedure :: get_value_from_indices => grid_get_value_from_indices

<Grids: procedures>+≡
  function grid_get_value_from_indices (grid, indices)
    real(default) :: grid_get_value_from_indices
    class(grid_t), intent(in) :: grid
    integer, dimension(:), intent(in) :: indices
    grid_get_value_from_indices = grid%values(grid%get_index(indices))
  end function grid_get_value_from_indices
```

```

⟨Grids: procedures⟩+≡
function grid_get_value_from_x (grid, x)
  real(default) :: grid_get_value_from_x
  class(grid_t), intent(in) :: grid
  real(default), dimension(:), intent(in) :: x
  grid_get_value_from_x = grid_get_value_from_indices &
    (grid, grid_get_segment (grid, x))
end function grid_get_value_from_x

```

The segment is the part of the grid that contains the point x and is identified by a tuple of indices. This is just a brute force search, for fine grids one could also implement a binary search for $\mathcal{O}(\log N)$ behavior instead of $\mathcal{O}(N)$.

```

⟨Grids: grid: TBP⟩+≡
  procedure :: get_segment => grid_get_segment

⟨Grids: procedures⟩+≡
function grid_get_segment (grid, x, unit)
  class(grid_t), intent(in) :: grid
  real(default), dimension(:), intent(in) :: x
  integer, intent(in), optional :: unit
  integer, dimension(1:size (x)) :: grid_get_segment
  integer :: dim, i
  real(default) :: segment_width
  grid_get_segment = 0
  do dim = 1, size (grid%points)
    segment_width = one / grid%points (dim)
    SEARCH: do i = 1, grid%points (dim)
      if (x (dim) <= i * segment_width + tiny_07) then
        grid_get_segment (dim) = i
        exit SEARCH
      end if
    end do SEARCH
    if (grid_get_segment (dim) == 0) then
      do i = 1, size(x)
        write (msg_buffer, "(A," // DEFAULT_OUTPUT_PRECISION // ")") &
          "x[i] = ", x(i)
        call msg_message ()
      end do
      call msg_error ("grid_get_segment: Did not find x in [0,1]^d", &
        unit=unit)
    end if
  end do
end function grid_get_segment

```

This is a simple storage mapping function but more sophisticated ideas like hashing could be implemented.

$$\begin{aligned}
\text{index} = & \text{indices}(1) + \\
& \text{indices}(2) * \text{size}(1) + \\
& \text{indices}(3) * \text{size}(1) * \text{size}(2) + \dots
\end{aligned} \tag{6.1}$$

```

⟨Grids: grid: TBP⟩+≡
  procedure :: get_index => grid_get_index

```

```

⟨Grids: procedures⟩+≡
  pure function grid_get_index (grid, indices) result (grid_index)
    integer :: grid_index
    class(grid_t), intent(in) :: grid
    integer, dimension(:), intent(in) :: indices
    integer :: dim_innerloop, dim_outerloop, multiplier
    grid_index = 1
    do dim_outerloop = 1, size(indices)
      multiplier = 1
      do dim_innerloop = 1, dim_outerloop - 1
        multiplier = multiplier * grid%points (dim_innerloop)
      end do
      grid_index = grid_index + (indices(dim_outerloop) - 1) * multiplier
    end do
  end function grid_get_index

```

6.6.3 Grid manipulations

Given a point in the hypercube x and its value y , we update the grids, such that the stepwise function f defined by the grid is $f(x_i) \geq y_i \forall \{x_i, y_i\}$.

```

⟨Grids: grid: TBP⟩+≡
  procedure :: update_maxima => grid_update_maxima

⟨Grids: procedures⟩+≡
  subroutine grid_update_maxima (grid, x, y)
    class(grid_t), intent(inout) :: grid
    real(default), dimension(:), intent(in) :: x
    real(default), intent(in) :: y
    integer, dimension(1:size(x)) :: indices
    indices = grid%get_segment (x)
    if (grid%get_value (indices) < y) then
      grid%values (grid%get_index (indices)) = y
    end if
  end subroutine grid_update_maxima

```

More general cases have to be thought through when they are needed. *This is inefficient and non-general.*

```

⟨Grids: grid: TBP⟩+≡
  procedure :: get_maximum_in_3d => grid_get_maximum_in_3d

⟨Grids: procedures⟩+≡
  function grid_get_maximum_in_3d (grid, projected_index) result (maximum)
    real(default) :: maximum
    class(grid_t), intent(in) :: grid
    integer, intent(in) :: projected_index
    real(default) :: val
    integer :: i, j
    maximum = zero
    do i = 1, grid%points(1)
      do j = 1, grid%points(2)
        val = grid%get_value ([i, j, projected_index])
        if (val > maximum) then

```



```

        maximum = val
    end if
end do
end do

end function grid_get_maximum_in_3d

```

```

⟨Grids: grid: TBP⟩+≡
  procedure :: is_non_zero_everywhere => grid_is_non_zero_everywhere
⟨Grids: procedures⟩+≡
  pure function grid_is_non_zero_everywhere (grid) result (yorn)
    logical :: yorn
    class(grid_t), intent(in) :: grid
    yorn = all (abs (grid%values) > zero)
  end function grid_is_non_zero_everywhere

```

Returns true if any value of the grid is non-zero. We need this to determine whether the grid has been filled during integration.

```

⟨Grids: grid: TBP⟩+≡
  procedure :: has_non_zero_entries => grid_has_non_zero_entries
⟨Grids: procedures⟩+≡
  pure function grid_has_non_zero_entries (grid) result (non_zero)
    logical :: non_zero
    class(grid_t), intent(in) :: grid
    non_zero = any (abs (grid%values) > zero)
  end function grid_has_non_zero_entries

```

MPI: We allow for several grids in a parallelized run to be combined with MPI.reduce. The operator has to be specified. We do not check on any specifications.

```

⟨MPI: Grids: grid: TBP⟩≡
  procedure :: mpi_reduce => grid_mpi_reduce
⟨MPI: Grids: procedures⟩≡
  subroutine grid_mpi_reduce (grid, operator)
    class(grid_t), intent(inout) :: grid
    type(MPI_op), intent(in) :: operator
    real(default), dimension(size (grid%values)) :: root_values
    integer :: rank
    call MPI_Comm_rank (MPI_COMM_WORLD, rank)
    call MPI_Reduce (grid%values, root_values, size (grid%values), &
      & MPI_DOUBLE_PRECISION, operator, 0, MPI_COMM_WORLD)
    if (rank == 0) then
      grid%values = root_values
    end if
  end subroutine grid_mpi_reduce

```

6.6.4 Input and Output to screen and disk

```

⟨Grids: grid: TBP⟩+≡
  procedure :: write => grid_write

```

```

<Grids: procedures>+≡
subroutine grid_write (grid, unit)
  class(grid_t), intent(in) :: grid
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1X,A)") "Grid"
  write (u, "(2X,A,2X)", advance='no') "Number of points per dimension:"
  if (allocated (grid%points)) then
    do i = 1, size (grid%points)
      write (u, "(I12,1X)", advance='no') &
        grid%points (i)
    end do
  end if
  write (u, *)
  write (u, "(2X,A)") "Values of the grid:"
  if (allocated (grid%values)) then
    do i = 1, size (grid%values)
      write (u, "(" // DEFAULT_OUTPUT_PRECISION // ",1X)") &
        grid%values (i)
    end do
  end if
  call grid%compute_and_write_mean_and_max (u)
end subroutine grid_write

```

```

<Grids: grid: TBP>+≡
procedure :: compute_and_write_mean_and_max => &
  grid_compute_and_write_mean_and_max

```

```

<Grids: procedures>+≡
subroutine grid_compute_and_write_mean_and_max (grid, unit)
  class(grid_t), intent(in) :: grid
  integer, intent(in), optional :: unit
  integer :: u, i, n_values
  real(default) :: mean, val, maximum
  u = given_output_unit (unit); if (u < 0) return
  mean = zero
  maximum = zero
  if (allocated (grid%values)) then
    n_values = size (grid%values)
    do i = 1, n_values
      val = grid%values (i)
      mean = mean + val / n_values
      if (val > maximum) then
        maximum = val
      end if
    end do
    write (msg_buffer, "(A," // DEFAULT_OUTPUT_PRECISION // ")") &
      "Grid: Mean value of the grid: ", mean
    call msg_message ()
    write (msg_buffer, "(A," // DEFAULT_OUTPUT_PRECISION // ")") &
      "Grid: Max value of the grid: ", maximum
    call msg_message ()
    if (maximum > zero) then

```

```

        write (msg_buffer, "(A," // DEFAULT_OUTPUT_PRECISION // ")") &
        "Grid: Mean/Max value of the grid: ", mean / maximum
        call msg_message ()
    end if
else
    call msg_warning ("Grid: Grid is not allocated!")
end if
end subroutine grid_compute_and_write_mean_and_max

<Grids: grid: TBP>+≡
    procedure :: save_to_file => grid_save_to_file

<Grids: procedures>+≡
    subroutine grid_save_to_file (grid, file)
        class(grid_t), intent(in) :: grid
        character(len=*), intent(in) :: file
        integer :: iostat, u, i
        u = free_unit ()
        open (file=file, unit=u, action='write')
        if (allocated (grid%points)) then
            write (u, "(I12)") size (grid%points)
            do i = 1, size (grid%points)
                write (u, "(I12,1X)", advance='no', iostat=iostat) &
                    grid%points (i)
            end do
        end if
        write (u, *)
        if (allocated (grid%values)) then
            do i = 1, size (grid%values)
                write (u, "(" // DEFAULT_OUTPUT_PRECISION // ",1X)", &
                    advance='no', iostat=iostat) grid%values (i)
            end do
        end if
        if (iostat /= 0) then
            call msg_warning &
                ('grid_save_to_file: Could not save grid to file')
        end if
        close (u)
    end subroutine grid_save_to_file

<Grids: parameters>+≡
    character(len=*), parameter :: DEFAULT_OUTPUT_PRECISION = FMT_16

<Grids: public>+≡
    public :: verify_points_for_grid

<Grids: procedures>+≡
    function verify_points_for_grid (file, points) result (valid)
        logical :: valid
        character(len=*), intent(in) :: file
        integer, dimension(:), intent(in) :: points
        integer, dimension(:), allocatable :: points_from_file
        integer :: u
        call load_points_from_file (file, u, points_from_file)

```

```

close (u)
if (allocated (points_from_file)) then
    valid = all (points == points_from_file)
else
    valid = .false.
end if
end function verify_points_for_grid

```

Returns the `unit` that has opened the input file and read the first two lines. The caller has to close it. Furthermore, we return `points` containing the number of points in each dimension.

<Grids: procedures>+≡

```

subroutine load_points_from_file (file, unit, points)
character(len=*), intent(in) :: file
integer, intent(out) :: unit
integer, dimension(:), allocatable :: points
integer :: iostat, n_dimensions, i_dim
unit = free_unit ()
open (file=file, unit=unit, action='read', iostat=iostat)
if (iostat /= 0) return
read (unit, "(I12)", iostat=iostat) n_dimensions
if (iostat /= 0) return
allocate (points (n_dimensions))
do i_dim = 1, size (points)
    read (unit, "(I12,1X)", advance='no', iostat=iostat) &
        points (i_dim)
end do
if (iostat /= 0) return
read (unit, *)
if (iostat /= 0) return
end subroutine load_points_from_file

```

<Grids: grid: TBP>+≡

```

procedure :: load_from_file => grid_load_from_file

```

<Grids: procedures>+≡

```

subroutine grid_load_from_file (grid, file)
class(grid_t), intent(out) :: grid
character(len=*), intent(in) :: file
integer :: iostat, u, i
integer, dimension(:), allocatable :: points
call load_points_from_file (file, u, points)
if (.not. allocated (points)) return
call grid%init (points)
do i = 1, size (grid%values)
    read (u, "(" // DEFAULT_OUTPUT_PRECISION // ",1X)", advance='no', iostat=iostat) &
        grid%values (i)
end do
if (iostat /= 0) then
    call msg_warning ('grid_load_from_file: Could not load grid from file')
end if
close (u)
end subroutine grid_load_from_file

```

6.6.5 Unit tests

Test module, followed by the corresponding implementation module.

```
<grids.ut.f90>≡
  <File header>

  module grids_ut
    use unit_tests
    use grids_uti

    <Standard module head>

    <Grids: public test>

    contains

    <Grids: test driver>

  end module grids_ut

<grids.uti.f90>≡
  <File header>

  module grids_uti

    <Use kinds>
    use constants, only: zero, one, two, three, four, tiny_07
    use file_utils, only: delete_file
    use numeric_utils

    use grids

    <Standard module head>

    <Grids: test declarations>

    contains

    <Grids: tests>

  end module grids_uti

API: driver for the unit tests below.
<Grids: public test>≡
  public :: grids_test

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

Test Index Function

```
(Grids: execute tests)≡
  call test(grid_1, "grid_1", &
    "Test Index Function", u, results)

(Grids: test declarations)≡
  public :: grid_1

(Grids: tests)≡
  subroutine grid_1 (u)
    integer, intent(in) :: u
    type(grid_t) :: grid
    write (u, "(A)")  "* Test output: grid_1"
    write (u, "(A)")  "* Purpose: Test Index Function"
    write (u, "(A)")

    call grid%init ([3])
    call grid%write(u)
    call assert (u, grid%get_index([1]) == 1, "grid%get_index(1) == 1")
    call assert (u, grid%get_index([2]) == 2, "grid%get_index(2) == 2")
    call assert (u, grid%get_index([3]) == 3, "grid%get_index(3) == 3")
    call grid%final ()

    call grid%init ([3,3])
    call grid%write(u)
    call assert (u, grid%get_index([1,1]) == 1, "grid%get_index(1,1) == 1")
    call assert (u, grid%get_index([2,1]) == 2, "grid%get_index(2,1) == 2")
    call assert (u, grid%get_index([3,1]) == 3, "grid%get_index(3,1) == 3")
    call assert (u, grid%get_index([1,2]) == 4, "grid%get_index(1,2) == 4")
    call assert (u, grid%get_index([2,2]) == 5, "grid%get_index(2,2) == 5")
    call assert (u, grid%get_index([3,2]) == 6, "grid%get_index(3,2) == 6")
    call assert (u, grid%get_index([1,3]) == 7, "grid%get_index(1,3) == 7")
    call assert (u, grid%get_index([2,3]) == 8, "grid%get_index(2,3) == 8")
    call assert (u, grid%get_index([3,3]) == 9, "grid%get_index(3,3) == 9")
    call grid%final ()

    call grid%init ([3,3,2])
    call grid%write(u)
    call assert (u, grid%get_index([1,1,1]) == 1, "grid%get_index(1,1,1) == 1")
    call assert (u, grid%get_index([2,1,2]) == 2+9, "grid%get_index(2,1,2) == 2+9")
    call assert (u, grid%get_index([3,3,1]) == 9, "grid%get_index(3,3,1) == 3")
    call assert (u, grid%get_index([3,1,2]) == 3+9, "grid%get_index(3,1,2) == 4+9")
    call assert (u, grid%get_index([2,2,1]) == 5, "grid%get_index(2,2,1) == 5")
    call assert (u, grid%get_index([3,2,2]) == 6+9, "grid%get_index(3,2,2) == 6+9")
    call assert (u, grid%get_index([1,3,1]) == 7, "grid%get_index(1,3,1) == 7")
    call assert (u, grid%get_index([2,3,2]) == 8+9, "grid%get_index(2,3,2) == 8+9")
    call assert (u, grid%get_index([3,3,2]) == 9+9, "grid%get_index(3,3,2) == 9+9")
    call grid%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: grid_1"
  end subroutine grid_1
```

Saving and Loading

```
(Grids: execute tests)+≡
    call test(grid_2, "grid_2", &
        "Saving and Loading", u, results)

(Grids: test declarations)+≡
    public :: grid_2

(Grids: tests)+≡
    subroutine grid_2 (u)
        integer, intent(in) :: u
        type(grid_t) :: grid
        write (u, "(A)")  "* Test output: grid_2"
        write (u, "(A)")  "* Purpose: Saving and Loading"
        write (u, "(A)")

        call grid%init ([3])
        call grid%set_values ([one, two, three])
        call grid%save_to_file ('grid_2_test')
        call grid%final ()

        call assert (u, verify_points_for_grid('grid_2_test', [3]), &
            "verify_points_for_grid")
        call grid%load_from_file ('grid_2_test')
        call grid%write (u)
        call assert (u, nearly_equal (grid%get_value([1]), one),  "grid%get_value(1) == 1")
        call assert (u, nearly_equal (grid%get_value([2]), two),  "grid%get_value(2) == 2")
        call assert (u, nearly_equal (grid%get_value([3]), three), "grid%get_value(3) == 3")
        call grid%final ()

        call grid%init ([3,3])
        call grid%set_values ([one, two, three, four, zero, zero, zero, zero, zero])
        call grid%save_to_file ('grid_2_test')
        call grid%final ()

        call assert (u, verify_points_for_grid('grid_2_test', [3,3]), &
            "verify_points_for_grid")
        call grid%load_from_file ('grid_2_test')
        call grid%write (u)
        call assert (u, nearly_equal (grid%get_value([1,1]), one),  "grid%get_value(1,1) == 1")
        call assert (u, nearly_equal (grid%get_value([2,1]), two),  "grid%get_value(2,1) == 2")
        call assert (u, nearly_equal (grid%get_value([3,1]), three), "grid%get_value(3,1) == 3")
        call assert (u, nearly_equal (grid%get_value([1,2]), four),  "grid%get_value(1,2) == 4")
        call delete_file ('grid_2_test')

        call grid%load_from_file ('grid_2_test')
        call assert (u, .not. verify_points_for_grid('grid_2_test', [3,3]), &
            "verify_points_for_grid")
        call grid%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: grid_2"
    end subroutine grid_2
```

Get Segments

```
<Grids: execute tests>+≡
    call test(grid3_3, "grid3_3", &
              "Get Segments", u, results)

<Grids: test declarations>+≡
    public :: grid3_3

<Grids: tests>+≡
    subroutine grid3_3 (u)
        integer, intent(in) :: u
        type(grid_t) :: grid
        integer, dimension(2) :: fail
        write (u, "(A)")  "* Test output: grid3_3"
        write (u, "(A)")  "*   Purpose: Get Segments"
        write (u, "(A)")

        call grid%init ([3])
        call assert (u, all(grid%get_segment([0.00_default]) == [1]), &
                     "all(grid%get_segment([0.00_default]) == [1])")
        call assert (u, all(grid%get_segment([0.32_default]) == [1]), &
                     "all(grid%get_segment([0.32_default]) == [1])")
        call assert (u, all(grid%get_segment([0.52_default]) == [2]), &
                     "all(grid%get_segment([0.52_default]) == [2])")
        call assert (u, all(grid%get_segment([1.00_default]) == [3]), &
                     "all(grid%get_segment([1.00_default]) == [3])")
        call grid%final ()

        call grid%init ([3,3])
        call assert (u, all(grid%get_segment([0.00_default,0.00_default]) == [1,1]), &
                     "all(grid%get_segment([0.00_default,0.00_default]) == [1,1])")
        call assert (u, all(grid%get_segment([0.32_default,0.32_default]) == [1,1]), &
                     "all(grid%get_segment([0.32_default,0.32_default]) == [1,1])")
        call assert (u, all(grid%get_segment([0.52_default,0.52_default]) == [2,2]), &
                     "all(grid%get_segment([0.52_default,0.52_default]) == [2,2])")
        call assert (u, all(grid%get_segment([1.00_default,1.00_default]) == [3,3]), &
                     "all(grid%get_segment([1.00_default,1.00_default]) == [3,3])")
        write (u, "(A)")  "* A double error is expected"
        fail = grid%get_segment([1.10_default,1.10_default], u)
        call grid%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: grid3_3"
    end subroutine grid3_3
```

Update Maxima

```
<Grids: execute tests>+≡
    call test(grid4_4, "grid4_4", &
              "Update Maxima", u, results)

<Grids: test declarations>+≡
    public :: grid4_4
```



```

<Grids: tests>+≡
subroutine grids_4 (u)
  integer, intent(in) :: u
  type(grid_t) :: grid
  write (u, "(A)")  "* Test output: grids_4"
  write (u, "(A)")  "* Purpose: Update Maxima"
  write (u, "(A)")

  call grid%init ([4,4])
  call grid%update_maxima ([0.1_default, 0.0_default], 0.3_default)
  call grid%update_maxima ([0.9_default, 0.95_default], 1.7_default)
  call grid%write (u)
  call assert_equal (u, grid%get_value([1,1]), 0.3_default, &
    "grid%get_value([1,1]")
  call assert_equal (u, grid%get_value([2,2]), 0.0_default, &
    "grid%get_value([2,2]")
  call assert_equal (u, grid%get_value([4,4]), 1.7_default, &
    "grid%get_value([4,4]")

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: grids_4"
end subroutine grids_4

```

Finding and checking

```

<Grids: execute tests>+≡
  call test(grids_5, "grids_5", &
    "Finding and checking", u, results)

<Grids: test declarations>+≡
  public :: grids_5

<Grids: tests>+≡
subroutine grids_5 (u)
  integer, intent(in) :: u
  type(grid_t) :: grid
  real(default) :: first, second
  write (u, "(A)")  "* Test output: grids_5"
  write (u, "(A)")  "* Purpose: Finding and checking"
  write (u, "(A)")

  call grid%init ([2,2,2])
  first = one / two - tiny_07
  second = two / two - tiny_07
  call grid%update_maxima ([0.1_default, 0.0_default, first], 0.3_default)
  call grid%update_maxima ([0.9_default, 0.95_default, second], 1.7_default)
  call grid%write (u)
  call assert (u, .not. grid%is_non_zero_everywhere (), &
    ".not. grid%is_non_zero_everywhere (")
  call assert_equal (u, grid%get_maximum_in_3d (1), 0.3_default, &
    "grid%get_maximum_in_3d (1)")
  call assert_equal (u, grid%get_maximum_in_3d (2), 1.7_default, &
    "grid%get_maximum_in_3d (2)")

```

```

call grid%update_maxima ([0.9_default, 0.95_default, first], 1.8_default)
call grid%update_maxima ([0.1_default, 0.95_default, first], 1.5_default)
call grid%update_maxima ([0.9_default, 0.15_default, first], 1.5_default)
call grid%update_maxima ([0.1_default, 0.0_default, second], 0.2_default)
call grid%update_maxima ([0.1_default, 0.9_default, second], 0.2_default)
call grid%update_maxima ([0.9_default, 0.0_default, second], 0.2_default)
call grid%write (u)
call assert (u, grid%is_non_zero_everywhere (), &
             "grid%is_non_zero_everywhere ()")
call assert_equal (u, grid%get_maximum_in_3d (1), 1.8_default, &
                  "grid%get_maximum_in_3d (1)")
call assert_equal (u, grid%get_maximum_in_3d (2), 1.7_default, &
                  "grid%get_maximum_in_3d (2)")

write (u, "(A)")
write (u, "(A)")  "* Test output end: grids_5"
end subroutine grids_5

```

One could think of multiple implementations of a generic type.

```

<solver.f90>≡
  <File header>

  module solver

    <Use kinds>
    use constants, only: tiny_10
    use numeric_utils
    use diagnostics

    <Standard module head>

    <solver: public>

    <solver: parameters>

    <solver: types>

    <solver: interfaces>

    contains

    <solver: procedures>

  end module solver

<solver: public>≡
  public :: solver_function_t

<solver: types>≡
  type, abstract :: solver_function_t
  contains
    procedure(solver_function_evaluate), deferred :: evaluate
  end type solver_function_t

```

```

<solver: interfaces>≡
    abstract interface
        function solver_function_evaluate (solver_f, x) result (f)
            import
            complex(default) :: f
            class(solver_function_t), intent(in) :: solver_f
            real(default), intent(in) :: x
        end function
    end interface

<solver: public>+≡
    public :: solve_secant

<solver: procedures>≡
    function solve_secant (func, lower_start, upper_start, success, precision) result (x0)
        class(solver_function_t), intent(in) :: func
        real(default) :: x0
        real(default), intent(in) :: lower_start, upper_start
        real(default), intent(in), optional :: precision
        logical, intent(out) :: success
        real(default) :: desired, x_curr, x_next, f_curr, f_next, x_new
        integer :: n_iter
        desired = DEFAULT_PRECISION; if (present(precision)) desired = precision
        x_curr = lower_start
        x_next = upper_start
        n_iter = 0
        success = .false.
        SEARCH: do
            n_iter = n_iter + 1
            f_curr = real( func%evaluate (x_curr) )
            f_next = real( func%evaluate (x_next) )
            <Exit if close to zero and handle exceptions>
            x_new = x_next - (x_next - x_curr) / (f_next - f_curr) * f_next
            x_curr = x_next
            x_next = x_new
        end do SEARCH
        if (x0 < lower_start .or. x0 > upper_start) then
            call msg_warning ("solve: The root of the function is not in boundaries")
            return
        end if
        success = .true.
    end function solve_secant

<Exit if close to zero and handle exceptions>≡
    if (abs (f_next) < desired) then
        x0 = x_next
        exit
    end if
    if (n_iter > MAX_TRIES) then
        call msg_warning ("solve: Couldn't find root of function")
        return
    end if
    if (vanishes (f_next - f_curr)) then
        x_next = x_next + (x_next - x_curr) / 10

```

```

        cycle
    end if

```

Implements the bisection root-finding method to find a root of `func` between `lower_start` and `upper_start` with tolerance `precision`.

```

<solver: public>+≡
    public :: solve_interval

<solver: procedures>+≡
    function solve_interval (func, lower_start, upper_start, success, precision) &
                                                result (x0)

        class(solver_function_t), intent(in) :: func
        real(default) :: x0
        real(default), intent(in) :: lower_start, upper_start
        real(default), intent(in), optional :: precision
        logical, intent(out) :: success
        real(default) :: desired
        real(default) :: x_low, x_high, x_half
        real(default) :: f_low, f_high, f_half
        integer :: n_iter
        success = .false.
        desired = DEFAULT_PRECISION; if (present(precision)) desired = precision
        x0 = lower_start
        x_low = lower_start
        x_high = upper_start
        f_low = real( func%evaluate (x_low) )
        f_high = real( func%evaluate (x_high) )
        if (f_low * f_high > 0) return
        if (x_low > x_high) then
            call display_solver_status()
            call msg_fatal ("Interval solver: Upper bound must be &
                            &greater than lower bound")
        end if
        n_iter = 0
        do n_iter = 1, MAX_TRIES
            x_half = (x_high + x_low)/2
            f_half = real( func%evaluate (x_half) )
            if (abs (f_half) <= desired) then
                x0 = x_half
                exit
            end if
            if (f_low * f_half > 0._default) then
                x_low = x_half
                f_low = f_half
            else
                x_high = x_half
                f_high = f_half
            end if
        end do
        if (x0 < lower_start .or. x0 > upper_start) then
            call msg_warning ("Interval solver: The root of the function&
                              & is out of boundaries")
        return
    end if

```

```

        success = .true.
contains
  subroutine display_solver_status ()
    print *, '=====
    print *, 'Status of interval solver: '
    print *, 'initial values: ', lower_start, upper_start
    print *, 'iteration: ', n_iter
    print *, 'x_low: ', x_low, 'f_low: ', f_low
    print *, 'x_high: ', x_high, 'f_high: ', f_high
    print *, 'x_half: ', x_half, 'f_half: ', f_half
  end subroutine display_solver_status
end function solve_interval

<solver: public>+≡
  public :: solve_qgaus

<solver: procedures>+≡
  function solve_qgaus (integrand, grid) result (integral)
    class(solver_function_t), intent(in) :: integrand
    complex(default) :: integral
    real(default), dimension(:), intent(in) :: grid
    integer :: i, j
    real(default) :: xm, xr
    real(default), dimension(5) :: dx, &
      w = (/ 0.2955242247_default, 0.2692667193_default, &
        0.2190863625_default, 0.1494513491_default, 0.0666713443_default /), &
      x = (/ 0.1488743389_default, 0.4333953941_default, 0.6794095682_default, &
        0.8650633666_default, 0.9739065285_default /)
    integral = 0.0_default
    if ( size(grid) < 2 ) then
      call msg_warning ("solve_qgaus: size of integration grid smaller than 2.")
      return
    end if
    do i=1, size(grid)-1
      xm = 0.5_default * ( grid(i+1) + grid(i) )
      xr = 0.5_default * ( grid(i+1) - grid(i) )
      do j=1, 5
        dx(j) = xr * x(j)
        integral = integral + xr * w(j) * &
          ( integrand%evaluate (xm+dx(j)) + integrand%evaluate (xm-dx(j)) )
      end do
    end do
  end function solve_qgaus

<solver: parameters>≡
  real(default), parameter, public :: DEFAULT_PRECISION = tiny_10

<solver: parameters>+≡
  integer, parameter :: MAX_TRIES = 10000

```

6.6.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<solver_ut.f90>≡

```

```

    <File header>

    module solver_ut
        use unit_tests
        use solver_util

    <Standard module head>

    <solver: public test>

    contains

    <solver: test driver>

    end module solver_ut
<solver_util.f90>≡
    <File header>

    module solver_util

    <Use kinds>
        use constants, only: zero, one, two
        use numeric_utils

        use solver

    <Standard module head>

    <solver: test declarations>

    <solver: test types>

    contains

    <solver: tests>

    <solver: test auxiliary>

    end module solver_util
API: driver for the unit tests below.
<solver: public test>≡
    public :: solver_test
<solver: test driver>≡
    subroutine solver_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <solver: execute tests>
    end subroutine solver_test

```

Test functions

```

<solver: test types>≡

```

```

type, extends (solver_function_t) :: test_function_1_t
contains
  procedure :: evaluate => test_func_1
end type test_function_1_t

<solver: test types>+≡
type, extends (solver_function_t) :: test_function_2_t
contains
  procedure :: evaluate => test_func_2
end type test_function_2_t

<solver: test types>+≡
type, extends (solver_function_t) :: test_function_3_t
contains
  procedure :: evaluate => test_func_3
end type test_function_3_t

<solver: test types>+≡
type, extends (solver_function_t) :: test_function_4_t
contains
  procedure :: evaluate => test_func_4
end type test_function_4_t

<solver: test auxiliary>≡
function test_func_1 (solver_f, x) result (f)
  complex(default) :: f
  class(test_function_1_t), intent(in) :: solver_f
  real(default), intent(in) :: x
  f = x
end function test_func_1

function test_func_2 (solver_f, x) result (f)
  complex(default) :: f
  class(test_function_2_t), intent(in) :: solver_f
  real(default), intent(in) :: x
  f = x ** 2
end function test_func_2

function test_func_3 (solver_f, x) result (f)
  complex(default) :: f
  class(test_function_3_t), intent(in) :: solver_f
  real(default), intent(in) :: x
  f = x ** 3
end function test_func_3

function test_func_4 (solver_f, x) result (f)
  complex(default) :: f
  class(test_function_4_t), intent(in) :: solver_f
  real(default), intent(in) :: x
  real(default) :: s, cutoff
  s = 100.0_default
  cutoff = 1.01_default

```

```

    if (x < cutoff) then
      f = - (log (s) * log (log (s) / log(cutoff**2)) - log (s / cutoff**2)) - &
        log (one/two)
    else
      f = - (log (s) * log (log (s) / log(x**2)) - log (s / x**2)) - &
        log (one/two)
    end if
  end function test_func_4

```

Solve trivial functions

```

<solver: execute tests>≡
  call test(solver_1, "solver_1", &
    "Solve trivial functions", u, results)

<solver: test declarations>≡
  public :: solver_1

<solver: tests>≡
  subroutine solver_1 (u)
    integer, intent(in) :: u
    real(default) :: zero_position
    logical :: success
    type(test_function_1_t) :: test_func_1
    type(test_function_2_t) :: test_func_2
    type(test_function_3_t) :: test_func_3
    type(test_function_4_t) :: test_func_4
    write (u, "(A)")  "* Test output: solver_1"
    write (u, "(A)")  "* Purpose: Solve trivial functions"
    write (u, "(A)")

    zero_position = solve_interval (test_func_1, -one, one, success)
    call assert (u, success, "success")
    call assert_equal (u, zero_position, zero, "test_func_1: zero_position")

    zero_position = solve_interval (test_func_4, two, 10.0_default, success)
    call assert (u, success, "success")
    call assert_equal (u, zero_position, &
      3.5216674011865940283397224_default, &
      "test_func_4: zero_position", rel_smallness=1000*DEFAULT_PRECISION)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: solver_1"
  end subroutine solver_1

```


Chapter 7

Text handling

WHIZARD has to handle complex structures in input (and output) data. Doing this in a generic and transparent way requires a generic lexer and parser. The necessary modules are implemented here:

ifiles Implementation of line-oriented internal files in a more flexible way (linked lists of variable-length strings) than the Fortran builtin features.

lexers Read text and transform it into a token stream.

syntax_rules Define the rules for interpreting tokens, to be used by the WHIZARD parser.

parser Categorize tokens (keyword, string, number etc.) and use a set of syntax rules to transform the input into a parse tree.

xml Read and parse XML text, separate from the WHIZARD parser.

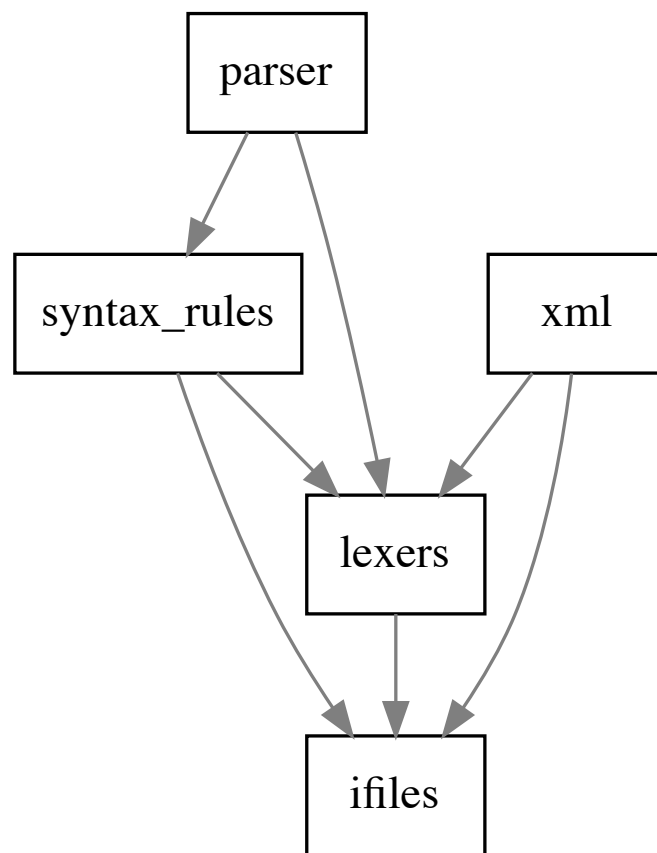


Figure 7.1: Module dependencies in `src/parsing`.

7.1 Internal files

The internal files introduced here (`ifile`) are a replacement for the built-in internal files, which are fixed-size arrays of fixed-length character strings. The `ifile` type is a doubly-linked list of variable-length character strings with line numbers.

```
<ifiles.f90>≡  
  <File header>  
  
  module ifiles  
  
    <Use strings>  
    use io_units  
    use system_defs, only: EOF  
  
    <Standard module head>  
  
    <Ifiles: public>  
  
    <Ifiles: types>  
  
    <Ifiles: interfaces>  
  
    contains  
  
    <Ifiles: subroutines>  
  
  end module ifiles
```

7.1.1 The line type

The line entry type is for internal use, it is the list entry to be collected in an `ifile` object.

```
<Ifiles: types>≡  
  type :: line_entry_t  
  private  
  type(line_entry_t), pointer :: previous => null ()  
  type(line_entry_t), pointer :: next => null ()  
  type(string_t) :: string  
  integer :: index  
end type line_entry_t
```

Create a new list entry, given a varying string as input. The line number and pointers are not set, these make sense only within an `ifile`.

```
<Ifiles: subroutines>≡  
  subroutine line_entry_create (line, string)  
    type(line_entry_t), pointer :: line  
    type(string_t), intent(in) :: string  
    allocate (line)  
    line%string = string  
  end subroutine line_entry_create
```

Destroy a single list entry: Since the pointer components should not be deallocated explicitly, just deallocate the object itself.

```

<Ifiles: subroutines>+≡
  subroutine line_entry_destroy (line)
    type(line_entry_t), pointer :: line
    deallocate (line)
  end subroutine line_entry_destroy

```

7.1.2 The ifile type

The internal file is a linked list of line entries.

```

<Ifiles: public>≡
  public :: ifile_t
<Ifiles: types>+≡
  type :: ifile_t
    private
    type(line_entry_t), pointer :: first => null ()
    type(line_entry_t), pointer :: last => null ()
    integer :: n_lines = 0
    contains
    <Ifiles: ifile: TBP>
  end type ifile_t

```

We need no explicit initializer, but a routine which recursively deallocates the contents may be appropriate. After this, existing line pointers may become undefined, so they should be nullified before the file is destroyed.

```

<Ifiles: public>+≡
  public :: ifile_clear
<Ifiles: subroutines>+≡
  subroutine ifile_clear (ifile)
    class(ifile_t), intent(inout) :: ifile
    type(line_entry_t), pointer :: current
    do while (associated (ifile%first))
      current => ifile%first
      ifile%first => current%next
      call line_entry_destroy (current)
    end do
    nullify (ifile%last)
    ifile%n_lines = 0
  end subroutine ifile_clear

```

The finalizer is just an alias for the above.

```

<Ifiles: public>+≡
  public :: ifile_final
<Ifiles: ifile: TBP>≡
  procedure :: final => ifile_clear
<Ifiles: interfaces>≡
  interface ifile_final
    module procedure ifile_clear
  end interface

```

7.1.3 I/O on ifiles

Fill an ifile from an ordinary external file, i.e., I/O unit. If the ifile is not empty, the old contents will be destroyed. We can read a fixed-length character string, an ISO varying string, an ordinary internal file (character-string array), or from an external unit. In the latter case, lines are appended until EOF is reached. Finally, there is a variant which reads from another ifile, effectively copying it.

```
(Ifiles: public)+≡
    public :: ifile_read

(Ifiles: interfaces)+≡
    interface ifile_read
        module procedure ifile_read_from_string
        module procedure ifile_read_from_char
        module procedure ifile_read_from_unit
        module procedure ifile_read_from_char_array
        module procedure ifile_read_from_ifile
    end interface

(Ifiles: subroutines)+≡
    subroutine ifile_read_from_string (ifile, string)
        type(ifile_t), intent(inout) :: ifile
        type(string_t), intent(in) :: string
        call ifile_clear (ifile)
        call ifile_append (ifile, string)
    end subroutine ifile_read_from_string

    subroutine ifile_read_from_char (ifile, char)
        type(ifile_t), intent(inout) :: ifile
        character(*), intent(in) :: char
        call ifile_clear (ifile)
        call ifile_append (ifile, char)
    end subroutine ifile_read_from_char

    subroutine ifile_read_from_char_array (ifile, char)
        type(ifile_t), intent(inout) :: ifile
        character(*), dimension(:), intent(in) :: char
        call ifile_clear (ifile)
        call ifile_append (ifile, char)
    end subroutine ifile_read_from_char_array

    subroutine ifile_read_from_unit (ifile, unit, iostat)
        type(ifile_t), intent(inout) :: ifile
        integer, intent(in) :: unit
        integer, intent(out), optional :: iostat
        call ifile_clear (ifile)
        call ifile_append (ifile, unit, iostat)
    end subroutine ifile_read_from_unit

    subroutine ifile_read_from_ifile (ifile, ifile_in)
        type(ifile_t), intent(inout) :: ifile
        type(ifile_t), intent(in) :: ifile_in
        call ifile_clear (ifile)
        call ifile_append (ifile, ifile_in)
    end subroutine ifile_read_from_ifile
```

Append to an ifile. The same as reading, but without resetting the ifile. In addition, there is a routine for appending a whole ifile.

```

<Ifiles: public>+≡
    public :: ifile_append

<Ifiles: ifile: TBP>+≡
    generic :: append => &
        ifile_append_from_char
    procedure, private :: ifile_append_from_char

<Ifiles: interfaces>+≡
    interface ifile_append
        module procedure ifile_append_from_string
        module procedure ifile_append_from_char
        module procedure ifile_append_from_unit
        module procedure ifile_append_from_char_array
        module procedure ifile_append_from_ifile
    end interface

<Ifiles: subroutines>+≡
    subroutine ifile_append_from_string (ifile, string)
        class(ifile_t), intent(inout) :: ifile
        type(string_t), intent(in) :: string
        type(line_entry_t), pointer :: current
        call line_entry_create (current, string)
        current%index = ifile%n_lines + 1
        if (associated (ifile%last)) then
            current%previous => ifile%last
            ifile%last%next => current
        else
            ifile%first => current
        end if
        ifile%last => current
        ifile%n_lines = current%index
    end subroutine ifile_append_from_string

    subroutine ifile_append_from_char (ifile, char)
        class(ifile_t), intent(inout) :: ifile
        character(*), intent(in) :: char
        call ifile_append_from_string (ifile, var_str (trim (char)))
    end subroutine ifile_append_from_char

    subroutine ifile_append_from_char_array (ifile, char)
        class(ifile_t), intent(inout) :: ifile
        character(*), dimension(:), intent(in) :: char
        integer :: i
        do i = 1, size (char)
            call ifile_append_from_string (ifile, var_str (trim (char(i))))
        end do
    end subroutine ifile_append_from_char_array

    subroutine ifile_append_from_unit (ifile, unit, iostat)
        class(ifile_t), intent(inout) :: ifile
        integer, intent(in) :: unit

```

```

integer, intent(out), optional :: iostat
type(string_t) :: buffer
integer :: ios
ios = 0
READ_LOOP: do
    call get (unit, buffer, iostat = ios)
    if (ios == EOF .or. ios > 0) exit READ_LOOP
    call ifile_append_from_string (ifile, buffer)
end do READ_LOOP
if (present (iostat)) then
    iostat = ios
else if (ios > 0) then
    call get (unit, buffer) ! trigger error again
end if
end subroutine ifile_append_from_unit

subroutine ifile_append_from_ifile (ifile, ifile_in)
    class(ifile_t), intent(inout) :: ifile
    type(ifile_t), intent(in) :: ifile_in
    type(line_entry_t), pointer :: current
    current => ifile_in%first
    do while (associated (current))
        call ifile_append_from_string (ifile, current%string)
        current => current%next
    end do
end subroutine ifile_append_from_ifile

```

Write the ifile contents to an external unit

```

<Ifiles: public>+≡
    public :: ifile_write

<Ifiles: subroutines>+≡
    subroutine ifile_write (ifile, unit, iostat)
        type(ifile_t), intent(in) :: ifile
        integer, intent(in), optional :: unit
        integer, intent(out), optional :: iostat
        integer :: u
        type(line_entry_t), pointer :: current
        u = given_output_unit (unit); if (u < 0) return
        current => ifile%first
        do while (associated (current))
            call put_line (u, current%string, iostat)
            current => current%next
        end do
    end subroutine ifile_write

```

Convert the ifile to an array of strings, which is allocated by this function:

```

<Ifiles: public>+≡
    public :: ifile_to_string_array

<Ifiles: subroutines>+≡
    subroutine ifile_to_string_array (ifile, string)
        type(ifile_t), intent(in) :: ifile
        type(string_t), dimension(:), intent(inout), allocatable :: string

```

```

    type(line_entry_t), pointer :: current
    integer :: i
    allocate (string (ifile_get_length (ifile)))
    current => ifile%first
    do i = 1, ifile_get_length (ifile)
        string(i) = current%string
        current => current%next
    end do
end subroutine ifile_to_string_array

```

7.1.4 Ifile tools

```

<Ifiles: public>+≡
    public :: ifile_get_length

<Ifiles: subroutines>+≡
    function ifile_get_length (ifile) result (length)
        integer :: length
        type(ifile_t), intent(in) :: ifile
        length = ifile%n_lines
    end function ifile_get_length

```

7.1.5 Line pointers

Instead of the implicit pointer used in ordinary file access, we define explicit pointers, so there can be more than one at a time.

```

<Ifiles: public>+≡
    public :: line_p

<Ifiles: types>+≡
    type :: line_p
    private
    type(line_entry_t), pointer :: p => null ()
end type line_p

```

Assign a file pointer to the first or last line in an ifile:

```

<Ifiles: public>+≡
    public :: line_init

<Ifiles: subroutines>+≡
    subroutine line_init (line, ifile, back)
        type(line_p), intent(inout) :: line
        type(ifile_t), intent(in) :: ifile
        logical, intent(in), optional :: back
        if (present (back)) then
            if (back) then
                line%p => ifile%last
            else
                line%p => ifile%first
            end if
        else
            line%p => ifile%first
        end if
    end subroutine line_init

```



```

        end if
    end subroutine line_init

```

Remove the pointer association:

```

<Ifiles: public>+≡
    public :: line_final

<Ifiles: subroutines>+≡
    subroutine line_final (line)
        type(line_p), intent(inout) :: line
        nullify (line%p)
    end subroutine line_final

```

Go one step forward

```

<Ifiles: public>+≡
    public :: line_advance

<Ifiles: subroutines>+≡
    subroutine line_advance (line)
        type(line_p), intent(inout) :: line
        if (associated (line%p)) line%p => line%p%next
    end subroutine line_advance

```

Go one step backward

```

<Ifiles: public>+≡
    public :: line_backspace

<Ifiles: subroutines>+≡
    subroutine line_backspace (line)
        type(line_p), intent(inout) :: line
        if (associated (line%p)) line%p => line%p%previous
    end subroutine line_backspace

```

Check whether we are accessing a valid line

```

<Ifiles: public>+≡
    public :: line_is_associated

<Ifiles: subroutines>+≡
    function line_is_associated (line) result (ok)
        logical :: ok
        type(line_p), intent(in) :: line
        ok = associated (line%p)
    end function line_is_associated

```

7.1.6 Access lines via pointers

We do not need the ifile as an argument to these functions, because the `line` type will point to an existing ifile.

```

<Ifiles: public>+≡
    public :: line_get_string

```

```

<Ifiles: subroutines>+=
function line_get_string (line) result (string)
  type(string_t) :: string
  type(line_p), intent(in) :: line
  if (associated (line%p)) then
    string = line%p%string
  else
    string = ""
  end if
end function line_get_string

```

Variant where the line pointer is advanced after reading.

```

<Ifiles: public>+=
public :: line_get_string_advance
<Ifiles: subroutines>+=
function line_get_string_advance (line) result (string)
  type(string_t) :: string
  type(line_p), intent(inout) :: line
  if (associated (line%p)) then
    string = line%p%string
    call line_advance (line)
  else
    string = ""
  end if
end function line_get_string_advance

```

```

<Ifiles: public>+=
public :: line_get_index
<Ifiles: subroutines>+=
function line_get_index (line) result (index)
  integer :: index
  type(line_p), intent(in) :: line
  if (associated (line%p)) then
    index = line%p%index
  else
    index = 0
  end if
end function line_get_index

```

```

<Ifiles: public>+=
public :: line_get_length
<Ifiles: subroutines>+=
function line_get_length (line) result (length)
  integer :: length
  type(line_p), intent(in) :: line
  if (associated (line%p)) then
    length = len (line%p%string)
  else
    length = 0
  end if
end function line_get_length

```

7.2 Lexer

The lexer purpose is to read from a line-separated character input stream (usually a file) and properly chop the stream into lexemes (tokens). [The parser will transform lexemes into meaningful tokens, to be stored in a parse tree, therefore we do not use the term 'token' here.] The input is read line-by-line, but interpreted free-form, except for quotes and the comment syntax. (Fortran 2003 would allow us to use a stream type for reading.)

In an object-oriented approach, we can dynamically create and destroy lexers, including the lexer setup.

The main lexer function is to return a lexeme according to the basic lexer rules (quotes, comments, whitespace, special classes). There is also a routine to write back a lexeme to the input stream (but only once).

For the rules, we separate the possible characters into classes. Whitespace usually consists of blank, tab, and line-feed, where any number of consecutive whitespace is equivalent to one. Quoted strings are enclosed by a pair of quote characters, possibly multiline. Comments are similar to quotes, but interpreted as whitespace. Numbers are identified (not distinguishing real and integer) but not interpreted. Other character classes make up identifiers.

```
<lexers.f90>≡  
  <File header>  
  
  module lexers  
  
    <Use strings>  
    use io_units  
    use string_utils  
    use system_defs, only: EOF, EOR  
    use system_defs, only: LF  
    use system_defs, only: WHITESPACE_CHARS, LCLETTERS, UCLETTERS, DIGITS  
    use diagnostics  
    use ifiles, only: ifile_t  
    use ifiles, only: line_p, line_is_associated, line_init, line_final  
    use ifiles, only: line_get_string_advance  
  
    <Standard module head>  
  
    <Lexer: public>  
  
    <Lexer: parameters>  
  
    <Lexer: types>  
  
    <Lexer: interfaces>  
  
    contains  
  
    <Lexer: procedures>  
  
  end module lexers
```

7.2.1 Input streams

For flexible input, we define a generic stream type that refers to either an external file, an external unit which is already open, a string, an `ifile` object (internal file, i.e., string list), or a line pointer to an `ifile` object. The stream type actually follows the idea of a formatted external file, which is line-oriented. Thus, the stream reader always returns a whole record (input line).

Note that only in the string version, the stream contents are stored inside the stream object. In the `ifile` version, the stream contains only the line pointer, while in the external-file case, the line pointer is implicitly created by the runtime library.

```
<Lexer: public>≡
  public :: stream_t

<Lexer: types>≡
  type :: stream_t
    type(string_t), pointer :: filename => null ()
    integer, pointer :: unit => null ()
    type(string_t), pointer :: string => null ()
    type(ifile_t), pointer :: ifile => null ()
    type(line_p), pointer :: line => null ()
    integer :: record = 0
    logical :: eof = .false.
  contains
    <Lexer: stream: TBP>
  end type stream_t
```

The initializers refer to the specific version. The stream should be undefined before calling this.

```
<Lexer: public>+≡
  public :: stream_init

<Lexer: stream: TBP>≡
  generic :: init => &
    stream_init_filename, &
    stream_init_unit, &
    stream_init_string, &
    stream_init_ifile, &
    stream_init_line
  procedure, private :: stream_init_filename
  procedure, private :: stream_init_unit
  procedure, private :: stream_init_string
  procedure, private :: stream_init_ifile
  procedure, private :: stream_init_line

<Lexer: interfaces>≡
  interface stream_init
    module procedure stream_init_filename
    module procedure stream_init_unit
    module procedure stream_init_string
    module procedure stream_init_ifile
    module procedure stream_init_line
  end interface
```

```

<Lexer: procedures>+≡
  subroutine stream_init_filename (stream, filename)
    class(stream_t), intent(out) :: stream
    character(*), intent(in) :: filename
    integer :: unit
    unit = free_unit ()
    open (unit=unit, file=filename, status="old", action="read")
    call stream_init_unit (stream, unit)
    allocate (stream%filename)
    stream%filename = filename
  end subroutine stream_init_filename

  subroutine stream_init_unit (stream, unit)
    class(stream_t), intent(out) :: stream
    integer, intent(in) :: unit
    allocate (stream%unit)
    stream%unit = unit
    stream%eof = .false.
  end subroutine stream_init_unit

  subroutine stream_init_string (stream, string)
    class(stream_t), intent(out) :: stream
    type(string_t), intent(in) :: string
    allocate (stream%string)
    stream%string = string
  end subroutine stream_init_string

  subroutine stream_init_ifile (stream, ifile)
    class(stream_t), intent(out) :: stream
    type(ifile_t), intent(in) :: ifile
    type(line_p) :: line
    call line_init (line, ifile)
    call stream_init_line (stream, line)
    allocate (stream%ifile)
    stream%ifile = ifile
  end subroutine stream_init_ifile

  subroutine stream_init_line (stream, line)
    class(stream_t), intent(out) :: stream
    type(line_p), intent(in) :: line
    allocate (stream%line)
    stream%line = line
  end subroutine stream_init_line

```

The finalizer restores the initial state. If an external file was opened, it is closed.

```

<Lexer: public>+≡
  public :: stream_final

<Lexer: stream: TBP>+≡
  procedure :: final => stream_final

<Lexer: procedures>+≡
  subroutine stream_final (stream)
    class(stream_t), intent(inout) :: stream
    if (associated (stream%filename)) then

```

```

        close (stream%unit)
        deallocate (stream%unit)
        deallocate (stream%filename)
    else if (associated (stream%unit)) then
        deallocate (stream%unit)
    else if (associated (stream%string)) then
        deallocate (stream%string)
    else if (associated (stream%ifile)) then
        call line_final (stream%line)
        deallocate (stream%line)
        deallocate (stream%ifile)
    else if (associated (stream%line)) then
        call line_final (stream%line)
        deallocate (stream%line)
    end if
end subroutine stream_final

```

This returns the next record from the input stream. Depending on the stream type, the stream pointers are modified: Reading from external unit, the external file is advanced (implicitly). Reading from string, the string is replaced by an empty string. Reading from ifile, the line pointer is advanced. Note that the `iostat` argument is mandatory.

```

<Lexer: public>+≡
    public :: stream_get_record

<Lexer: procedures>+≡
    subroutine stream_get_record (stream, string, iostat)
        type(stream_t), intent(inout) :: stream
        type(string_t), intent(out) :: string
        integer, intent(out) :: iostat
        if (associated (stream%unit)) then
            if (stream%eof) then
                iostat = EOF
            else
                call get (stream%unit, string, iostat=iostat)
                if (iostat == EOR) then
                    iostat = 0
                    stream%record = stream%record + 1
                end if
                if (iostat == EOF) then
                    iostat = 0
                    stream%eof = .true.
                    if (len (string) /= 0) stream%record = stream%record + 1
                end if
            end if
        else if (associated (stream%string)) then
            if (len (stream%string) /= 0) then
                string = stream%string
                stream%string = ""
                iostat = 0
                stream%record = stream%record + 1
            else
                string = ""
                iostat = EOF
            end if
        end if
    end subroutine stream_get_record

```

```

        end if
    else if (associated (stream%line)) then
        if (line_is_associated (stream%line)) then
            string = line_get_string_advance (stream%line)
            iostat = 0
            stream%record = stream%record + 1
        else
            string = ""
            iostat = EOF
        end if
    else
        call msg_bug (" Attempt to read from uninitialized input stream")
    end if
end subroutine stream_get_record

```

Return the current stream source as a message string.

<Lexer: public>+≡

```
public :: stream_get_source_info_string
```

<Lexer: procedures>+≡

```

function stream_get_source_info_string (stream) result (string)
    type(string_t) :: string
    type(stream_t), intent(in) :: stream
    character(20) :: buffer
    if (associated (stream%filename)) then
        string = "File '" // stream%filename // "' (unit = "
        write (buffer, "(I0)") stream%unit
        string = string // trim (buffer) // ")"
    else if (associated (stream%unit)) then
        write (buffer, "(I0)") stream%unit
        string = "Unit " // trim (buffer)
    else if (associated (stream%string)) then
        string = "Input string"
    else if (associated (stream%ifile) .or. associated (stream%line)) then
        string = "Internal file"
    else
        string = ""
    end if
end function stream_get_source_info_string

```

Return the index of the record just read as a message string.

<Lexer: public>+≡

```
public :: stream_get_record_info_string
```

<Lexer: procedures>+≡

```

function stream_get_record_info_string (stream) result (string)
    type(string_t) :: string
    type(stream_t), intent(in) :: stream
    character(20) :: buffer
    string = stream_get_source_info_string (stream)
    if (string /= "") string = string // ", "
    write (buffer, "(I0)") stream%record
    string = string // "line " // trim (buffer)
end function stream_get_record_info_string

```

7.2.2 Keyword list

The lexer should be capable of identifying a token as a known keyword. To this end, we store a list of keywords:

```
<Lexer: public>+≡
    public :: keyword_list_t

<Lexer: types>+≡
    type :: keyword_entry_t
        private
            type(string_t) :: string
            type(keyword_entry_t), pointer :: next => null ()
        end type keyword_entry_t

    type :: keyword_list_t
        private
            type(keyword_entry_t), pointer :: first => null ()
            type(keyword_entry_t), pointer :: last => null ()
        end type keyword_list_t
```

Add a new string to the keyword list, unless it is already there:

```
<Lexer: public>+≡
    public :: keyword_list_add

<Lexer: procedures>+≡
    subroutine keyword_list_add (keylist, string)
        type(keyword_list_t), intent(inout) :: keylist
        type(string_t), intent(in) :: string
        type(keyword_entry_t), pointer :: k_entry_new
        if (.not. keyword_list_contains (keylist, string)) then
            allocate (k_entry_new)
            k_entry_new%string = string
            if (associated (keylist%first)) then
                keylist%last%next => k_entry_new
            else
                keylist%first => k_entry_new
            end if
            keylist%last => k_entry_new
        end if
    end subroutine keyword_list_add
```

Return true if a string is a keyword.

```
<Lexer: public>+≡
    public :: keyword_list_contains

<Lexer: procedures>+≡
    function keyword_list_contains (keylist, string) result (found)
        type(keyword_list_t), intent(in) :: keylist
        type(string_t), intent(in) :: string
        logical :: found
        found = .false.
```



```

        call check_rec (keylist%first)
contains
    recursive subroutine check_rec (k_entry)
        type(keyword_entry_t), pointer :: k_entry
        if (associated (k_entry)) then
            if (k_entry%string /= string) then
                call check_rec (k_entry%next)
            else
                found = .true.
            end if
        end if
    end subroutine check_rec
end function keyword_list_contains

```

Write the keyword list

```

<Lexer: public>+≡
    public :: keyword_list_write

<Lexer: interfaces>+≡
    interface keyword_list_write
        module procedure keyword_list_write_unit
    end interface

<Lexer: procedures>+≡
    subroutine keyword_list_write_unit (keylist, unit)
        type(keyword_list_t), intent(in) :: keylist
        integer, intent(in) :: unit
        write (unit, "(A)") "Keyword list:"
        if (associated (keylist%first)) then
            call keyword_write_rec (keylist%first)
            write (unit, *)
        else
            write (unit, "(1x,A)") "[empty]"
        end if
    contains
        recursive subroutine keyword_write_rec (k_entry)
            type(keyword_entry_t), intent(in), pointer :: k_entry
            if (associated (k_entry)) then
                write (unit, "(1x,A)", advance="no") char (k_entry%string)
                call keyword_write_rec (k_entry%next)
            end if
        end subroutine keyword_write_rec
    end subroutine keyword_list_write_unit

```

Clear the keyword list

```

<Lexer: public>+≡
    public :: keyword_list_final

<Lexer: procedures>+≡
    subroutine keyword_list_final (keylist)
        type(keyword_list_t), intent(inout) :: keylist
        call keyword_destroy_rec (keylist%first)
        nullify (keylist%last)
    contains

```

```

recursive subroutine keyword_destroy_rec (k_entry)
  type(keyword_entry_t), pointer :: k_entry
  if (associated (k_entry)) then
    call keyword_destroy_rec (k_entry%next)
    deallocate (k_entry)
  end if
end subroutine keyword_destroy_rec
end subroutine keyword_list_final

```

7.2.3 Lexeme templates

This type is handled like a rudimentary regular expression. It determines the lexer behavior when matching a string. The actual objects made from this type and the corresponding matching routines are listed below.

```

<Lexer: types>+≡
  type :: template_t
  private
  integer :: type
  character(256) :: charset1, charset2
  integer :: len1, len2
end type template_t

```

These are the types that valid lexemes can have:

```

<Lexer: public>+≡
  public :: T_KEYWORD, T_IDENTIFIER, T_QUOTED, T_NUMERIC

<Lexer: parameters>≡
  integer, parameter :: T_KEYWORD = 1
  integer, parameter :: T_IDENTIFIER = 2, T_QUOTED = 3, T_NUMERIC = 4

```

These are special types:

```

<Lexer: parameters>+≡
  integer, parameter :: EMPTY = 0, WHITESPACE = 10
  integer, parameter :: NO_MATCH = 11, IO_ERROR = 12, OVERFLOW = 13
  integer, parameter :: UNMATCHED_QUOTE = 14

```

In addition, we have EOF which is a negative integer, normally -1 . Printout for debugging:

```

<Lexer: procedures>+≡
  subroutine lexeme_type_write (type, unit)
    integer, intent(in) :: type
    integer, intent(in) :: unit
    select case (type)
    case (EMPTY);      write(unit,"(A)",advance="no") " EMPTY      "
    case (WHITESPACE); write(unit,"(A)",advance="no") " WHITESPACE "
    case (T_IDENTIFIER);write(unit,"(A)",advance="no") " IDENTIFIER "
    case (T_QUOTED);   write(unit,"(A)",advance="no") " QUOTED      "
    case (T_NUMERIC);  write(unit,"(A)",advance="no") " NUMERIC      "
    case (IO_ERROR);   write(unit,"(A)",advance="no") " IO_ERROR     "
    case (OVERFLOW);   write(unit,"(A)",advance="no") " OVERFLOW    "
    case (UNMATCHED_QUOTE); write(unit,"(A)",advance="no") " UNMATCHEDQ "
    case (NO_MATCH);   write(unit,"(A)",advance="no") " NO_MATCH     "
    case (EOF);        write(unit,"(A)",advance="no") " EOF         "

```

```

        case default;      write(unit,"(A)",advance="no") " [illegal] "
    end select
end subroutine lexeme_type_write

subroutine template_write (tt, unit)
    type(template_t), intent(in) :: tt
    integer, intent(in) :: unit
    call lexeme_type_write (tt%type, unit)
    write (unit, "(A)", advance="no") "' " // tt%charset1(1:tt%len1) // "' "
    write (unit, "(A)", advance="no") " ' " // tt%charset2(1:tt%len2) // "' "
end subroutine template_write

```

The matching functions all return the number of matched characters in the provided string. If this number is zero, the match has failed.

The `template` functions are declared `pure` because they appear in `forall` loops below.

A template for whitespace:

```

<Lexer: procedures>+≡
pure function template_whitespace (chars) result (tt)
    character(*), intent(in) :: chars
    type(template_t) :: tt
    tt = template_t (WHITESPACE, chars, "", len (chars), 0)
end function template_whitespace

```

Just match the string against the character set.

```

<Lexer: procedures>+≡
subroutine match_whitespace (tt, s, n)
    type(template_t), intent(in) :: tt
    character(*), intent(in) :: s
    integer, intent(out) :: n
    n = verify (s, tt%charset1(1:tt%len1)) - 1
    if (n < 0) n = len (s)
end subroutine match_whitespace

```

A template for normal identifiers. To match, a lexeme should have a first character in class `chars1` and an arbitrary number of further characters in class `chars2`. If the latter is empty, we are looking for a single-character lexeme.

```

<Lexer: procedures>+≡
pure function template_identifier (chars1, chars2) result (tt)
    character(*), intent(in) :: chars1, chars2
    type(template_t) :: tt
    tt = template_t (T_IDENTIFIER, chars1, chars2, len(chars1), len(chars2))
end function template_identifier

```

Here, the first letter must match, the others may or may not.

```

<Lexer: procedures>+≡
subroutine match_identifier (tt, s, n)
    type(template_t), intent(in) :: tt
    character(*), intent(in) :: s
    integer, intent(out) :: n
    if (verify (s(1:1), tt%charset1(1:tt%len1)) == 0) then

```

```

        n = verify (s(2:), tt%charset2(1:tt%len2))
        if (n == 0) n = len (s)
    else
        n = 0
    end if
end subroutine match_identifier

```

A template for quoted strings. The same template applies for comments. The first character set indicates the left quote (could be a sequence of several characters), the second one the matching right quote.

```

<Lexer: procedures>+≡
pure function template_quoted (chars1, chars2) result (tt)
character(*), intent(in) :: chars1, chars2
type(template_t) :: tt
tt = template_t (T_QUOTED, chars1, chars2, len (chars1), len (chars2))
end function template_quoted

```

Here, the beginning of the string must exactly match the first character set, then we look for the second one. If found, return. If there is a first quote but no second one, return a negative number, indicating this error condition.

```

<Lexer: procedures>+≡
subroutine match_quoted (tt, s, n, range)
type(template_t), intent(in) :: tt
character(*), intent(in) :: s
integer, intent(out) :: n
integer, dimension(2), intent(out) :: range
character(tt%len1) :: ch1
character(tt%len2) :: ch2
integer :: i
ch1 = tt%charset1
if (s(1:tt%len1) == ch1) then
    ch2 = tt%charset2
    do i = tt%len1 + 1, len (s) - tt%len2 + 1
        if (s(i:i+tt%len2-1) == ch2) then
            n = i + tt%len2 - 1
            range(1) = tt%len1 + 1
            range(2) = i - 1
            return
        end if
    end do
    n = -1
    range = 0
else
    n = 0
    range = 0
end if
end subroutine match_quoted

```

A template for real numbers. The first character set is the set of allowed exponent letters. In accordance with the other functions we return the lexeme as a string but do not read it.

```

<Lexer: procedures>+≡

```

```

pure function template_numeric (chars) result (tt)
  character(*), intent(in) :: chars
  type(template_t) :: tt
  tt = template_t (T_NUMERIC, chars, "", len (chars), 0)
end function template_numeric

```

A numeric lexeme may be real or integer. We purposely do not allow for a preceding sign. If the number is followed by an exponent, this is included, otherwise the rest is ignored.

There is a possible pitfall with this behavior: while the string `1e3` will be interpreted as a single number, the analogous string `1a3` will be split into the number `1` and an identifier `a3`. There is no easy way around such an ambiguity. We should make sure that the syntax does not contain identifiers like `a3` or `e3`.

(Lexer: procedures)+≡

```

subroutine match_numeric (tt, s, n)
  type(template_t), intent(in) :: tt
  character(*), intent(in) :: s
  integer, intent(out) :: n
  integer :: i, n0
  character(10), parameter :: digits = "0123456789"
  character(2), parameter :: signs = "-+"
  n = verify (s, digits) - 1
  if (n < 0) then
    n = 0
    return
  else if (s(n+1:n+1) == ".") then
    i = verify (s(n+2:), digits) - 1
    if (i < 0) then
      n = len (s)
      return
    else if (i > 0 .or. n > 0) then
      n = n + 1 + i
    end if
  end if
  n0 = n
  if (n > 0) then
    if (verify (s(n+1:n+1), tt%charset1(1:tt%len1)) == 0) then
      n = n + 1
      if (verify (s(n+1:n+1), signs) == 0) n = n + 1
      i = verify (s(n+1:), digits) - 1
      if (i < 0) then
        n = len (s)
      else if (i == 0) then
        n = n0
      else
        n = n + i
      end if
    end if
  end if
end subroutine match_numeric

```

The generic matching routine. With Fortran 2003 we would define separate types and use a `SELECT TYPE` instead.

```

<Lexer: procedures>+≡
subroutine match_template (tt, s, n, range)
  type(template_t), intent(in) :: tt
  character(*), intent(in) :: s
  integer, intent(out) :: n
  integer, dimension(2), intent(out) :: range
  select case (tt%type)
  case (WHITESPACE)
    call match_whitespace (tt, s, n)
    range = 0
  case (T_IDENTIFIER)
    call match_identifier (tt, s, n)
    range(1) = 1
    range(2) = len_trim (s)
  case (T_QUOTED)
    call match_quoted (tt, s, n, range)
  case (T_NUMERIC)
    call match_numeric (tt, s, n)
    range(1) = 1
    range(2) = len_trim (s)
  case default
    call msg_bug ("Invalid lexeme template encountered")
  end select
end subroutine match_template

```

Match against an array of templates. Return the index of the first template that matches together with the number of characters matched and the range of the relevant substring. If all fails, these numbers are zero.

```

<Lexer: procedures>+≡
subroutine match (tt, s, n, range, ii)
  type(template_t), dimension(:), intent(in) :: tt
  character(*), intent(in) :: s
  integer, intent(out) :: n
  integer, dimension(2), intent(out) :: range
  integer, intent(out) :: ii
  integer :: i
  do i = 1, size (tt)
    call match_template (tt(i), s, n, range)
    if (n /= 0) then
      ii = i
      return
    end if
  end do
  n = 0
  ii = 0
end subroutine match

```

7.2.4 The lexer setup

This object contains information about character classes. As said above, one class consists of quoting chars (matching left and right), another one of comment chars (similar), a class of whitespace, and several classes of characters

that make up identifiers. When creating the lexer setup, the character classes are transformed into lexeme templates which are to be matched in a certain predefined order against the input stream.

BLANK should always be taken as whitespace, some things may depend on this. TAB is also fixed by convention, but may in principle be modified. Newline (DOS!) and linefeed are also defined as whitespace. The lexer setup, containing the list of lexeme templates. No defaults yet. The type with index zero will be assigned to the NO_MATCH lexeme.

The keyword list is not stored, just a pointer to it. We anticipate that the keyword list is part of the syntax table, and the lexer needs not alter it. Furthermore, the lexer is typically finished before the syntax table is.

```
<Lexer: parameters>+≡
    integer, parameter :: CASE_KEEP = 0, CASE_UP = 1, CASE_DOWN = 2
```

```
<Lexer: types>+≡
    type :: lexer_setup_t
    private
    type(template_t), dimension(:), allocatable :: tt
    integer, dimension(:), allocatable :: type
    integer :: keyword_case = CASE_KEEP
    type(keyword_list_t), pointer :: keyword_list => null ()
end type lexer_setup_t
```

Fill the lexer setup object. Some things are hardcoded here (whitespace, alphanumeric identifiers), some are free: comment chars (but these must be single, and comments must be terminated by line-feed), quote chars and matches (must be single), characters to be read as one-character lexeme, special classes (characters of one class that should be glued together as identifiers).

```
<Lexer: procedures>+≡
    subroutine lexer_setup_init (setup, &
        comment_chars, quote_chars, quote_match, &
        single_chars, special_class, &
        keyword_list, upper_case_keywords)
    type(lexer_setup_t), intent(inout) :: setup
    character(*), intent(in) :: comment_chars
    character(*), intent(in) :: quote_chars, quote_match
    character(*), intent(in) :: single_chars
    character(*), dimension(:), intent(in) :: special_class
    type(keyword_list_t), pointer :: keyword_list
    logical, intent(in), optional :: upper_case_keywords
    integer :: n, i
    if (present (upper_case_keywords)) then
        if (upper_case_keywords) then
            setup%keyword_case = CASE_UP
        else
            setup%keyword_case = CASE_DOWN
        end if
    else
        setup%keyword_case = CASE_KEEP
    end if
    n = 1 + len (comment_chars) + len (quote_chars) + 1 &
```

```

        + len (single_chars) + size (special_class) + 1
allocate (setup%tt(n))
allocate (setup%type(0:n))
n = 0
setup%type(n) = NO_MATCH
n = n + 1
setup%tt(n) = template_whitespace (WHITESPACE_CHARS)
setup%type(n) = EMPTY
forall (i = 1:len(comment_chars))
    setup%tt(n+i) = template_quoted (comment_chars(i:i), LF)
    setup%type(n+i) = EMPTY
end forall
n = n + len (comment_chars)
forall (i = 1:len(quote_chars))
    setup%tt(n+i) = template_quoted (quote_chars(i:i), quote_match(i:i))
    setup%type(n+i) = T_QUOTED
end forall
n = n + len (quote_chars)
setup%tt(n+1) = template_numeric ("EeDd")
setup%type(n+1) = T_NUMERIC
n = n + 1
forall (i = 1:len (single_chars))
    setup%tt(n+i) = template_identifier (single_chars(i:i), "")
    setup%type(n+i) = T_IDENTIFIER
end forall
n = n + len (single_chars)
forall (i = 1:size (special_class))
    setup%tt(n+i) = template_identifier &
        (trim (special_class(i)), trim (special_class(i)))
    setup%type(n+i) = T_IDENTIFIER
end forall
n = n + size (special_class)
setup%tt(n+1) = template_identifier &
    (LCLETTERS//UCLETTERS, LCLETTERS//DIGITS//"_"/UCLETTERS)
setup%type(n+1) = T_IDENTIFIER
n = n + 1
if (n /= size (setup%tt)) &
    call msg_bug ("Size mismatch in lexer setup")
setup%keyword_list => keyword_list
end subroutine lexer_setup_init

```

The destructor is needed only if the object is not itself part of an allocatable array

```

<Lexer: procedures>+≡
subroutine lexer_setup_final (setup)
    type(lexer_setup_t), intent(inout) :: setup
    deallocate (setup%tt, setup%type)
    setup%keyword_list => null ()
end subroutine lexer_setup_final

```

For debugging: Write the lexer setup

```

<Lexer: procedures>+≡
subroutine lexer_setup_write (setup, unit)

```



```

type(lexer_setup_t), intent(in) :: setup
integer, intent(in) :: unit
integer :: i
write (unit, "(A)") "Lexer setup:"
if (allocated (setup%tt)) then
  do i = 1, size (setup%tt)
    call template_write (setup%tt(i), unit)
    write (unit, '(A)', advance = "no") " -> "
    call lexeme_type_write (setup%type(i), unit)
    write (unit, *)
  end do
else
  write (unit, *) "[empty]"
end if
if (associated (setup%keyword_list)) then
  call keyword_list_write (setup%keyword_list, unit)
end if
end subroutine lexer_setup_write

```

7.2.5 The lexeme type

An object of this type is returned by the lexer. Apart from the lexeme string, it gives information about the relevant substring (first and last character index) and the lexeme type. Interpreting the string is up to the parser.

```

<Lexer: public>+≡
  public :: lexeme_t
<Lexer: types>+≡
  type :: lexeme_t
  private
  integer :: type = EMPTY
  type(string_t) :: s
  integer :: b = 0, e = 0
end type lexeme_t

```

Debugging aid:

```

<Lexer: public>+≡
  public :: lexeme_write
<Lexer: procedures>+≡
  subroutine lexeme_write (t, unit)
    type(lexeme_t), intent(in) :: t
    integer, intent(in) :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    select case (t%type)
    case (T_KEYWORD)
      write (u, *) "KEYWORD:  ' " // char (t%s) // "' "
    case (T_IDENTIFIER)
      write (u, *) "IDENTIFIER: ' " // char (t%s) // "' "
    case (T_QUOTED)
      write (u, *) "QUOTED:   ' " // char (t%s) // "' "
    case (T_NUMERIC)

```

```

        write (u, *) "NUMERIC:      '" // char (t%s) // "'"
case (UNMATCHED_QUOTE)
    write (u, *) "Unmatched quote: "// char (t%s)
case (OVERFLOW); write (u, *) "Overflow: "// char (t%s)
case (EMPTY);    write (u, *) "Empty lexeme"
case (NO_MATCH); write (u, *) "No match"
case (IO_ERROR); write (u, *) "IO error"
case (EOF);      write (u, *) "EOF"
case default
    write (u, *) "Error"
end select
end subroutine lexeme_write

```

Store string and type in a lexeme. The range determines the beginning and end of the relevant part of the string. Check for a keyword.

<Lexer: procedures>+≡

```

subroutine lexeme_set (t, keyword_list, s, range, type, keyword_case)
    type(lexeme_t), intent(out) :: t
    type(keyword_list_t), pointer :: keyword_list
    type(string_t), intent(in) :: s
    type(string_t) :: keyword
    integer, dimension(2), intent(in) :: range
    integer, intent(in) :: type
    integer, intent(in), optional :: keyword_case
    t%type = type
    if (present (keyword_case)) then
        select case (keyword_case)
            case (CASE_KEEP); keyword = s
            case (CASE_UP);   keyword = upper_case (s)
            case (CASE_DOWN); keyword = lower_case (s)
        end select
    else
        keyword = s
    end if
    if (type == T_IDENTIFIER) then
        if (associated (keyword_list)) then
            if (keyword_list_contains (keyword_list, keyword)) &
                t%type = T_KEYWORD
        end if
    end if
    select case (t%type)
        case (T_KEYWORD); t%s = keyword
        case default;    t%s = s
    end select
    t%b = range(1)
    t%e = range(2)
end subroutine lexeme_set

subroutine lexeme_clear (t)
    type(lexeme_t), intent(out) :: t
    t%type = EMPTY
    t%s = ""
end subroutine lexeme_clear

```

Retrieve the lexeme string, the relevant part of it, and the type. The last function returns true if there is a break condition reached (error or EOF).

```

<Lexer: public>+≡
    public :: lexeme_get_string
    public :: lexeme_get_contents
    public :: lexeme_get_delimiters
    public :: lexeme_get_type

<Lexer: procedures>+≡
    function lexeme_get_string (t) result (s)
        type(string_t) :: s
        type(lexeme_t), intent(in) :: t
        s = t%s
    end function lexeme_get_string

    function lexeme_get_contents (t) result (s)
        type(string_t) :: s
        type(lexeme_t), intent(in) :: t
        s = extract (t%s, t%b, t%e)
    end function lexeme_get_contents

    function lexeme_get_delimiters (t) result (del)
        type(string_t), dimension(2) :: del
        type(lexeme_t), intent(in) :: t
        del(1) = extract (t%s, finish = t%b-1)
        del(2) = extract (t%s, start = t%e+1)
    end function lexeme_get_delimiters

    function lexeme_get_type (t) result (type)
        integer :: type
        type(lexeme_t), intent(in) :: t
        type = t%type
    end function lexeme_get_type

```

Check for a generic break condition (error/eof) and for eof in particular.

```

<Lexer: public>+≡
    public :: lexeme_is_break
    public :: lexeme_is_eof

<Lexer: procedures>+≡
    function lexeme_is_break (t) result (break)
        logical :: break
        type(lexeme_t), intent(in) :: t
        select case (t%type)
            case (EOF, IO_ERROR, OVERFLOW, NO_MATCH)
                break = .true.
            case default
                break = .false.
        end select
    end function lexeme_is_break

    function lexeme_is_eof (t) result (ok)
        logical :: ok

```

```

    type(lexeme_t), intent(in) :: t
    ok = t%type == EOF
end function lexeme_is_eof

```

7.2.6 The lexer object

We store the current lexeme and the current line. The line buffer is set each time a new line is read from file. The working buffer has one character more, to hold any trailing blank. Pointers to line and column are for debugging, they will be used to make up readable error messages for the parser.

```

<Lexer: public>+≡
    public :: lexer_t

<Lexer: types>+≡
    type :: lexer_t
    private
    type(lexer_setup_t) :: setup
    type(stream_t), pointer :: stream => null ()
    type(lexeme_t) :: lexeme
    type(string_t) :: previous_line2
    type(string_t) :: previous_line1
    type(string_t) :: current_line
    integer :: lines_read = 0
    integer :: current_column = 0
    integer :: previous_column = 0
    type(string_t) :: buffer
    type(lexer_t), pointer :: parent => null ()
    contains
    <Lexer: lexer: TBP>
end type lexer_t

Create-setup wrapper

<Lexer: public>+≡
    public :: lexer_init

<Lexer: lexer: TBP>≡
    procedure :: init => lexer_init

<Lexer: procedures>+≡
    subroutine lexer_init (lexer, &
        comment_chars, quote_chars, quote_match, &
        single_chars, special_class, &
        keyword_list, upper_case_keywords, &
        parent)
    class(lexer_t), intent(inout) :: lexer
    character(*), intent(in) :: comment_chars
    character(*), intent(in) :: quote_chars, quote_match
    character(*), intent(in) :: single_chars
    character(*), dimension(:), intent(in) :: special_class
    type(keyword_list_t), pointer :: keyword_list
    logical, intent(in), optional :: upper_case_keywords
    type(lexer_t), target, intent(in), optional :: parent
    call lexer_setup_init (lexer%setup, &
        comment_chars = comment_chars, &

```

```

        quote_chars = quote_chars, &
        quote_match = quote_match, &
        single_chars = single_chars, &
        special_class = special_class, &
        keyword_list = keyword_list, &
        upper_case_keywords = upper_case_keywords)
    if (present (parent)) lexer%parent => parent
    call lexer_clear (lexer)
end subroutine lexer_init

```

Clear the lexer state, but not the setup. This should be done when the lexing starts, but it is not known whether the lexer was used before.

```

<Lexer: public>+≡
    public :: lexer_clear

<Lexer: lexer: TBP>+≡
    procedure :: clear => lexer_clear

<Lexer: procedures>+≡
    subroutine lexer_clear (lexer)
        class(lexer_t), intent(inout) :: lexer
        call lexeme_clear (lexer%lexeme)
        lexer%previous_line2 = ""
        lexer%previous_line1 = ""
        lexer%current_line = ""
        lexer%lines_read = 0
        lexer%current_column = 0
        lexer%previous_column = 0
        lexer%buffer = ""
    end subroutine lexer_clear

```

Reset lexer state and delete setup

```

<Lexer: public>+≡
    public :: lexer_final

<Lexer: lexer: TBP>+≡
    procedure :: final => lexer_final

<Lexer: procedures>+≡
    subroutine lexer_final (lexer)
        class(lexer_t), intent(inout) :: lexer
        call lexer%clear ()
        call lexer_setup_final (lexer%setup)
    end subroutine lexer_final

```

7.2.7 The lexer routine

For lexing we need to associate an input stream to the lexer.

```

<Lexer: public>+≡
    public :: lexer_assign_stream

<Lexer: lexer: TBP>+≡
    procedure :: assign_stream => lexer_assign_stream

```

```

<Lexer: procedures>+≡
  subroutine lexer_assign_stream (lexer, stream)
    class(lexer_t), intent(inout) :: lexer
    type(stream_t), intent(in), target :: stream
    lexer%stream => stream
  end subroutine lexer_assign_stream

```

The lexer. The `lexer` function takes the lexer and returns the currently stored lexeme. If there is none, it is read from buffer, matching against the lexeme templates in the lexer setup. Empty lexemes, i.e., comments and whitespace, are discarded and the buffer is read again until we have found a nonempty lexeme (which may also be EOF or an error condition).

The initial state of the lexer contains an empty lexeme, so reading from buffer is forced. The empty state is restored after returning the lexeme. A nonempty lexeme is present in the lexer only if `lex_back` has been executed before.

The workspace is the `lexer%buffer`, treated as a sort of input stream. We chop off lexemes from the beginning, adjusting the buffer to the left. Whenever the buffer is empty, or we are matching against an open quote which has not terminated, we read a new line and append it to the right. This may result in special conditions, which for simplicity are also returned as lexemes: I/O error, buffer overflow, end of file. If the latter happens during reading a quoted string, we return an unmatched-quote lexeme. Obviously, the special-condition lexemes have to be caught by the parser.

Note that reading further lines is only necessary when reading a quoted string. Otherwise, the line-feed that ends each line is interpreted as whitespace which terminates a preceding lexeme, so there are no other valid multiline lexemes.

To enable meaningful error messages, we also keep track of the line number of the last line read, and the beginning and the end of the current lexeme with respect to this line.

The lexer is implemented as a function that returns the next lexeme (i.e., token). It uses the `lexer` setup and modifies the buffers and pointers stored within the lexer, a side effect. The lexer reads from an input stream object, which also is modified by this reading, e.g., a line pointer is advanced.

```

<Lexer: public>+≡
  public :: lex

<Lexer: procedures>+≡
  subroutine lex (lexeme, lexer)
    type(lexeme_t), intent(out) :: lexeme
    type(lexer_t), intent(inout) :: lexer
    integer :: iostat1, iostat2
    integer :: pos
    integer, dimension(2) :: range
    integer :: template_index, type
    if (.not. associated (lexer%stream)) &
      call msg_bug ("Lexer called without assigned stream")
    GET_LEXEME: do while (lexeme_get_type (lexer%lexeme) == EMPTY)
      if (len (lexer%buffer) /= 0) then
        iostat1 = 0

```

```

else
  call lexer_read_line (lexer, iostat1)
end if
select case (iostat1)
case (0)
  MATCH_BUFFER: do
    call match (lexer%setup%tt, char (lexer%buffer), &
               pos, range, template_index)
    if (pos >= 0) then
      type = lexer%setup%type(template_index)
      exit MATCH_BUFFER
    else
      pos = 0
      call lexer_read_line (lexer, iostat2)
      select case (iostat2)
      case (EOF); type = UNMATCHED_QUOTE; exit MATCH_BUFFER
      case (1);   type = IO_ERROR;       exit MATCH_BUFFER
      case (2);   type = OVERFLOW;       exit MATCH_BUFFER
      end select
    end if
  end do MATCH_BUFFER
case (EOF); type = EOF
case (1);   type = IO_ERROR
case (2);   type = OVERFLOW
end select
call lexeme_set (lexer%lexeme, lexer%setup%keyword_list, &
                 extract (lexer%buffer, finish=pos), range, type, &
                 lexer%setup%keyword_case)
lexer%buffer = remove (lexer%buffer, finish=pos)
lexer%previous_column = lexer%current_column
lexer%current_column = lexer%current_column + pos
end do GET_LEXEME
lexeme = lexer%lexeme
call lexeme_clear (lexer%lexeme)
end subroutine lex

```

Read a line and append it to the input buffer. If the input buffer overflows, return `iostat=2`. Otherwise, `iostat=1` indicates an I/O error, and `iostat=-1` the EOF.

The input stream may either be an external unit or a `ifile` object. In the latter case, a line is read and the line pointer is advanced.

Note that inserting LF between input lines is the Unix convention. Since we are doing this explicitly when gluing lines together, we can pattern-match against LF without having to worry about the system.

(Lexer: procedures)+≡

```

subroutine lexer_read_line (lexer, iostat)
  type(lexer_t), intent(inout) :: lexer
  integer, intent(out) :: iostat
  type(string_t) :: current_line
  current_line = lexer%current_line
  call stream_get_record (lexer%stream, lexer%current_line, iostat)
  if (iostat == 0) then
    lexer%lines_read = lexer%lines_read + 1
  end if
end subroutine lexer_read_line

```

```

        lexer%previous_line2 = lexer%previous_line1
        lexer%previous_line1 = current_line
        lexer%buffer = lexer%buffer // lexer%current_line // LF
        lexer%previous_column = 0
        lexer%current_column = 0
    end if
end subroutine lexer_read_line

```

Once in a while we have read one lexeme to many, which can be pushed back into the input stream. Do not do this more than once.

```

<Lexer: public>+≡
    public :: lexer_put_back

<Lexer: procedures>+≡
    subroutine lexer_put_back (lexer, lexeme)
        type(lexer_t), intent(inout) :: lexer
        type(lexeme_t), intent(in) :: lexeme
        if (lexeme_get_type (lexer%lexeme) == EMPTY) then
            lexer%lexeme = lexeme
        else
            call msg_bug (" Lexer: lex_back fails; probably called twice")
        end if
    end subroutine lexer_put_back

```

7.2.8 Diagnostics

For debugging: print just the setup

```

<Lexer: public>+≡
    public :: lexer_write_setup

<Lexer: procedures>+≡
    subroutine lexer_write_setup (lexer, unit)
        type(lexer_t), intent(in) :: lexer
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call lexer_setup_write (lexer%setup, u)
    end subroutine lexer_write_setup

```

This is useful for error printing: show the current line with index and a pointer to the current column within the line.

```

<Lexer: public>+≡
    public :: lexer_show_location

<Lexer: procedures>+≡
    subroutine lexer_show_location (lexer)
        type(lexer_t), intent(in) :: lexer
        type(string_t) :: loc_str
        if (associated (lexer%parent)) then
            call lexer_show_source (lexer%parent)
            call msg_message ("[includes]")
        else

```



```

        call msg_message ()
    end if
    if (associated (lexer%stream)) then
        call msg_message &
            (char (stream_get_record_info_string (lexer%stream)) // ":")
    end if
    if (lexer%lines_read >= 4) call msg_result ("[...]")
    if (lexer%lines_read >= 3) call msg_result (char (lexer%previous_line2))
    if (lexer%lines_read >= 2) call msg_result (char (lexer%previous_line1))
    if (lexer%lines_read >= 1) then
        call msg_result (char (lexer%current_line))
        loc_str = repeat (" ", lexer%previous_column)
        loc_str = loc_str // "^"
        if (lexer%current_column > lexer%previous_column) then
            loc_str = loc_str &
                // repeat ("-", max (lexer%current_column &
                    - lexer%previous_column - 1, 0)) &
                // "^"
        end if
        call msg_result (char (loc_str))
    end if
end subroutine lexer_show_location

```

This just prints the current stream source.

<Lexer: procedures>+≡

```

recursive subroutine lexer_show_source (lexer)
    type(lexer_t), intent(in) :: lexer
    if (associated (lexer%parent)) then
        call lexer_show_source (lexer%parent)
        call msg_message ("[includes]")
    else
        call msg_message ()
    end if
    if (associated (lexer%stream)) then
        call msg_message &
            (char (stream_get_source_info_string (lexer%stream)) // ":")
    end if
end subroutine lexer_show_source

```

7.2.9 Unit tests

Test module, followed by the corresponding implementation module.

<lexers_ut.f90>≡

<File header>

```

module lexers_ut
    use unit_tests
    use lexers_uti

```

<Standard module head>

<Lexer: public test>

```

contains

  <Lexer: test driver>

  end module lexers_ut

<lexers_uti.f90>≡
  <File header>

  module lexers_uti

    <Use strings>

    use lexers

    <Standard module head>

    <Lexer: test declarations>

    contains

    <Lexer: tests>

    end module lexers_uti
API: driver for the unit tests below.
<Lexer: public test>≡
  public :: lexer_test
<Lexer: test driver>≡
  subroutine lexer_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Lexer: execute tests>
  end subroutine lexer_test

```

Test the lexer by lexing and printing all lexemes from unit `u`, one per line, using preset conventions.

```

<Lexer: execute tests>≡
  call test (lexer_1, "lexer_1", &
    "check lexer", u, results)

<Lexer: test declarations>≡
  public :: lexer_1

<Lexer: tests>≡
  subroutine lexer_1 (u)
    integer, intent(in) :: u
    type(lexer_t), target :: lexer
    type(stream_t), target :: stream
    type(string_t) :: string
    type(lexeme_t) :: lexeme
    string = "abcdefghij"
    call lexer_init (lexer, &
      comment_chars = "", &

```

```

        quote_chars = "<'\"", &
        quote_match = ">'\"", &
        single_chars = "?*+|=,()", &
        special_class = ["."], &
        keyword_list = null ()
    call stream_init (stream, string)
    call lexer_assign_stream (lexer, stream)
do
    call lex (lexeme, lexer)
    call lexeme_write (lexeme, u)
    if (lexeme_is_break (lexeme)) exit
end do
    call stream_final (stream)
    call lexer_final (lexer)
end subroutine lexer_1

```

7.3 Syntax rules

This module provides tools to handle syntax rules in an abstract way.

```
<syntax_rules.f90>≡  
  <File header>  
  
  module syntax_rules  
  
    <Use strings>  
    use io_units  
    use diagnostics  
    use system_defs, only: LCLETTERS, UCLETTERS, DIGITS  
    use ifiles, only: line_p, line_init, line_get_string_advance, line_final  
    use ifiles, only: ifile_t, ifile_get_length  
    use lexers  
  
    <Standard module head>  
  
    <Syntax: public>  
  
    <Syntax: parameters>  
  
    <Syntax: types>  
  
    <Syntax: interfaces>  
  
    contains  
  
    <Syntax: subroutines>  
  
  end module syntax_rules
```

7.3.1 Syntax rules

Syntax rules are used by the parser. They determine how to translate the stream of lexemes as returned by the lexer into the parse tree node. A rule may be terminal, i.e., replace a matching lexeme into a terminal node. The node will contain the lexeme interpreted as a recognized token:

- a keyword: unquoted fixed character string;
- a real number, to be determined at runtime;
- an integer, to be determined at runtime;
- a boolean value, to be determined at runtime;
- a quoted token (e.g., string), to be determined at runtime;
- an identifier (unquoted string that is not a recognized keyword), to be determined at runtime.

It may be nonterminal, i.e., contain a sequence of child rules. These are matched consecutively (and recursively) against the input stream; the resulting node will be a branch node.

- the file, i.e., the input stream as a whole;
- a sequence of syntax elements, where the last syntax element may be optional, or optional repetitive;

Sequences carry a flag that tells whether the last child is optional or may be repeated an arbitrary number of times, corresponding to the regexp modifiers `?`, `*`, and `+`.

We also need an alternative rule; this will be replaced by the node generated by one of its children that matches; thus, it does not create a node of its own.

- an alternative of syntax elements.

We also define special types of sequences as convenience macros:

- a list: a sequence where the elements are separated by a separator keyword (e.g., commas), the separators are thrown away when parsing the list;
- a group: a sequence of three tokens, where the first and third ones are left and right delimiters, the delimiters are thrown away;
- an argument list: a delimited list, containing both delimiters and separators.

It would be great to have a polymorphic type for this purpose, but until Fortran 2003 is out we have to emulate this.

Here are the syntax element codes:

```

<Syntax: public>≡
  public :: S_UNKNOWN
  public :: S_LOGICAL, S_INTEGER, S_REAL, S_COMPLEX, S_QUOTED
  public :: S_IDENTIFIER, S_KEYWORD
  public :: S_SEQUENCE, S_LIST, S_GROUP, S_ARGS
  public :: S_ALTERNATIVE
  public :: S_IGNORE

<Syntax: parameters>≡
  integer, parameter :: &
    S_UNKNOWN = 0, &
    S_LOGICAL = 1, S_INTEGER = 2, S_REAL = 3, S_COMPLEX = 4, &
    S_QUOTED = 5, S_IDENTIFIER = 6, S_KEYWORD = 7, &
    S_SEQUENCE = 8, S_LIST = 9, S_GROUP = 10, S_ARGS = 11, &
    S_ALTERNATIVE = 12, &
    S_IGNORE = 99

```

We need arrays of rule pointers, therefore this construct.

```

<Syntax: types>≡
  type :: rule_p
  private
    type(syntax_rule_t), pointer :: p => null ()
  end type rule_p

```

Return the association status of the rule pointer:

```

<Syntax: subroutines>≡
  elemental function rule_is_associated (rp) result (ok)
    logical :: ok
    type (rule_p), intent(in) :: rp
    ok = associated (rp%p)
  end function rule_is_associated

```

The rule type is one of the types listed above, represented by an integer code. The keyword, for a non-keyword rule, is an identifier used for the printed syntax table. The array of children is needed for nonterminal rules. In that case, there is a modifier for the last element (blank, "?", "*", or "+"), mirrored in the flags `opt` and `rep`. Then, we have the character constants used as separators and delimiters for this rule. Finally, the `used` flag can be set to indicate that this rule is the child of another rule.

```

<Syntax: types>+≡
  public :: syntax_rule_t

<Syntax: types>+≡
  type :: syntax_rule_t
    private
    integer :: type = S_UNKNOWN
    logical :: used = .false.
    type(string_t) :: keyword
    type(string_t) :: separator
    type(string_t), dimension(2) :: delimiter
    type(rule_p), dimension(:), allocatable :: child
    character(1) :: modifier = ""
    logical :: opt = .false., rep = .false.
  contains
    <Syntax: syntax rule: TBP>
  end type syntax_rule_t

```

Initializer: Set type and key for a rule, but do not (yet) allocate anything.

Finalizer: not needed (no pointer components).

```

<Syntax: subroutines>+≡
  subroutine syntax_rule_init (rule, key, type)
    type(syntax_rule_t), intent(inout) :: rule
    type(string_t), intent(in) :: key
    integer, intent(in) :: type
    rule%keyword = key
    rule%type = type
    select case (rule%type)
    case (S_GROUP)
      call syntax_rule_set_delimiter (rule)
    case (S_LIST)
      call syntax_rule_set_separator (rule)
    case (S_ARGS)
      call syntax_rule_set_delimiter (rule)
      call syntax_rule_set_separator (rule)
    end select
  end subroutine syntax_rule_init

```

These characters will not be enclosed in quotes when writing syntax rules:

```
<Syntax: parameters>+≡
    character(*), parameter :: &
        UNQUOTED = "(),|_//LCLETTERS//UCLETTERS//DIGITS"
```

7.3.2 I/O

Write an account of the rule. Setting `short` true will suppress the node type. Setting `key_only` true will suppress the definition. Setting `advance` false will suppress the trailing newline.

```
<Syntax: public>+≡
    public :: syntax_rule_write

<Syntax: syntax rule: TBP>≡
    procedure :: write => syntax_rule_write

<Syntax: subroutines>+≡
    subroutine syntax_rule_write (rule, unit, short, key_only, advance)
        class(syntax_rule_t), intent(in) :: rule
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: short, key_only, advance
        logical :: typ, def, adv
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        typ = .true.; if (present (short)) typ = .not. short
        def = .true.; if (present (key_only)) def = .not. key_only
        adv = .true.; if (present (advance)) adv = advance
        select case (rule%type)
        case (S_UNKNOWN); call write_atom ("???", typ)
        case (S_IGNORE); call write_atom ("IGNORE", typ)
        case (S_LOGICAL); call write_atom ("LOGICAL", typ)
        case (S_INTEGER); call write_atom ("INTEGER", typ)
        case (S_REAL); call write_atom ("REAL", typ)
        case (S_COMPLEX); call write_atom ("COMPLEX", typ)
        case (S_IDENTIFIER); call write_atom ("IDENTIFIER", typ)
        case (S_KEYWORD); call write_atom ("KEYWORD", typ)
        case (S_QUOTED)
            call write_quotes (typ, def, &
                del = rule%delimiter)
        case (S_SEQUENCE)
            call write_sequence ("SEQUENCE", typ, def, size (rule%child))
        case (S_GROUP)
            call write_sequence ("GROUP", typ, def, size (rule%child), &
                del = rule%delimiter)
        case (S_LIST)
            call write_sequence ("LIST", typ, def, size (rule%child), &
                sep = rule%separator)
        case (S_ARGS)
            call write_sequence ("ARGUMENTS", typ, def, size (rule%child), &
                del = rule%delimiter, &
                sep = rule%separator)
        case (S_ALTERNATIVE)
            call write_sequence ("ALTERNATIVE", typ, def, size (rule%child), &
                sep = var_str ("|"))
```

```

end select
if (adv) write (u, *)
contains
subroutine write_type (type)
  character(*), intent(in) :: type
  character(11) :: str
  str = type
  write (u, "(1x,A)", advance="no") str
end subroutine write_type
subroutine write_key
  write (u, "(1x,A)", advance="no") char (wkey (rule))
end subroutine write_key
subroutine write_atom (type, typ)
  character(*), intent(in) :: type
  logical, intent(in) :: typ
  if (typ) call write_type (type)
  call write_key
end subroutine write_atom
subroutine write_maybe_quoted (string)
  character(*), intent(in) :: string
  character, parameter :: q = '"'
  character, parameter :: qq = '''
  if (verify (string, UNQUOTED) == 0) then
    write (u, "(1x,A)", advance = "no") trim (string)
  else if (verify (string, q) == 0) then
    write (u, "(1x,A)", advance = "no") qq // trim (string) // qq
  else
    write (u, "(1x,A)", advance = "no") q // trim (string) // q
  end if
end subroutine write_maybe_quoted
subroutine write_quotes (typ, def, del)
  logical, intent(in) :: typ, def
  type(string_t), dimension(2), intent(in) :: del
  if (typ) call write_type ("QUOTED")
  call write_key
  if (def) then
    write (u, "(1x,'=')", advance="no")
    call write_maybe_quoted (char (del(1)))
    write (u, "(1x,A)", advance="no") "... "
    call write_maybe_quoted (char (del(2)))
  end if
end subroutine write_quotes
subroutine write_sequence (type, typ, def, n, del, sep)
  character(*), intent(in) :: type
  logical, intent(in) :: typ, def
  integer, intent(in) :: n
  type(string_t), dimension(2), intent(in), optional :: del
  type(string_t), intent(in), optional :: sep
  integer :: i
  if (typ) call write_type (type)
  call write_key
  if (def) then
    write (u, "(1x,'=')", advance="no")
    if (present (del)) call write_maybe_quoted (char (del(1)))

```



```

do i = 1, n
  if (i > 1 .and. present (sep)) &
    call write_maybe_quoted (char (sep))
  write (u, "(1x,A)", advance="no") &
    char (wkey (syntax_rule_get_sub_ptr(rule, i)))
  if (i == n) write (u, "(A)", advance="no") trim (rule%modifier)
end do
if (present (del)) call write_maybe_quoted (char (del(2)))
end if
end subroutine write_sequence
end subroutine syntax_rule_write

```

In the printed representation, the keyword strings are enclosed as <...>, unless they are bare keywords. Bare keywords are enclosed as '...' if they contain a character which is not a letter, digit, or underscore. If they contain a single-quote character, they are enclosed as "...". (A keyword must not contain both single- and double-quotes.)

```

<Syntax: subroutines>+≡
function wkey (rule) result (string)
  type(string_t) :: string
  type(syntax_rule_t), intent(in) :: rule
  select case (rule%type)
  case (S_KEYWORD)
    if (verify (rule%keyword, UNQUOTED) == 0) then
      string = rule%keyword
    else if (scan (rule%keyword, "'") == 0) then
      string = "'" // rule%keyword // "'"
    else
      string = '"' // rule%keyword // '"'
    end if
  case default
    string = "<" // rule%keyword // ">"
  end select
end function wkey

```

7.3.3 Completing syntax rules

Set the separator and delimiter entries, using defaults:

```

<Syntax: subroutines>+≡
subroutine syntax_rule_set_separator (rule, separator)
  type(syntax_rule_t), intent(inout) :: rule
  type(string_t), intent(in), optional :: separator
  if (present (separator)) then
    rule%separator = separator
  else
    rule%separator = ","
  end if
end subroutine syntax_rule_set_separator

subroutine syntax_rule_set_delimiter (rule, delimiter)
  type(syntax_rule_t), intent(inout) :: rule

```

```

type(string_t), dimension(2), intent(in), optional :: delimiter
if (present (delimiter)) then
    rule%delimiter = delimiter
else
    rule%delimiter(1) = "("
    rule%delimiter(2) = ")"
end if
end subroutine syntax_rule_set_delimiter

```

Set the modifier entry and corresponding flags:

(Syntax: subroutines) +=

```

function is_modifier (string) result (ok)
    logical :: ok
    type(string_t), intent(in) :: string
    select case (char (string))
    case (" ", "?", "*", "+"); ok = .true.
    case default; ok = .false.
    end select
end function is_modifier

subroutine syntax_rule_set_modifier (rule, modifier)
    type(syntax_rule_t), intent(inout) :: rule
    type(string_t), intent(in) :: modifier
    rule%modifier = char (modifier)
    select case (rule%modifier)
    case (" ")
    case ("?"); rule%opt = .true.
    case ("*"); rule%opt = .true.; rule%rep = .true.
    case ("+"); rule%rep = .true.
    case default
        call msg_bug (" Syntax: sequence modifier '" // rule%modifier &
            // "' is not one of '+' '*' '?'")
    end select
end subroutine syntax_rule_set_modifier

```

Check a finalized rule for completeness

(Syntax: subroutines) +=

```

subroutine syntax_rule_check (rule)
    type(syntax_rule_t), intent(in) :: rule
    if (rule%keyword == "") call msg_bug ("Rule key not set")
    select case (rule%type)
    case (S_UNKNOWN); call bug (" Undefined rule")
    case (S_IGNORE, S_LOGICAL, S_INTEGER, S_REAL, S_COMPLEX, &
        S_IDENTIFIER, S_KEYWORD)
    case (S_QUOTED)
        if (rule%delimiter(1) == "" .or. rule%delimiter(2) == "") &
            call bug (" Missing quote character(s)")
    case (S_SEQUENCE)
    case (S_GROUP)
        if (rule%delimiter(1) == "" .or. rule%delimiter(2) == "") &
            call bug (" Missing delimiter(s)")
    case (S_LIST)
        if (rule%separator == "") call bug (" Missing separator")
    end select
end subroutine syntax_rule_check

```

```

case (S_ARGS)
  if (rule%delimiter(1) == "" .or. rule%delimiter(2) == "") &
    call bug (" Missing delimiter(s)")
  if (rule%separator == "") call bug (" Missing separator")
case (S_ALTERNATIVE)
case default
  call bug (" Undefined syntax code")
end select
select case (rule%type)
case (S_SEQUENCE, S_GROUP, S_LIST, S_ARGS, S_ALTERNATIVE)
  if (allocated (rule%child)) then
    if (.not.all (rule_is_associated (rule%child))) &
      call bug (" Child rules not all associated")
  else
    call bug (" Parent rule without children")
  end if
case default
  if (allocated (rule%child)) call bug (" Non-parent rule with children")
end select
contains
subroutine bug (string)
  character(*), intent(in) :: string
  call msg_bug (" Syntax table: Rule " // char (rule%keyword) // ": " &
    // string)
end subroutine bug
end subroutine syntax_rule_check

```

7.3.4 Accessing rules

This is the API for syntax rules:

```

<Syntax: public>+≡
public :: syntax_rule_get_type

<Syntax: subroutines>+≡
function syntax_rule_get_type (rule) result (type)
  integer :: type
  type(syntax_rule_t), intent(in) :: rule
  type = rule%type
end function syntax_rule_get_type

<Syntax: public>+≡
public :: syntax_rule_get_key

<Syntax: syntax rule: TBP>+≡
procedure :: get_key => syntax_rule_get_key

<Syntax: subroutines>+≡
function syntax_rule_get_key (rule) result (key)
  class(syntax_rule_t), intent(in) :: rule
  type(string_t) :: key
  key = rule%keyword
end function syntax_rule_get_key

```

```

<Syntax: public>+≡
    public :: syntax_rule_get_separator
    public :: syntax_rule_get_delimiter

<Syntax: subroutines>+≡
    function syntax_rule_get_separator (rule) result (separator)
        type(string_t) :: separator
        type(syntax_rule_t), intent(in) :: rule
        separator = rule%separator
    end function syntax_rule_get_separator

    function syntax_rule_get_delimiter (rule) result (delimiter)
        type(string_t), dimension(2) :: delimiter
        type(syntax_rule_t), intent(in) :: rule
        delimiter = rule%delimiter
    end function syntax_rule_get_delimiter

```

Accessing child rules. If we use `syntax_rule_get_n_sub` for determining loop bounds, we do not need a check in the second routine.

```

<Syntax: public>+≡
    public :: syntax_rule_get_n_sub
    public :: syntax_rule_get_sub_ptr

<Syntax: subroutines>+≡
    function syntax_rule_get_n_sub (rule) result (n)
        integer :: n
        type(syntax_rule_t), intent(in) :: rule
        if (allocated (rule%child)) then
            n = size (rule%child)
        else
            n = 0
        end if
    end function syntax_rule_get_n_sub

    function syntax_rule_get_sub_ptr (rule, i) result (sub)
        type(syntax_rule_t), pointer :: sub
        type(syntax_rule_t), intent(in), target :: rule
        integer, intent(in) :: i
        sub => rule%child(i)%p
    end function syntax_rule_get_sub_ptr

    subroutine syntax_rule_set_sub (rule, i, sub)
        type(syntax_rule_t), intent(inout) :: rule
        integer, intent(in) :: i
        type(syntax_rule_t), intent(in), target :: sub
        rule%child(i)%p => sub
    end subroutine syntax_rule_set_sub

```

Return the modifier flags:

```

<Syntax: public>+≡
    public :: syntax_rule_last_optional
    public :: syntax_rule_last_repetitive

```

```

<Syntax: subroutines>+≡
function syntax_rule_last_optional (rule) result (opt)
  logical :: opt
  type(syntax_rule_t), intent(in) :: rule
  opt = rule%opt
end function syntax_rule_last_optional
function syntax_rule_last_repetitive (rule) result (rep)
  logical :: rep
  type(syntax_rule_t), intent(in) :: rule
  rep = rule%rep
end function syntax_rule_last_repetitive

```

Return true if the rule is atomic, i.e., logical, real, keyword etc.

```

<Syntax: public>+≡
public :: syntax_rule_is_atomic

<Syntax: subroutines>+≡
function syntax_rule_is_atomic (rule) result (atomic)
  logical :: atomic
  type(syntax_rule_t), intent(in) :: rule
  select case (rule%type)
    case (S_LOGICAL, S_INTEGER, S_REAL, S_COMPLEX, S_IDENTIFIER, &
          S_KEYWORD, S_QUOTED)
      atomic = .true.
    case default
      atomic = .false.
  end select
end function syntax_rule_is_atomic

```

7.3.5 Syntax tables

A syntax table contains the tree of syntax rules and, for direct parser access, the list of valid keywords.

Types

The syntax contains an array of rules and a list of keywords. The array is actually used as a tree, where the top rule is the first array element, and the other rules are recursively pointed to by this first rule. (No rule should be used twice or be unused.) The keyword list is derived from the rule tree.

Objects of this type need the target attribute if they are associated with a lexer. The keyword list will be pointed to by this lexer.

```

<Syntax: public>+≡
public :: syntax_t

<Syntax: types>+≡
type :: syntax_t
private
  type(syntax_rule_t), dimension(:), allocatable :: rule
  type(keyword_list_t) :: keyword_list
end type syntax_t

```

Constructor/destructor

Initialize and finalize syntax tables

```
<Syntax: public>+≡  
public :: syntax_init  
public :: syntax_final
```

There are two ways to create a syntax: hard-coded from rules or dynamically from file.

```
<Syntax: interfaces>≡  
interface syntax_init  
  module procedure syntax_init_from_ifile  
end interface
```

The syntax definition is read from an ifile object which contains the syntax definitions in textual form, one rule per line. This interface allows for determining the number of rules beforehand.

To parse the rule definitions, we make up a temporary lexer. Obviously, we cannot use a generic parser yet, so we have to hardcode the parsing process.

```
<Syntax: subroutines>+≡  
subroutine syntax_init_from_ifile (syntax, ifile)  
  type(syntax_t), intent(out), target :: syntax  
  type(ifile_t), intent(in) :: ifile  
  type(lexer_t) :: lexer  
  type(line_p) :: line  
  type(string_t) :: string  
  integer :: n_token  
  integer :: i  
  call lexer_init (lexer, &  
    comment_chars = "", &  
    quote_chars = "<'\"", &  
    quote_match = ">'\"", &  
    single_chars = "?*+=,()", &  
    special_class = ["."], &  
    keyword_list = null ())  
  allocate (syntax%rule (ifile_get_length (ifile)))  
  call line_init (line, ifile)  
  do i = 1, size (syntax%rule)  
    string = line_get_string_advance (line)  
    call set_rule_type_and_key (syntax%rule(i), string, lexer)  
  end do  
  call line_init (line, ifile)  
  do i = 1, size (syntax%rule)  
    string = line_get_string_advance (line)  
    select case (syntax%rule(i)%type)  
    case (S_QUOTED, S_SEQUENCE, S_GROUP, S_LIST, S_ARGS, S_ALTERNATIVE)  
      n_token = get_n_token (string, lexer)  
      call set_rule_contents &  
        (syntax%rule(i), syntax, n_token, string, lexer)  
    end select  
  end do  
  call line_final (line)  
  call lexer_final (lexer)  
  call syntax_make_keyword_list (syntax)
```

```

if (.not. all (syntax%rule%used)) then
  do i = 1, size (syntax%rule)
    if (.not. syntax%rule(i)%used) then
      call syntax_rule_write (syntax%rule(i), 6)
    end if
  end do
  call msg_bug (" Syntax table: unused rules")
end if
end subroutine syntax_init_from_ifile

```

For a given rule defined in the input, the first task is to determine its type and key. With these, we can initialize the rule in the table, postponing the association of children.

(Syntax: subroutines) +=

```

subroutine set_rule_type_and_key (rule, string, lexer)
  type(syntax_rule_t), intent(inout) :: rule
  type(string_t), intent(in) :: string
  type(lexer_t), intent(inout) :: lexer
  type(stream_t), target :: stream
  type(lexeme_t) :: lexeme
  type(string_t) :: key
  character(2) :: type
  call lexer_clear (lexer)
  call stream_init (stream, string)
  call lexer_assign_stream (lexer, stream)
  call lex (lexeme, lexer)
  type = lexeme_get_string (lexeme)
  call lex (lexeme, lexer)
  key = lexeme_get_contents (lexeme)
  call stream_final (stream)
  if (trim (key) /= "") then
    select case (type)
      case ("IG"); call syntax_rule_init (rule, key, S_IGNORE)
      case ("LO"); call syntax_rule_init (rule, key, S_LOGICAL)
      case ("IN"); call syntax_rule_init (rule, key, S_INTEGER)
      case ("RE"); call syntax_rule_init (rule, key, S_REAL)
      case ("CO"); call syntax_rule_init (rule, key, S_COMPLEX)
      case ("ID"); call syntax_rule_init (rule, key, S_IDENTIFIER)
      case ("KE"); call syntax_rule_init (rule, key, S_KEYWORD)
      case ("QU"); call syntax_rule_init (rule, key, S_QUOTED)
      case ("SE"); call syntax_rule_init (rule, key, S_SEQUENCE)
      case ("GR"); call syntax_rule_init (rule, key, S_GROUP)
      case ("LI"); call syntax_rule_init (rule, key, S_LIST)
      case ("AR"); call syntax_rule_init (rule, key, S_ARGS)
      case ("AL"); call syntax_rule_init (rule, key, S_ALTERNATIVE)
      case default
        call lexer_show_location (lexer)
        call msg_bug (" Syntax definition: unknown type '" // type // "'")
      end select
    else
      print *, char (string)
      call msg_bug (" Syntax definition: empty rule key")
    end if
  end if
end if

```

```
end subroutine set_rule_type_and_key
```

This function returns the number of tokens in an input line.

(Syntax: subroutines)+≡

```
function get_n_token (string, lexer) result (n)
  integer :: n
  type(string_t), intent(in) :: string
  type(lexer_t), intent(inout) :: lexer
  type(stream_t), target :: stream
  type(lexeme_t) :: lexeme
  integer :: i
  call lexer_clear (lexer)
  call stream_init (stream, string)
  call lexer_assign_stream (lexer, stream)
  i = 0
  do
    call lex (lexeme, lexer)
    if (lexeme_is_break (lexeme)) exit
    i = i + 1
  end do
  n = i
  call stream_final (stream)
end function get_n_token
```

This subroutine extracts the rule contents for an input line. There are three tasks: (1) determine the number of children, depending on the rule type; (2) find and set the separator and delimiter strings, if required; (3) scan the child rules, find them in the syntax table and associate the parent rule with them.

(Syntax: subroutines)+≡

```
subroutine set_rule_contents (rule, syntax, n_token, string, lexer)
  type(syntax_rule_t), intent(inout) :: rule
  type(syntax_t), intent(in), target :: syntax
  integer, intent(in) :: n_token
  type(string_t), intent(in) :: string
  type(lexer_t), intent(inout) :: lexer
  type(stream_t), target :: stream
  type(lexeme_t), dimension(n_token) :: lexeme
  integer :: i, n_children
  call lexer_clear (lexer)
  call stream_init (stream, string)
  call lexer_assign_stream (lexer, stream)
  do i = 1, n_token
    call lex (lexeme(i), lexer)
  end do
  call stream_final (stream)
  n_children = get_n_children ()
  call set_delimiters
  if (n_children > 1) call set_separator
  if (n_children > 0) call set_children
contains
  function get_n_children () result (n_children)
    integer :: n_children
    select case (rule%type)
```



```

case (S_QUOTED)
  if (n_token /= 6) call broken_rule (rule)
  n_children = 0
case (S_GROUP)
  if (n_token /= 6) call broken_rule (rule)
  n_children = 1
case (S_SEQUENCE)
  if (is_modifier (lexeme_get_string (lexeme(n_token)))) then
    if (n_token <= 4) call broken_rule (rule)
    call syntax_rule_set_modifier &
      (rule, lexeme_get_string (lexeme(n_token)))
    n_children = n_token - 4
  else
    if (n_token <= 3) call broken_rule (rule)
    n_children = n_token - 3
  end if
case (S_LIST)
  if (is_modifier (lexeme_get_string (lexeme(n_token)))) then
    if (n_token <= 4 .or. mod (n_token, 2) /= 1) &
      call broken_rule (rule)
    call syntax_rule_set_modifier &
      (rule, lexeme_get_string (lexeme(n_token)))
  else if (n_token <= 3 .or. mod (n_token, 2) /= 0) then
    call broken_rule (rule)
  end if
  n_children = (n_token - 2) / 2
case (S_ARGS)
  if (is_modifier (lexeme_get_string (lexeme(n_token-1)))) then
    if (n_token <= 6 .or. mod (n_token, 2) /= 1) &
      call broken_rule (rule)
    call syntax_rule_set_modifier &
      (rule, lexeme_get_string (lexeme(n_token-1)))
  else if (n_token <= 5 .or. mod (n_token, 2) /= 0) then
    call broken_rule (rule)
  end if
  n_children = (n_token - 4) / 2
case (S_ALTERNATIVE)
  if (n_token <= 3 .or. mod (n_token, 2) /= 0) call broken_rule (rule)
  n_children = (n_token - 2) / 2
end select
end function get_n_children
subroutine set_delimiters
  type(string_t), dimension(2) :: delimiter
  select case (rule%type)
  case (S_QUOTED, S_GROUP, S_ARGS)
    delimiter(1) = lexeme_get_contents (lexeme(4))
    delimiter(2) = lexeme_get_contents (lexeme(n_token))
    call syntax_rule_set_delimiter (rule, delimiter)
  end select
end subroutine set_delimiters
subroutine set_separator
  type(string_t) :: separator
  select case (rule%type)
  case (S_LIST)

```

```

        separator = lexeme_get_contents (lexeme(5))
        call syntax_rule_set_separator (rule, separator)
    case (S_ARGS)
        separator = lexeme_get_contents (lexeme(6))
        call syntax_rule_set_separator (rule, separator)
    end select
end subroutine set_separator
subroutine set_children
    allocate (rule%child(n_children))
    select case (rule%type)
    case (S_GROUP)
        call syntax_rule_set_sub (rule, 1, syntax_get_rule_ptr (syntax, &
            lexeme_get_contents (lexeme(5))))
    case (S_SEQUENCE)
        do i = 1, n_children
            call syntax_rule_set_sub (rule, i, syntax_get_rule_ptr (syntax, &
                lexeme_get_contents (lexeme(i+3))))
        end do
    case (S_LIST, S_ALTERNATIVE)
        do i = 1, n_children
            call syntax_rule_set_sub (rule, i, syntax_get_rule_ptr (syntax, &
                lexeme_get_contents (lexeme(2*i+2))))
        end do
    case (S_ARGS)
        do i = 1, n_children
            call syntax_rule_set_sub (rule, i, syntax_get_rule_ptr (syntax, &
                lexeme_get_contents (lexeme(2*i+3))))
        end do
    end select
end subroutine set_children
subroutine broken_rule (rule)
    type(syntax_rule_t), intent(in) :: rule
    call lexer_show_location (lexer)
    call msg_bug (" Syntax definition: broken rule '" &
        // char (wkey (rule)) // "'")
end subroutine broken_rule
end subroutine set_rule_contents

```

This routine completes the syntax table object. We assume that the rule array is set up. We associate the top rule with the first entry in the rule array and build up the keyword list.

The keyword list includes delimiters and separators. Filling it can only be done after all rules are set. We scan the rule tree. For each keyword that we find, we try to add it to the keyword list; the pointer to the last element is carried along with the recursive scanning. Before appending a keyword, we check whether it is already in the list.

<Syntax: subroutines>+≡

```

subroutine syntax_make_keyword_list (syntax)
    type(syntax_t), intent(inout), target :: syntax
    type(syntax_rule_t), pointer :: rule
    rule => syntax%rule(1)
    call rule_scan_rec (rule, syntax%keyword_list)
contains

```

```

recursive subroutine rule_scan_rec (rule, keyword_list)
  type(syntax_rule_t), pointer :: rule
  type(keyword_list_t), intent(inout) :: keyword_list
  integer :: i
  if (rule%used) return
  rule%used = .true.
  select case (rule%type)
  case (S_UNKNOWN)
    call msg_bug (" Syntax: rule tree contains undefined rule")
  case (S_KEYWORD)
    call keyword_list_add (keyword_list, rule%keyword)
  end select
  select case (rule%type)
  case (S_LIST, S_ARGS)
    call keyword_list_add (keyword_list, rule%separator)
  end select
  select case (rule%type)
  case (S_GROUP, S_ARGS)
    call keyword_list_add (keyword_list, rule%delimiter(1))
    call keyword_list_add (keyword_list, rule%delimiter(2))
  end select
  select case (rule%type)
  case (S_SEQUENCE, S_GROUP, S_LIST, S_ARGS, S_ALTERNATIVE)
    if (.not. allocated (rule%child)) &
      call msg_bug (" Syntax: Non-terminal rule without children")
  case default
    if (allocated (rule%child)) &
      call msg_bug (" Syntax: Terminal rule with children")
  end select
  if (allocated (rule%child)) then
    do i = 1, size (rule%child)
      call rule_scan_rec (rule%child(i)%p, keyword_list)
    end do
  end if
end subroutine rule_scan_rec
end subroutine syntax_make_keyword_list

```

The finalizer deallocates the rule pointer array and deletes the keyword list.

```

<Syntax: subroutines>+≡
subroutine syntax_final (syntax)
  type(syntax_t), intent(inout) :: syntax
  if (allocated (syntax%rule)) deallocate (syntax%rule)
  call keyword_list_final (syntax%keyword_list)
end subroutine syntax_final

```

7.3.6 Accessing the syntax table

Return a pointer to the top rule

```

<Syntax: public>+≡
public :: syntax_get_top_rule_ptr

```

```

<Syntax: subroutines>+≡
function syntax_get_top_rule_ptr (syntax) result (rule)
  type(syntax_rule_t), pointer :: rule
  type(syntax_t), intent(in), target :: syntax
  if (allocated (syntax%rule)) then
    rule => syntax%rule(1)
  else
    rule => null ()
  end if
end function syntax_get_top_rule_ptr

```

Assign the pointer to the rule associated with a given key (assumes that the rule array is allocated)

```

<Syntax: public>+≡
  public :: syntax_get_rule_ptr

<Syntax: subroutines>+≡
function syntax_get_rule_ptr (syntax, key) result (rule)
  type(syntax_rule_t), pointer :: rule
  type(syntax_t), intent(in), target :: syntax
  type(string_t), intent(in) :: key
  integer :: i
  do i = 1, size (syntax%rule)
    if (syntax%rule(i)%keyword == key) then
      rule => syntax%rule(i)
      return
    end if
  end do
  call msg_bug (" Syntax table: Rule " // char (key) // " not found")
end function syntax_get_rule_ptr

```

Return a pointer to the keyword list

```

<Syntax: public>+≡
  public :: syntax_get_keyword_list_ptr

<Syntax: subroutines>+≡
function syntax_get_keyword_list_ptr (syntax) result (keyword_list)
  type(keyword_list_t), pointer :: keyword_list
  type(syntax_t), intent(in), target :: syntax
  keyword_list => syntax%keyword_list
end function syntax_get_keyword_list_ptr

```

7.3.7 I/O

Write a readable representation of the syntax table

```

<Syntax: public>+≡
  public :: syntax_write

<Syntax: subroutines>+≡
subroutine syntax_write (syntax, unit)
  type(syntax_t), intent(in) :: syntax
  integer, intent(in), optional :: unit

```

```

integer :: u
integer :: i
u = given_output_unit (unit); if (u < 0) return
write (u, "(A)") "Syntax table:"
if (allocated (syntax%rule)) then
  do i = 1, size (syntax%rule)
    call syntax_rule_write (syntax%rule(i), u)
  end do
else
  write (u, "(1x,A)") "[not allocated]"
end if
call keyword_list_write (syntax%keyword_list, u)
end subroutine syntax_write

```

7.4 The parser

On a small scale, the parser interprets the string tokens returned by the lexer; they are interpreted as numbers, keywords and such and stored as a typed object. On a large scale, a text is read, parsed, and a syntax rule set is applied such that the tokens are stored as a parse tree. Syntax errors are spotted in this process, so the resulting parse tree is syntactically correct by definition.

```
<parser.f90>≡
  <File header>

  module parser

    <Use kinds>
    <Use strings>
    use io_units
    use format_defs, only: FMT_19
    use system_defs, only: DIGITS
    use diagnostics
    use md5
    use lexers
    use syntax_rules

    <Standard module head>

    <Parser: public>

    <Parser: types>

    <Parser: interfaces>

    contains

    <Parser: procedures>

  end module parser
```

7.4.1 The token type

Tokens are elements of the parsed input that carry a value: logical, integer, real, quoted string, (unquoted) identifier, or known keyword. Note that non-keyword tokens also have an abstract key attached to them.

This is an obvious candidate for polymorphism.

```
<Parser: types>≡
  type :: token_t
    private
    integer :: type = S_UNKNOWN
    logical, pointer :: lval => null ()
    integer, pointer :: ival => null ()
    real(default), pointer :: rval => null ()
    complex(default), pointer :: cval => null ()
    type(string_t), pointer :: sval => null ()
    type(string_t), pointer :: kval => null ()
```

```

        type(string_t), dimension(:), pointer :: quote => null ()
    end type token_t

```

Create a token from the lexeme returned by the lexer: Allocate storage and try to interpret the lexeme according to the type that is requested by the parser. For a keyword token, match the lexeme against the requested key. If successful, set the token type, value, and key. Otherwise, set the type to S_UNKNOWN.

(Parser: procedures)≡

```

subroutine token_init (token, lexeme, requested_type, key)
    type(token_t), intent(out) :: token
    type(lexeme_t), intent(in) :: lexeme
    integer, intent(in) :: requested_type
    type(string_t), intent(in) :: key
    integer :: type
    type = lexeme_get_type (lexeme)
    token%type = S_UNKNOWN
    select case (requested_type)
    case (S_LOGICAL)
        if (type == T_IDENTIFIER) call read_logical &
            (char (lexeme_get_string (lexeme)))
    case (S_INTEGER)
        if (type == T_NUMERIC) call read_integer &
            (char (lexeme_get_string (lexeme)))
    case (S_REAL)
        if (type == T_NUMERIC) call read_real &
            (char (lexeme_get_string (lexeme)))
    case (S_COMPLEX)
        if (type == T_NUMERIC) call read_complex &
            (char (lexeme_get_string (lexeme)))
    case (S_IDENTIFIER)
        if (type == T_IDENTIFIER) call read_identifier &
            (lexeme_get_string (lexeme))
    case (S_KEYWORD)
        if (type == T_KEYWORD) call check_keyword &
            (lexeme_get_string (lexeme), key)
    case (S_QUOTED)
        if (type == T_QUOTED) call read_quoted &
            (lexeme_get_contents (lexeme), lexeme_get_delimiters (lexeme))
    case default
        print *, requested_type
        call msg_bug (" Invalid token type code requested by the parser")
    end select
    if (token%type /= S_UNKNOWN) then
        allocate (token%kval)
        token%kval = key
    end if
contains
    subroutine read_logical (s)
        character(*), intent(in) :: s
        select case (s)
        case ("t", "T", "true", "TRUE", "y", "Y", "yes", "YES")
            allocate (token%lval)
            token%lval = .true.

```

```

        token%type = S_LOGICAL
    case ("f", "F", "false", "FALSE", "n", "N", "no", "NO")
        allocate (token%lval)
        token%lval = .false.
        token%type = S_LOGICAL
    end select
end subroutine read_logical
subroutine read_integer (s)
    character(*), intent(in) :: s
    integer :: tmp, iostat
    if (verify (s, DIGITS) == 0) then
        read (s, *, iostat=iostat) tmp
        if (iostat == 0) then
            allocate (token%ival)
            token%ival = tmp
            token%type = S_INTEGER
        end if
    end if
end subroutine read_integer
subroutine read_real (s)
    character(*), intent(in) :: s
    real(default) :: tmp
    integer :: iostat
    read (s, *, iostat=iostat) tmp
    if (iostat == 0) then
        allocate (token%rval)
        token%rval = tmp
        token%type = S_REAL
    end if
end subroutine read_real
subroutine read_complex (s)
    character(*), intent(in) :: s
    complex(default) :: tmp
    integer :: iostat
    read (s, *, iostat=iostat) tmp
    if (iostat == 0) then
        allocate (token%cval)
        token%cval = tmp
        token%type = S_COMPLEX
    end if
end subroutine read_complex
subroutine read_identifier (s)
    type(string_t), intent(in) :: s
    allocate (token%sval)
    token%sval = s
    token%type = S_IDENTIFIER
end subroutine read_identifier
subroutine check_keyword (s, key)
    type(string_t), intent(in) :: s
    type(string_t), intent(in) :: key
    if (key == s) token%type = S_KEYWORD
end subroutine check_keyword
subroutine read_quoted (s, del)
    type(string_t), intent(in) :: s

```



```

        type(string_t), dimension(2), intent(in) :: del
        allocate (token%sval, token%quote(2))
        token%sval = s
        token%quote(1) = del(1)
        token%quote(2) = del(2)
        token%type = S_QUOTED
    end subroutine read_quoted
end subroutine token_init

```

Manually set a token to a keyword.

```

<Parser: procedures>+≡
    subroutine token_init_key (token, key)
        type(token_t), intent(out) :: token
        type(string_t), intent(in) :: key
        token%type = S_KEYWORD
        allocate (token%kval)
        token%kval = key
    end subroutine token_init_key

```

Reset a token to an empty state, freeing allocated memory, and deallocate the token itself.

```

<Parser: procedures>+≡
    subroutine token_final (token)
        type(token_t), intent(inout) :: token
        token%type = S_UNKNOWN
        if (associated (token%lval)) deallocate (token%lval)
        if (associated (token%ival)) deallocate (token%ival)
        if (associated (token%rval)) deallocate (token%rval)
        if (associated (token%sval)) deallocate (token%sval)
        if (associated (token%kval)) deallocate (token%kval)
        if (associated (token%quote)) deallocate (token%quote)
    end subroutine token_final

```

Check for empty=valid token:

```

<Parser: procedures>+≡
    function token_is_valid (token) result (valid)
        logical :: valid
        type(token_t), intent(in) :: token
        valid = token%type /= S_UNKNOWN
    end function token_is_valid

```

Write the contents of a token.

```

<Parser: procedures>+≡
    subroutine token_write (token, unit)
        type(token_t), intent(in) :: token
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        select case (token%type)
        case (S_LOGICAL)
            write (u, "(L1)") token%lval
        case (S_INTEGER)

```

```

        write (u, "(I0)") token%ival
    case (S_REAL)
        write (u, "(" // FMT_19 // ")") token%rval
    case (S_COMPLEX)
        write (u, "('('," // FMT_19 // "',''," // FMT_19 // "',')')" token%cval
    case (S_IDENTIFIER)
        write (u, "(A)") char (token%sval)
    case (S_KEYWORD)
        write (u, "(A,A)" '[keyword]' // char (token%kval)
    case (S_QUOTED)
        write (u, "(A)" &
            char (token%quote(1)) // char (token%sval) // char (token%quote(2))
    case default
        write (u, "(A)" '[empty]'
    end select
end subroutine token_write

```

Token assignment via deep copy. This is useful to avoid confusion when the token is transferred to some parse-tree node.

```

(Parser: interfaces)≡
    interface assignment(=)
        module procedure token_assign
        module procedure token_assign_integer
        module procedure token_assign_real
        module procedure token_assign_complex
        module procedure token_assign_logical
        module procedure token_assign_string
    end interface

```

We need to copy only the contents that are actually assigned, the other pointers remain disassociated.

```

(Parser: procedures)+≡
    subroutine token_assign (token, token_in)
        type(token_t), intent(out) :: token
        type(token_t), intent(in) :: token_in
        token%type = token_in%type
        select case (token%type)
            case (S_LOGICAL);    allocate (token%lval); token%lval = token_in%lval
            case (S_INTEGER);    allocate (token%ival); token%ival = token_in%ival
            case (S_REAL);       allocate (token%rval); token%rval = token_in%rval
            case (S_COMPLEX);    allocate (token%cval); token%cval = token_in%cval
            case (S_IDENTIFIER); allocate (token%sval); token%sval = token_in%sval
            case (S_QUOTED);     allocate (token%sval); token%sval = token_in%sval
                                allocate (token%quote(2)); token%quote = token_in%quote
        end select
        if (token%type /= S_UNKNOWN) then
            allocate (token%kval); token%kval = token_in%kval
        end if
    end subroutine token_assign

```

We need to copy only the contents that are actually assigned, the other pointers remain disassociated.

```

(Parser: procedures)+≡
subroutine token_assign_integer (token, ival)
  type(token_t), intent(out) :: token
  integer, intent(in) :: ival
  token%type = S_INTEGER
  allocate (token%ival)
  token%ival = ival
end subroutine token_assign_integer

subroutine token_assign_real (token, rval)
  type(token_t), intent(out) :: token
  real(default), intent(in) :: rval
  token%type = S_REAL
  allocate (token%rval)
  token%rval = rval
end subroutine token_assign_real

subroutine token_assign_complex (token, cval)
  type(token_t), intent(out) :: token
  complex(default), intent(in) :: cval
  token%type = S_COMPLEX
  allocate (token%cval)
  token%cval = cval
end subroutine token_assign_complex

subroutine token_assign_logical (token, lval)
  type(token_t), intent(out) :: token
  logical, intent(in) :: lval
  token%type = S_LOGICAL
  allocate (token%lval)
  token%lval = lval
end subroutine token_assign_logical

subroutine token_assign_string (token, sval)
  type(token_t), intent(out) :: token
  type(string_t), intent(in) :: sval
  token%type = S_QUOTED
  allocate (token%sval)
  token%sval = sval
  allocate (token%quote(2)); token%quote = '''
end subroutine token_assign_string

```

7.4.2 Retrieve token contents

These functions all do a trivial sanity check that should avoid crashes.

```

(Parser: procedures)+≡
function token_get_logical (token) result (lval)
  logical :: lval
  type(token_t), intent(in) :: token
  if (associated (token%lval)) then
    lval = token%lval
  else

```

```

        call token_mismatch (token, "logical")
    end if
end function token_get_logical

function token_get_integer (token) result (ival)
    integer :: ival
    type(token_t), intent(in) :: token
    if (associated (token%ival)) then
        ival = token%ival
    else
        call token_mismatch (token, "integer")
    end if
end function token_get_integer

function token_get_real (token) result (rval)
    real(default) :: rval
    type(token_t), intent(in) :: token
    if (associated (token%rval)) then
        rval = token%rval
    else
        call token_mismatch (token, "real")
    end if
end function token_get_real

function token_get_cmplx (token) result (cval)
    complex(default) :: cval
    type(token_t), intent(in) :: token
    if (associated (token%cval)) then
        cval = token%cval
    else
        call token_mismatch (token, "complex")
    end if
end function token_get_cmplx

function token_get_string (token) result (sval)
    type(string_t) :: sval
    type(token_t), intent(in) :: token
    if (associated (token%sval)) then
        sval = token%sval
    else
        call token_mismatch (token, "string")
    end if
end function token_get_string

function token_get_key (token) result (kval)
    type(string_t) :: kval
    type(token_t), intent(in) :: token
    if (associated (token%kval)) then
        kval = token%kval
    else
        call token_mismatch (token, "keyword")
    end if
end function token_get_key

```

```

function token_get_quote (token) result (quote)
  type(string_t), dimension(2) :: quote
  type(token_t), intent(in) :: token
  if (associated (token%quote)) then
    quote = token%quote
  else
    call token_mismatch (token, "quote")
  end if
end function token_get_quote

```

```

(Parser: procedures)+≡
subroutine token_mismatch (token, type)
  type(token_t), intent(in) :: token
  character(*), intent(in) :: type
  write (6, "(A)", advance="no") "Token: "
  call token_write (token)
  call msg_bug (" Token type mismatch; value required as " // type)
end subroutine token_mismatch

```

7.4.3 The parse tree: nodes

The parser will generate a parse tree from the input stream. Each node in this parse tree points to the syntax rule that was applied. (Since syntax rules are stored in a pointer-type array within the syntax table, they qualify as targets.) A leaf node contains a token. A branch node has subnodes. The subnodes are stored as a list, so each node also has a `next` pointer.

```

(Parser: public)≡
public :: parse_node_t

(Parser: types)+≡
type :: parse_node_t
private
  type(syntax_rule_t), pointer :: rule => null ()
  type(token_t) :: token
  integer :: n_sub = 0
  type(parse_node_t), pointer :: sub_first => null ()
  type(parse_node_t), pointer :: sub_last => null ()
  type(parse_node_t), pointer :: next => null ()
contains
  (Parser: parse node: TBP)
end type parse_node_t

```

Container for parse node pointers, useful for creating pointer arrays:

```

(Parser: public)+≡
public :: parse_node_p

(Parser: types)+≡
type :: parse_node_p
  type(parse_node_t), pointer :: ptr => null ()
end type parse_node_p

```

Output. The first version writes a node together with its sub-node tree, organized by indentation.

```

(Parser: parse node: TBP)≡
    procedure :: write => parse_node_write_rec

(Parser: public)+≡
    public :: parse_node_write_rec

(Parser: procedures)+≡
    recursive subroutine parse_node_write_rec (node, unit, short, depth)
        class(parse_node_t), intent(in), target :: node
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: short
        integer, intent(in), optional :: depth
        integer :: u, d
        type(parse_node_t), pointer :: current
        u = given_output_unit (unit); if (u < 0) return
        d = 0; if (present (depth)) d = depth
        call parse_node_write (node, u, short=short)
        current => node%sub_first
        do while (associated (current))
            write (u, "(A)", advance = "no") repeat ("| ", d)
            call parse_node_write_rec (current, unit, short, d+1)
            current => current%next
        end do
    end subroutine parse_node_write_rec

```

This does the actual output for a single node, without recursion.

```

(Parser: public)+≡
    public :: parse_node_write

(Parser: procedures)+≡
    subroutine parse_node_write (node, unit, short)
        class(parse_node_t), intent(in) :: node
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: short
        integer :: u
        type(parse_node_t), pointer :: current
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(' + ')", advance = "no")
        if (associated (node%rule)) then
            call syntax_rule_write (node%rule, u, &
                short=short, key_only=.true., advance=.false.)
        if (token_is_valid (node%token)) then
            write (u, "(' = ')", advance="no")
            call token_write (node%token, u)
        else if (associated (node%sub_first)) then
            write (u, "(' = ')", advance="no")
            current => node%sub_first
            do while (associated (current))
                call syntax_rule_write (current%rule, u, &
                    short=.true., key_only=.true., advance=.false.)
                current => current%next
            end do
        write (u, *)
    end subroutine parse_node_write

```

```

        else
            write (u, *)
        end if
    else
        write (u, *) "[empty]"
    end if
end subroutine parse_node_write

```

Finalize the token and recursively finalize and deallocate all sub-nodes.

```

<Parser: public>+≡
    public :: parse_node_final

<Parser: procedures>+≡
    recursive subroutine parse_node_final (node, recursive)
        type(parse_node_t), intent(inout) :: node
        type(parse_node_t), pointer :: current
        logical, intent(in), optional :: recursive
        logical :: rec
        rec = .true.; if (present (recursive)) rec = recursive
        call token_final (node%token)
        if (rec) then
            do while (associated (node%sub_first))
                current => node%sub_first
                node%sub_first => node%sub_first%next
                call parse_node_final (current)
                deallocate (current)
            end do
        end if
    end subroutine parse_node_final

```

7.4.4 Filling nodes

The constructors allocate and initialize the node. There are two possible initializers (in a later version, should correspond to different type extensions).

First, leaf (terminal) nodes. The token constructor does the actual work, looking at the requested type and key for the given rule and matching against the lexeme contents. If it fails, the token will keep the type `S_UNKNOWN` and remain empty. Otherwise, we have a valid node which contains the new token.

If the lexeme argument is absent, the token is left empty.

```

<Parser: procedures>+≡
    subroutine parse_node_create_leaf (node, rule, lexeme)
        type(parse_node_t), pointer :: node
        type(syntax_rule_t), intent(in), target :: rule
        type(lexeme_t), intent(in) :: lexeme
        allocate (node)
        node%rule => rule
        call token_init (node%token, lexeme, &
            syntax_rule_get_type (rule), syntax_rule_get_key (rule))
        if (.not. token_is_valid (node%token)) deallocate (node)
    end subroutine parse_node_create_leaf

```

This version allows us to manually create a leaf node that holds a keyword.

```

(Parser: public)+≡
    public :: parse_node_create_key

(Parser: procedures)+≡
    subroutine parse_node_create_key (node, rule)
        type(parse_node_t), intent(out) :: node
        type(syntax_rule_t), intent(in), target :: rule
        node%rule => rule
        call token_init_key (node%token, syntax_rule_get_key (rule))
    end subroutine parse_node_create_key

```

This version allows us to manually create a leaf node that holds a fixed value.
Only one of the optional values should be provided.

```

(Parser: public)+≡
    public :: parse_node_create_value

(Parser: procedures)+≡
    subroutine parse_node_create_value (node, rule, ival, rval, cval, sval, lval)
        type(parse_node_t), intent(out) :: node
        type(syntax_rule_t), intent(in), target :: rule
        integer, intent(in), optional :: ival
        real(default), intent(in), optional :: rval
        complex(default), intent(in), optional :: cval
        type(string_t), intent(in), optional :: sval
        logical, intent(in), optional :: lval
        node%rule => rule
        call parse_node_set_value (node, ival, rval, cval, sval, lval)
    end subroutine parse_node_create_value

```

Directly set the value without changing anything else.

```

(Parser: public)+≡
    public :: parse_node_set_value

(Parser: procedures)+≡
    subroutine parse_node_set_value (node, ival, rval, cval, sval, lval)
        type(parse_node_t), intent(inout) :: node
        integer, intent(in), optional :: ival
        real(default), intent(in), optional :: rval
        complex(default), intent(in), optional :: cval
        type(string_t), intent(in), optional :: sval
        logical, intent(in), optional :: lval
        if (present (ival)) then
            node%token = ival
        else if (present (rval)) then
            node%token = rval
        else if (present (cval)) then
            node%token = cval
        else if (present (lval)) then
            node%token = lval
        else if (present (sval)) then
            node%token = sval
        end if
    end subroutine parse_node_set_value

```


Second, branch nodes. We first assign the rule:

```

(Parser: public)+≡
    public :: parse_node_create_branch

(Parser: procedures)+≡
    subroutine parse_node_create_branch (node, rule)
        type(parse_node_t), pointer :: node
        type(syntax_rule_t), intent(in), target :: rule
        allocate (node)
        node%rule => rule
    end subroutine parse_node_create_branch

```

Copy a node. This is a shallow copy. Note that we have to nullify the `next` pointer if we don't want to inherit the context of the original node.

```

(Parser: parse node: TBP)+≡
    procedure :: copy => parse_node_copy

(Parser: procedures)+≡
    subroutine parse_node_copy (node, copy)
        class(parse_node_t), intent(in) :: node
        type(parse_node_t), pointer, intent(out) :: copy
        allocate (copy)
        select type (node)
            type is (parse_node_t)
                copy = node
        end select
        copy%next => null ()
    end subroutine parse_node_copy

```

Append a sub-node. The sub-node must exist and be a valid target, otherwise nothing is done.

```

(Parser: public)+≡
    public :: parse_node_append_sub

(Parser: parse node: TBP)+≡
    procedure :: append_sub => parse_node_append_sub

(Parser: procedures)+≡
    subroutine parse_node_append_sub (node, sub)
        class(parse_node_t), intent(inout) :: node
        type(parse_node_t), pointer :: sub
        if (associated (sub)) then
            if (associated (node%sub_last)) then
                node%sub_last%next => sub
            else
                node%sub_first => sub
            end if
            node%sub_last => sub
        end if
    end subroutine parse_node_append_sub

```

For easy access, once the list is complete we count the number of sub-nodes. If there are no subnodes, the whole node is deleted.

```

(Parser: public)+≡
    public :: parse_node_freeze_branch

```

```

(Parser: procedures)+≡
subroutine parse_node_freeze_branch (node)
  type(parse_node_t), pointer :: node
  type(parse_node_t), pointer :: current
  node%n_sub = 0
  current => node%sub_first
  do while (associated (current))
    node%n_sub = node%n_sub + 1
    current => current%next
  end do
  if (node%n_sub == 0) deallocate (node)
end subroutine parse_node_freeze_branch

```

Replace the syntax rule. This makes sense only if the parse node adheres to the syntax of the new rule.

```

(Parser: public)+≡
public :: parse_node_replace_rule

(Parser: procedures)+≡
subroutine parse_node_replace_rule (node, rule)
  type(parse_node_t), pointer :: node
  type(syntax_rule_t), intent(in), target :: rule
  node%rule => rule
end subroutine parse_node_replace_rule

```

Replace the last subnode by the target node. Since the subnodes are stored as a linked list, we can do this only if we copy the subnodes. Furthermore, the target node must also be copied, and the `next` pointer of the copy is nullified. This ensures that we cannot modify the originals at the subnode level.

All copies are shallow copies. This implies that further modifications at the sub-subnode level will affect the original nodes and must therefore be forbidden.

Use with care, this invites to memory mismanagement. The copy nodes can be deallocated, but not finalized, since its subnodes are the same objects as the subnodes of the target node.

```

(Parser: public)+≡
public :: parse_node_replace_last_sub

(Parser: procedures)+≡
subroutine parse_node_replace_last_sub (node, pn_target)
  type(parse_node_t), intent(inout), target :: node
  type(parse_node_t), intent(in), target :: pn_target
  type(parse_node_t), pointer :: current, current_copy, previous
  integer :: i
  select case (node%n_sub)
  case (1)
    allocate (current_copy)
    current_copy = pn_target
    node%sub_first => current_copy
  case (2:)
    current => node%sub_first
    allocate (current_copy)
    current_copy = current
    node%sub_first => current_copy
  end select
end subroutine parse_node_replace_last_sub

```

```

previous => current_copy
do i = 1, node%n_sub - 2
  current => current%next
  allocate (current_copy)
  current_copy = current
  previous%next => current_copy
  previous => current_copy
end do
allocate (current_copy)
current_copy = pn_target
previous%next => current_copy
case default
  call parse_node_write (node)
  call msg_bug ("replace_last_sub' called for non-branch parse node")
end select
current_copy%next => null ()
node%sub_last => current_copy
end subroutine parse_node_replace_last_sub

```

7.4.5 Accessing nodes

Return the node contents. Check if pointers are associated. No check when accessing a sub-node; assume that `parse_node_n_sub` is always used for the upper bound.

The token extractor returns a pointer.

(Parser: public)+≡

```

public :: parse_node_get_rule_ptr
public :: parse_node_get_n_sub
public :: parse_node_get_sub_ptr
public :: parse_node_get_next_ptr
public :: parse_node_get_last_sub_ptr

```

(Parser: parse node: TBP)+≡

```

procedure :: get_rule_ptr => parse_node_get_rule_ptr
procedure :: get_n_sub => parse_node_get_n_sub
procedure :: get_sub_ptr => parse_node_get_sub_ptr
procedure :: get_next_ptr => parse_node_get_next_ptr

```

(Parser: procedures)+≡

```

function parse_node_get_rule_ptr (node) result (rule)
  class(parse_node_t), intent(in) :: node
  type(syntax_rule_t), pointer :: rule
  if (associated (node%rule)) then
    rule => node%rule
  else
    rule => null ()
    call parse_node_undefined (node, "rule")
  end if
end function parse_node_get_rule_ptr

function parse_node_get_n_sub (node) result (n)
  class(parse_node_t), intent(in) :: node
  integer :: n

```

```

n = node%n_sub
end function parse_node_get_n_sub

function parse_node_get_sub_ptr (node, n, tag, required) result (sub)
  class(parse_node_t), intent(in), target :: node
  type(parse_node_t), pointer :: sub
  integer, intent(in), optional :: n
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
  integer :: i
  sub => node%sub_first
  if (present (n)) then
    do i = 2, n
      if (associated (sub)) then
        sub => sub%next
      else
        return
      end if
    end do
  end if
  call parse_node_check (sub, tag, required)
end function parse_node_get_sub_ptr

function parse_node_get_next_ptr (sub, n, tag, required) result (next)
  class(parse_node_t), intent(in), target :: sub
  type(parse_node_t), pointer :: next
  integer, intent(in), optional :: n
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
  integer :: i
  next => sub%next
  if (present (n)) then
    do i = 2, n
      if (associated (next)) then
        next => next%next
      else
        exit
      end if
    end do
  end if
  call parse_node_check (next, tag, required)
end function parse_node_get_next_ptr

function parse_node_get_last_sub_ptr (node, tag, required) result (sub)
  type(parse_node_t), pointer :: sub
  type(parse_node_t), intent(in), target :: node
  character(*), intent(in), optional :: tag
  logical, intent(in), optional :: required
  sub => node%sub_last
  call parse_node_check (sub, tag, required)
end function parse_node_get_last_sub_ptr

```

(Parser: procedures) +=
 subroutine parse_node_undefined (node, obj)

```

    type(parse_node_t), intent(in) :: node
    character(*), intent(in) :: obj
    call parse_node_write (node, 6)
    call msg_bug (" Parse-tree node: " // obj // " requested, but undefined")
end subroutine parse_node_undefined

```

Check if a parse node has a particular tag, and if it is associated:

```

(Parser: public)+≡
    public :: parse_node_check

(Parser: procedures)+≡
    subroutine parse_node_check (node, tag, required)
        type(parse_node_t), pointer :: node
        character(*), intent(in), optional :: tag
        logical, intent(in), optional :: required
        if (associated (node)) then
            if (present (tag)) then
                if (parse_node_get_rule_key (node) /= tag) &
                    call parse_node_mismatch (tag, node)
            end if
        else
            if (present (required)) then
                if (required) &
                    call msg_bug (" Missing node, expected <" // tag // ">")
            end if
        end if
    end subroutine parse_node_check

```

This is called by a parse-tree scanner if the expected and the actual nodes do not match

```

(Parser: public)+≡
    public :: parse_node_mismatch

(Parser: procedures)+≡
    subroutine parse_node_mismatch (string, parse_node)
        character(*), intent(in) :: string
        type(parse_node_t), intent(in) :: parse_node
        call parse_node_write (parse_node)
        call msg_bug (" Syntax mismatch, expected <" // string // ">.")
    end subroutine parse_node_mismatch

```

The following functions are wrappers for extracting the token contents.

```

(Parser: public)+≡
    public :: parse_node_get_logical
    public :: parse_node_get_integer
    public :: parse_node_get_real
    public :: parse_node_get_cmplx
    public :: parse_node_get_string
    public :: parse_node_get_key
    public :: parse_node_get_rule_key

(Parser: parse node: TBP)+≡
    procedure :: get_logical => parse_node_get_logical

```

```

procedure :: get_integer => parse_node_get_integer
procedure :: get_real => parse_node_get_real
procedure :: get_cmplx => parse_node_get_cmplx
procedure :: get_string => parse_node_get_string
procedure :: get_key => parse_node_get_key
procedure :: get_rule_key => parse_node_get_rule_key

(Parser: procedures) +=
  function parse_node_get_logical (node) result (lval)
    class(parse_node_t), intent(in), target :: node
    logical :: lval
    lval = token_get_logical (parse_node_get_token_ptr (node))
  end function parse_node_get_logical

  function parse_node_get_integer (node) result (ival)
    class(parse_node_t), intent(in), target :: node
    integer :: ival
    ival = token_get_integer (parse_node_get_token_ptr (node))
  end function parse_node_get_integer

  function parse_node_get_real (node) result (rval)
    class(parse_node_t), intent(in), target :: node
    real(default) :: rval
    rval = token_get_real (parse_node_get_token_ptr (node))
  end function parse_node_get_real

  function parse_node_get_cmplx (node) result (cval)
    class(parse_node_t), intent(in), target :: node
    complex(default) :: cval
    cval = token_get_cmplx (parse_node_get_token_ptr (node))
  end function parse_node_get_cmplx

  function parse_node_get_string (node) result (sval)
    class(parse_node_t), intent(in), target :: node
    type(string_t) :: sval
    sval = token_get_string (parse_node_get_token_ptr (node))
  end function parse_node_get_string

  function parse_node_get_key (node) result (kval)
    class(parse_node_t), intent(in), target :: node
    type(string_t) :: kval
    kval = token_get_key (parse_node_get_token_ptr (node))
  end function parse_node_get_key

  function parse_node_get_rule_key (node) result (kval)
    class(parse_node_t), intent(in), target :: node
    type(string_t) :: kval
    kval = syntax_rule_get_key (parse_node_get_rule_ptr (node))
  end function parse_node_get_rule_key

  function parse_node_get_token_ptr (node) result (token)
    type(token_t), pointer :: token
    type(parse_node_t), intent(in), target :: node
    if (token_is_valid (node%token)) then
      token => node%token
    end if
  end function parse_node_get_token_ptr

```

```

    else
        call parse_node_undefined (node, "token")
    end if
end function parse_node_get_token_ptr

```

Return a MD5 sum for a parse node. The method is to write the node to a scratch file and to evaluate the MD5 sum of that file.

```

<Parser: public>+≡
    public :: parse_node_get_md5sum

<Parser: procedures>+≡
    function parse_node_get_md5sum (pn) result (md5sum_pn)
        character(32) :: md5sum_pn
        type(parse_node_t), intent(in) :: pn
        integer :: u
        u = free_unit ()
        open (unit = u, status = "scratch", action = "readwrite")
        call parse_node_write_rec (pn, unit=u)
        rewind (u)
        md5sum_pn = md5sum (u)
        close (u)
    end function parse_node_get_md5sum

```

7.4.6 The parse tree

The parse tree is a tree of nodes, where leaf nodes hold a valid token, while branch nodes point to a list of sub-nodes.

```

<Parser: public>+≡
    public :: parse_tree_t

<Parser: types>+≡
    type :: parse_tree_t
    private
        type(parse_node_t), pointer :: root_node => null ()
    contains
        <Parser: parse tree: TBP>
    end type parse_tree_t

```

The parser. Its arguments are the parse tree (which should be empty initially), the lexer (which should be already set up), the syntax table (which should be valid), and the input stream. The input stream is completely parsed, using the lexer setup and the syntax rules as given, and the parse tree is built accordingly.

If `check_eof` is absent or true, the parser will complain about trailing garbage. Otherwise, it will ignore it.

By default, the input stream is matched against the top rule in the specified syntax. If `key` is given, it is matched against the rule with the specified key instead.

Failure at the top level means that no rule could match at all; in this case the error message will show the top rule.

```

<Parser: public>+≡
    public :: parse_tree_init

```

```

<Parser: parse tree: TBP>≡
    procedure :: parse => parse_tree_init

<Parser: procedures>+≡
    subroutine parse_tree_init &
        (parse_tree, syntax, lexer, key, check_eof)
        class(parse_tree_t), intent(inout) :: parse_tree
        type(lexer_t), intent(inout) :: lexer
        type(syntax_t), intent(in), target :: syntax
        type(string_t), intent(in), optional :: key
        logical, intent(in), optional :: check_eof
        type(syntax_rule_t), pointer :: rule
        type(lexeme_t) :: lexeme
        type(parse_node_t), pointer :: node
        logical :: ok, check
        check = .true.; if (present (check_eof)) check = check_eof
        call lexer_clear (lexer)
        if (present (key)) then
            rule => syntax_get_rule_ptr (syntax, key)
        else
            rule => syntax_get_top_rule_ptr (syntax)
        end if
        if (associated (rule)) then
            call parse_node_match_rule (node, rule, ok)
            if (ok) then
                parse_tree%root_node => node
            else
                call parse_error (rule, lexeme)
            end if
            if (check) then
                call lex (lexeme, lexer)
                if (.not. lexeme_is_eof (lexeme)) then
                    call lexer_show_location (lexer)
                    call msg_fatal (" Syntax error " &
                        // "(at or before the location indicated above)")
                end if
            end if
        end if
        else
            call msg_bug (" Parser failed because syntax is empty")
        end if
    contains
    <Parser: internal subroutines of parse_tree_init>
    end subroutine parse_tree_init

```

The parser works recursively, following the rule tree, building the tree of nodes on the fly. If the given rule matches, the node is filled on return. If not, the node remains empty.

```

<Parser: internal subroutines of parse_tree_init>≡
    recursive subroutine parse_node_match_rule (node, rule, ok)
        type(parse_node_t), pointer :: node
        type(syntax_rule_t), intent(in), target :: rule
        logical, intent(out) :: ok
        logical, parameter :: debug = .false.
        integer :: type

```



```

if (debug) write (6, "(A)", advance="no") "Parsing rule: "
if (debug) call syntax_rule_write (rule, 6)
node => null ()
type = syntax_rule_get_type (rule)
if (syntax_rule_is_atomic (rule)) then
  call lex (lexeme, lexer)
  if (debug) write (6, "(A)", advance="no") "Token: "
  if (debug) call lexeme_write (lexeme, 6)
  call parse_node_create_leaf (node, rule, lexeme)
  ok = associated (node)
  if (.not. ok) call lexer_put_back (lexer, lexeme)
else
  select case (type)
  case (S_ALTERNATIVE); call parse_alternative (node, rule, ok)
  case (S_GROUP);       call parse_group (node, rule, ok)
  case (S_SEQUENCE);    call parse_sequence (node, rule, .false., ok)
  case (S_LIST);        call parse_sequence (node, rule, .true., ok)
  case (S_ARGS);        call parse_args (node, rule, ok)
  case (S_IGNORE);      call parse_ignore (node, ok)
  end select
end if
if (debug) then
  if (ok) then
    write (6, "(A)", advance="no") "Matched rule: "
  else
    write (6, "(A)", advance="no") "Failed rule: "
  end if
  call syntax_rule_write (rule)
  if (associated (node)) call parse_node_write (node)
end if
end subroutine parse_node_match_rule

```

Parse an alternative: try each case. If the match succeeds, the node has been filled, so return. If nothing works, return failure.

(Parser: internal subroutines of parse.tree.init)+≡

```

recursive subroutine parse_alternative (node, rule, ok)
  type(parse_node_t), pointer :: node
  type(syntax_rule_t), intent(in), target :: rule
  logical, intent(out) :: ok
  integer :: i
  do i = 1, syntax_rule_get_n_sub (rule)
    call parse_node_match_rule (node, syntax_rule_get_sub_ptr (rule, i), ok)
    if (ok) return
  end do
  ok = .false.
end subroutine parse_alternative

```

Parse a group: the first and third lexemes have to be the delimiters, the second one is parsed as the actual node, using now the child rule. If the first match fails, return with failure. If the other matches fail, issue an error, since we cannot lex back more than one item.

(Parser: internal subroutines of parse.tree.init)+≡

```

recursive subroutine parse_group (node, rule, ok)
  type(parse_node_t), pointer :: node
  type(syntax_rule_t), intent(in), target :: rule

```

```

logical, intent(out) :: ok
type(string_t), dimension(2) :: delimiter
delimiter = syntax_rule_get_delimiter (rule)
call lex (lexeme, lexer)
if (lexeme_get_string (lexeme) == delimiter(1)) then
  call parse_node_match_rule (node, syntax_rule_get_sub_ptr (rule, 1), ok)
  if (ok) then
    call lex (lexeme, lexer)
    if (lexeme_get_string (lexeme) == delimiter(2)) then
      ok = .true.
    else
      call parse_error (rule, lexeme)
    end if
  else
    call parse_error (rule, lexeme)
  end if
else
  call lexer_put_back (lexer, lexeme)
  ok = .false.
end if
end subroutine parse_group

```

Parsing a sequence. The last rule element may be special: optional and/or repetitive. Each sub-node that matches is appended to the sub-node list of the parent node.

If `sep` is true, we look for a separator after each element.

(Parser: internal subroutines of parse_tree_init)+≡

```

recursive subroutine parse_sequence (node, rule, sep, ok)
  type(parse_node_t), pointer :: node
  type(syntax_rule_t), intent(in), target :: rule
  logical, intent(in) :: sep
  logical, intent(out) :: ok
  type(parse_node_t), pointer :: current
  integer :: i, n
  logical :: opt, rep, cont
  type(string_t) :: separator
  call parse_node_create_branch (node, rule)
  if (sep) separator = syntax_rule_get_separator (rule)
  n = syntax_rule_get_n_sub (rule)
  opt = syntax_rule_last_optional (rule)
  rep = syntax_rule_last_repetitive (rule)
  ok = .true.
  cont = .true.
SCAN_RULE: do i = 1, n
  call parse_node_match_rule &
    (current, syntax_rule_get_sub_ptr (rule, i), cont)
  if (cont) then
    call parse_node_append_sub (node, current)
    if (sep .and. (i < n .or. rep)) then
      call lex (lexeme, lexer)
      if (lexeme_get_string (lexeme) /= separator) then
        call lexer_put_back (lexer, lexeme)
        cont = .false.
      end if
    end if
    exit SCAN_RULE
  end if
end do

```

```

        end if
    end if
else
    if (i == n .and. opt) then
        exit SCAN_RULE
    else if (i == 1) then
        ok = .false.
        exit SCAN_RULE
    else
        call parse_error (rule, lexeme)
    end if
end if
end do SCAN_RULE
if (rep) then
    do while (cont)
        call parse_node_match_rule &
            (current, syntax_rule_get_sub_ptr (rule, n), cont)
        if (cont) then
            call parse_node_append_sub (node, current)
            if (sep) then
                call lex (lexeme, lexer)
                if (lexeme_get_string (lexeme) /= separator) then
                    call lexer_put_back (lexer, lexeme)
                    cont = .false.
                end if
            end if
        end if
    else
        if (sep) call parse_error (rule, lexeme)
    end if
end do
end if
call parse_node_freeze_branch (node)
end subroutine parse_sequence

```

Argument list: We use the `parse_group` code, but call `parse_sequence` inside.

(*Parser: internal subroutines of parse.tree.init*) \equiv

```

recursive subroutine parse_args (node, rule, ok)
    type(parse_node_t), pointer :: node
    type(syntax_rule_t), intent(in), target :: rule
    logical, intent(out) :: ok
    type(string_t), dimension(2) :: delimiter
    delimiter = syntax_rule_get_delimiter (rule)
    call lex (lexeme, lexer)
    if (lexeme_get_string (lexeme) == delimiter(1)) then
        call parse_sequence (node, rule, .true., ok)
        if (ok) then
            call lex (lexeme, lexer)
            if (lexeme_get_string (lexeme) == delimiter(2)) then
                ok = .true.
            else
                call parse_error (rule, lexeme)
            end if
        else
            call parse_error (rule, lexeme)
        end if
    end if
end if

```

```

    else
        call lexer_put_back (lexer, lexeme)
        ok = .false.
    end if
end subroutine parse_args

```

The IGNORE syntax reads one lexeme and discards it if it is numeric, logical or string/identifier (but not a keyword). This is a successful match. Otherwise, the match fails. The node pointer is returned disassociated in any case.

```

<Parser: internal subroutines of parse_tree_init>+≡
subroutine parse_ignore (node, ok)
    type(parse_node_t), pointer :: node
    logical, intent(out) :: ok
    call lex (lexeme, lexer)
    select case (lexeme_get_type (lexeme))
    case (T_NUMERIC, T_IDENTIFIER, T_QUOTED)
        ok = .true.
    case default
        ok = .false.
    end select
    node => null ()
end subroutine parse_ignore

```

If the match fails and we cannot step back:

```

<Parser: internal subroutines of parse_tree_init>+≡
subroutine parse_error (rule, lexeme)
    type(syntax_rule_t), intent(in) :: rule
    type(lexeme_t), intent(in) :: lexeme
    character(80) :: buffer
    integer :: u, iostat
    call lexer_show_location (lexer)
    u = free_unit ()
    open (u, status = "scratch")
    write (u, "(A)", advance="no") "Expected syntax:"
    call syntax_rule_write (rule, u)
    write (u, "(A)", advance="no") "Found token:"
    call lexeme_write (lexeme, u)
    rewind (u)
    do
        read (u, "(A)", iostat=iostat) buffer
        if (iostat /= 0) exit
        call msg_message (trim (buffer))
    end do
    call msg_fatal (" Syntax error " &
        // "(at or before the location indicated above)")
end subroutine parse_error

```

The finalizer recursively deallocates all nodes and their contents. For each node, `parse_node_final` is called on the sub-nodes, which in turn deallocates the token or sub-node array contained within each of them. At the end, only the top node remains to be deallocated.

```

<Parser: public>+≡
public :: parse_tree_final

<Parser: parse tree: TBP>+≡
procedure :: final => parse_tree_final

```

```

(Parser: procedures)+≡
  subroutine parse_tree_final (parse_tree)
    class(parse_tree_t), intent(inout) :: parse_tree
    if (associated (parse_tree%root_node)) then
      call parse_node_final (parse_tree%root_node)
      deallocate (parse_tree%root_node)
    end if
  end subroutine parse_tree_final

```

Print the parse tree. Print one token per line, indented according to the depth of the node.

The `verbose` version includes type identifiers for the nodes.

```

(Parser: public)+≡
  public :: parse_tree_write

(Parser: parse tree: TBP)+≡
  procedure :: write => parse_tree_write

(Parser: procedures)+≡
  subroutine parse_tree_write (parse_tree, unit, verbose)
    class(parse_tree_t), intent(in) :: parse_tree
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    logical :: short
    u = given_output_unit (unit); if (u < 0) return
    short = .true.; if (present (verbose)) short = .not. verbose
    write (u, "(A)") "Parse tree:"
    if (associated (parse_tree%root_node)) then
      call parse_node_write_rec (parse_tree%root_node, unit, short, 1)
    else
      write (u, *) "[empty]"
    end if
  end subroutine parse_tree_write

```

This is a generic error that can be issued if the parse tree does not meet the expectations of the parser. This most certainly indicates a bug.

```

(Parser: public)+≡
  public :: parse_tree_bug

(Parser: procedures)+≡
  subroutine parse_tree_bug (node, keys)
    type(parse_node_t), intent(in) :: node
    character(*), intent(in) :: keys
    call parse_node_write (node)
    call msg_bug (" Inconsistency in parse tree: expected " // keys)
  end subroutine parse_tree_bug

```

7.4.7 Access the parser

For scanning the parse tree we give access to the top node, as a node pointer. Of course, there should be no write access.

```

(Parser: parse tree: TBP)+≡

```

```

procedure :: get_root_ptr => parse_tree_get_root_ptr
<Parser: procedures>+≡
function parse_tree_get_root_ptr (parse_tree) result (node)
  class(parse_tree_t), intent(in) :: parse_tree
  type(parse_node_t), pointer :: node
  node => parse_tree%root_node
end function parse_tree_get_root_ptr

```

7.4.8 Tools

This operation traverses the parse tree and simplifies any occurrences of a set of syntax rules. If such a parse node has only one sub-node, it is replaced by that subnode. (This makes sense only of the rules to eliminate have no meaningful token.)

```

<Parser: public>+≡
public :: parse_tree_reduce

<Parser: procedures>+≡
subroutine parse_tree_reduce (parse_tree, rule_key)
  type(parse_tree_t), intent(inout) :: parse_tree
  type(string_t), dimension(:), intent(in) :: rule_key
  type(parse_node_t), pointer :: pn
  pn => parse_tree%root_node
  if (associated (pn)) then
    call parse_node_reduce (pn, null(), null())
  end if
contains
recursive subroutine parse_node_reduce (pn, pn_prev, pn_parent)
  type(parse_node_t), intent(inout), pointer :: pn
  type(parse_node_t), intent(in), pointer :: pn_prev, pn_parent
  type(parse_node_t), pointer :: pn_sub, pn_sub_prev, pn_tmp
  pn_sub_prev => null ()
  pn_sub => pn%sub_first
  do while (associated (pn_sub))
    call parse_node_reduce (pn_sub, pn_sub_prev, pn)
    pn_sub_prev => pn_sub
    pn_sub => pn_sub%next
  end do
  if (parse_node_get_n_sub (pn) == 1) then
    if (matches (parse_node_get_rule_key (pn), rule_key)) then
      pn_tmp => pn
      pn => pn%sub_first
      if (associated (pn_prev)) then
        pn_prev%next => pn
      else if (associated (pn_parent)) then
        pn_parent%sub_first => pn
      else
        parse_tree%root_node => pn
      end if
      if (associated (pn_tmp%next)) then
        pn%next => pn_tmp%next
      else if (associated (pn_parent)) then

```

```

        pn_parent%sub_last => pn
    end if
    call parse_node_final (pn_tmp, recursive=.false.)
    deallocate (pn_tmp)
end if
end if
end subroutine parse_node_reduce
function matches (key, key_list) result (flag)
    logical :: flag
    type(string_t), intent(in) :: key
    type(string_t), dimension(:), intent(in) :: key_list
    integer :: i
    flag = .true.
    do i = 1, size (key_list)
        if (key == key_list(i)) return
    end do
    flag = .false.
end function matches
end subroutine parse_tree_reduce

```

7.4.9 Applications

For a file of the form

```

process foo, bar
  <something>
process xyz
  <something>

```

get the <something> entry node for the first matching process tag. If no matching entry is found, the node pointer remains unassociated.

```

(Parser: public)+≡
    public :: parse_tree_get_process_ptr

(Parser: procedures)+≡
    function parse_tree_get_process_ptr (parse_tree, process) result (node)
        type(parse_node_t), pointer :: node
        type(parse_tree_t), intent(in), target :: parse_tree
        type(string_t), intent(in) :: process
        type(parse_node_t), pointer :: node_root, node_process_def
        type(parse_node_t), pointer :: node_process_phs, node_process_list
        integer :: j
        node_root => parse_tree%get_root_ptr ()
        if (associated (node_root)) then
            node_process_phs => parse_node_get_sub_ptr (node_root)
            SCAN_FILE: do while (associated (node_process_phs))
                node_process_def => parse_node_get_sub_ptr (node_process_phs)
                node_process_list => parse_node_get_sub_ptr (node_process_def, 2)
                do j = 1, parse_node_get_n_sub (node_process_list)
                    if (parse_node_get_string &
                        (parse_node_get_sub_ptr (node_process_list, j)) &
                        == process) then
                        node => parse_node_get_next_ptr (node_process_def)

```

```

        return
    end if
end do
    node_process_phs => parse_node_get_next_ptr (node_process_phs)
end do SCAN_FILE
node => null ()
else
    node => null ()
end if
end function parse_tree_get_process_ptr

```

7.4.10 Unit tests

Test module, followed by the corresponding implementation module.

<parser_ut.f90>≡
<File header>

```

module parser_ut
  use unit_tests
  use parser_uti

```

<Standard module head>

<Parser: public test>

contains

<Parser: test driver>

```

end module parser_ut

```

<parser_uti.f90>≡
<File header>

```

module parser_uti

  use syntax_rules

  use parser

```

<Standard module head>

<Parser: test declarations>

contains

<Parser: tests>

```

end module parser_uti

```

API: driver for the unit tests below.

<Parser: public test>≡
 public :: parse_test


```

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

```

This checks the parser.

```

<Parser: execute tests>≡
  call test (parse_1, "parse_1", &
    "check the parser", &
    u, results)

<Parser: test declarations>≡
  public :: parse_1

<Parser: tests>≡
  subroutine parse_1 (u)
    use ifiles
    use lexers
    integer, intent(in) :: u

    type(ifile_t) :: ifile
    type(syntax_t), target :: syntax
    type(lexer_t) :: lexer
    type(stream_t), target :: stream
    type(parse_tree_t), target :: parse_tree

    write (u, "(A)")  "* Test output: Parsing"
    write (u, "(A)")  "* Purpose: test parse routines"
    write (u, "(A)")

    call ifile_append (ifile, "SEQ expr = term addition*")
    call ifile_append (ifile, "SEQ addition = plus_or_minus term")
    call ifile_append (ifile, "SEQ term = factor multiplication*")
    call ifile_append (ifile, "SEQ multiplication = times_or_over factor")
    call ifile_append (ifile, "SEQ factor = atom exponentiation*")
    call ifile_append (ifile, "SEQ exponentiation = '^' atom")
    call ifile_append (ifile, "ALT atom = real | delimited_expr")
    call ifile_append (ifile, "GRO delimited_expr = ( expr )")
    call ifile_append (ifile, "ALT plus_or_minus = '+' | '-'")
    call ifile_append (ifile, "ALT times_or_over = '*' | '/'")
    call ifile_append (ifile, "KEY '+'")
    call ifile_append (ifile, "KEY '-'")
    call ifile_append (ifile, "KEY '*'")
    call ifile_append (ifile, "KEY '/'")
    call ifile_append (ifile, "KEY '^'")
    call ifile_append (ifile, "REA real")

    write (u, "(A)")  "* File contents (syntax definition):"
    call ifile_write (ifile, u)
    write (u, "(A)")  "EOF"
    write (u, "(A)")

    call syntax_init (syntax, ifile)

```

```

call ifile_final (ifile)
call syntax_write (syntax, u)
write (u, "(A)")

call lexer_init (lexer, &
    comment_chars = "", &
    quote_chars = "'", &
    quote_match = "'", &
    single_chars = "+-*/^()", &
    special_class = [""] , &
    keyword_list = syntax_get_keyword_list_ptr (syntax))
call lexer_write_setup (lexer, u)
write (u, "(A)")

call ifile_append (ifile, "(27+8^3-2/3)*(4+7)^2*99")
write (u, "(A)")  "* File contents (input file):"
call ifile_write (ifile, u)
write (u, "(A)")  "EOF"
print *

call stream_init (stream, ifile)
call lexer_assign_stream (lexer, stream)
call parse_tree_init (parse_tree, syntax, lexer)
call stream_final (stream)
call parse_tree_write (parse_tree, u, .true.)
print *

write (u, "(A)")  "* Cleanup, everything should now be empty:"
write (u, "(A)")

call parse_tree_final (parse_tree)
call parse_tree_write (parse_tree, u, .true.)
write (u, "(A)")

call lexer_final (lexer)
call lexer_write_setup (lexer, u)
write (u, "(A)")

call ifile_final (ifile)
write (u, "(A)")  "* File contents:"
call ifile_write (ifile, u)
write (u, "(A)")  "EOF"
write (u, "(A)")

call syntax_final (syntax)
call syntax_write (syntax, u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: parser_1"

end subroutine parse_1

```

7.5 XML Parser

The XML parser is actually independent from the previous modules of `lexer` and `parser`. However, for a generic I/O interface we make use of the `stream_t` facility.

We need the XML parser for reading and writing LHEF data files. Only a subset of XML is actually relevant. The parser is of the “pull” type, i.e., the program steers the reading of XML data in a context-sensitive manner.

```
<xml.f90>≡
  <File header>

  module xml

    <Use strings>
    use io_units
    use system_defs, only: BLANK, TAB
    use diagnostics
    use ifiles
    use lexers

    <Standard module head>

    <XML: public>

    <XML: types>

    contains

    <XML: procedures>

  end module xml
```

7.5.1 Cached Stream

The stream type as defined in the `lexer` module is versatile regarding the choice of input channel, but it does not allow reading a section more than once. Here, we define an extension where we can return a string to the stream, which is stored in a cache variable, and presented to the caller for the next read.

```
<XML: public>≡
  public :: cstream_t
<XML: types>≡
  type, extends (stream_t) :: cstream_t
    logical :: cache_is_empty = .true.
    type(string_t) :: cache
  contains
    <XML: cstream: TBP>
  end type cstream_t
```

The initializers are simply inherited.

Finalizer: also inherited, in essence:

```
<XML: cstream: TBP>≡
  procedure :: final => cstream_final
```

```

<XML: procedures>≡
  subroutine cstream_final (stream)
    class(cstream_t), intent(inout) :: stream
    stream%cache_is_empty = .true.
    call stream%stream_t%final ()
  end subroutine cstream_final

```

Get record: now, if there is a cache string, return this instead of the record from the stream.

```

<XML: cstream: TBP>+≡
  procedure :: get_record => cstream_get_record

<XML: procedures>+≡
  subroutine cstream_get_record (cstream, string, iostat)
    class(cstream_t), intent(inout) :: cstream
    type(string_t), intent(out) :: string
    integer, intent(out) :: iostat
    if (cstream%cache_is_empty) then
      call stream_get_record (cstream%stream_t, string, iostat)
    else
      string = cstream%cache
      cstream%cache_is_empty = .true.
      iostat = 0
    end if
  end subroutine cstream_get_record

```

Revert: return the (partially read) record to the stream, putting it in the cache.

```

<XML: cstream: TBP>+≡
  procedure :: revert_record => cstream_revert_record

<XML: procedures>+≡
  subroutine cstream_revert_record (cstream, string)
    class(cstream_t), intent(inout) :: cstream
    type(string_t), intent(in) :: string
    if (cstream%cache_is_empty) then
      cstream%cache = string
      cstream%cache_is_empty = .false.
    else
      call msg_bug ("CStream: attempt to revert twice")
    end if
  end subroutine cstream_revert_record

```

7.5.2 Attributes

A tag attribute has a name and a value; both are strings. When the attribute is defined, the `known` flag indicates this.

```

<XML: types>+≡
  type :: attribute_t
    type(string_t) :: name
    type(string_t) :: value
    logical :: known = .false.
  contains

```

```

    <XML: attribute: TBP>
end type attribute_t

```

Output in standard format, non-advancing. (If the value is unknown, we indicate this by a question mark, which is non-standard.)

```

<XML: attribute: TBP>≡
    procedure :: write => attribute_write

<XML: procedures>+≡
    subroutine attribute_write (object, unit)
        class(attribute_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(A,'=')", advance = "no") char (object%name)
        if (object%known) then
            write (u, "(A,A,A)", advance = "no") '""', char (object%value), ''
        else
            write (u, "(?'')", advance = "no")
        end if
    end subroutine attribute_write

```

This is a genuine constructor. The value is optional.

```

<XML: public>+≡
    public :: xml_attribute

<XML: procedures>+≡
    function xml_attribute (name, value) result (attribute)
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: value
        type(attribute_t) :: attribute
        attribute%name = name
        if (present (value)) then
            attribute%value = value
            attribute%known = .true.
        else
            attribute%known = .false.
        end if
    end function xml_attribute

```

Set a value explicitly.

```

<XML: attribute: TBP>+≡
    procedure :: set_value => attribute_set_value

<XML: procedures>+≡
    subroutine attribute_set_value (attribute, value)
        class(attribute_t), intent(inout) :: attribute
        type(string_t), intent(in) :: value
        attribute%value = value
        attribute%known = .true.
    end subroutine attribute_set_value

```

Extract a value. If unset, return "?"

```
<XML: attribute: TBP>+≡
    procedure :: get_value => attribute_get_value

<XML: procedures>+≡
    function attribute_get_value (attribute) result (value)
        class(attribute_t), intent(in) :: attribute
        type(string_t) :: value
        if (attribute%known) then
            value = attribute%value
        else
            value = "?"
        end if
    end function attribute_get_value
```

7.5.3 The Tag Type

The basic entity is the internal representation of an XML tag. The tag has a name, a well-defined set of attributes which may be mandatory or optional, and a flag that determines whether there is content or not. The content itself is not stored in the data structure.

```
<XML: public>+≡
    public :: xml_tag_t

<XML: types>+≡
    type :: xml_tag_t
        type(string_t) :: name
        type(attribute_t), dimension(:), allocatable :: attribute
        logical :: has_content = .false.
    contains
        <XML: tag: TBP>
    end type xml_tag_t
```

Initialization. There are different versions, depending on content.

```
<XML: tag: TBP>≡
    generic :: init => init_no_attributes
    procedure :: init_no_attributes => xml_tag_init_no_attributes

<XML: procedures>+≡
    subroutine xml_tag_init_no_attributes (tag, name, has_content)
        class(xml_tag_t), intent(out) :: tag
        type(string_t), intent(in) :: name
        logical, intent(in), optional :: has_content
        tag%name = name
        allocate (tag%attribute (0))
        if (present (has_content)) tag%has_content = has_content
    end subroutine xml_tag_init_no_attributes
```

This version sets attributes.

```
<XML: tag: TBP>+≡
    generic :: init => init_with_attributes
    procedure :: init_with_attributes => xml_tag_init_with_attributes
```

```

<XML: procedures>+≡
  subroutine xml_tag_init_with_attributes (tag, name, attribute, has_content)
    class(xml_tag_t), intent(out) :: tag
    type(string_t), intent(in) :: name
    type(attribute_t), dimension(:), intent(in) :: attribute
    logical, intent(in), optional :: has_content
    tag%name = name
    allocate (tag%attribute (size (attribute)))
    tag%attribute = attribute
    if (present (has_content)) tag%has_content = has_content
  end subroutine xml_tag_init_with_attributes

```

Set an attribute value explicitly.

```

<XML: tag: TBP>+≡
  procedure :: set_attribute => xml_tag_set_attribute

<XML: procedures>+≡
  subroutine xml_tag_set_attribute (tag, i, value)
    class(xml_tag_t), intent(inout) :: tag
    integer, intent(in) :: i
    type(string_t), intent(in) :: value
    call tag%attribute(i)%set_value (value)
  end subroutine xml_tag_set_attribute

```

Get an attribute value.

```

<XML: tag: TBP>+≡
  procedure :: get_attribute => xml_tag_get_attribute

<XML: procedures>+≡
  function xml_tag_get_attribute (tag, i) result (value)
    class(xml_tag_t), intent(in) :: tag
    integer, intent(in) :: i
    type(string_t) :: value
    value = tag%attribute(i)%get_value ()
  end function xml_tag_get_attribute

```

Output to an I/O unit, default STDOUT. We use non-advancing output.

```

<XML: tag: TBP>+≡
  generic :: write => write_without_content
  procedure :: write_without_content => xml_tag_write

<XML: procedures>+≡
  subroutine xml_tag_write (tag, unit)
    class(xml_tag_t), intent(in) :: tag
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "('<',A)", advance = "no") char (tag%name)
    do i = 1, size (tag%attribute)
      write (u, "(1x)", advance = "no")
      call tag%attribute(i)%write (u)
    end do
    if (tag%has_content) then
      write (u, "('>')", advance = "no")
    end if
  end subroutine xml_tag_write

```

```

    else
        write (u, "(' />')", advance = "no")
    end if
end subroutine xml_tag_write

```

If there is content, we should write the content next (arbitrary format), the write the corresponding closing tag. Again, non-advancing.

```

<XML: tag: TBP>+≡
    procedure :: close => xml_tag_close

<XML: procedures>+≡
    subroutine xml_tag_close (tag, unit)
        class(xml_tag_t), intent(in) :: tag
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "<'</',A,'>')", advance = "no") char (tag%name)
    end subroutine xml_tag_close

```

Given content as a single string, we can write tag, content, and closing at once

```

<XML: tag: TBP>+≡
    generic :: write => write_with_content
    procedure :: write_with_content => xml_tag_write_with_content

<XML: procedures>+≡
    subroutine xml_tag_write_with_content (tag, content, unit)
        class(xml_tag_t), intent(in) :: tag
        type(string_t), intent(in) :: content
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        call tag%write (u)
        write (u, "(A)", advance = "no") char (content)
        call tag%close (u)
    end subroutine xml_tag_write_with_content

```

Input from stream. We know what we are looking for, so we check if the name matches, then fill attributes. We report an error if (a) an I/O error occurs, (b) we reach EOF before encountering the tag, (c) if the tag is incomplete.

Trailing text after reading a tag is put back to the input stream.

We assume that the tag is not broken across records, and that there is only one tag within the record. This is more restricted than standard XML.

```

<XML: tag: TBP>+≡
    procedure :: read => xml_tag_read

<XML: procedures>+≡
    subroutine xml_tag_read (tag, cstream, success)
        class(xml_tag_t), intent(inout) :: tag
        type(cstream_t), intent(inout) :: cstream
        logical, intent(out) :: success
        type(string_t) :: string
        integer :: iostat, p1, p2
        character(2), parameter :: WS = BLANK // TAB

```



```

logical :: done

! Skip comments and blank lines
FIND_NON_COMMENT: do
  FIND_NONEMPTY_RECORD: do
    call cstream%get_record (string, iostat)
    if (iostat /= 0) call err_io ()
    p1 = verify (string, WS)
    if (p1 > 0) exit FIND_NONEMPTY_RECORD
  end do FIND_NONEMPTY_RECORD

  ! Look for comment beginning
  p2 = p1 + 3
  if (extract (string, p1, p2) /= "<!--") exit FIND_NON_COMMENT

  ! Look for comment end, then restart
  string = extract (string, p2 + 1)
  FIND_COMMENT_END: do
    do p1 = 1, len (string) - 2
      p2 = p1 + 2
      if (extract (string, p1, p2) == "-->") then

        ! Return trailing text to the stream
        string = extract (string, p2 + 1)
        if (string /= "") call cstream%revert_record (string)
        exit FIND_COMMENT_END

      end if
    end do
    call cstream%get_record (string, iostat)
    if (iostat /= 0) call err_io ()
  end do FIND_COMMENT_END
end do FIND_NON_COMMENT

! Look for opening <
p2 = p1
if (extract (string, p1, p2) /= "<") then
  call cstream%revert_record (string)
  success = .false.; return
else

  ! Look for tag name
  string = extract (string, p2 + 1)
  p1 = verify (string, WS); if (p1 == 0) call err_incomplete ()
  p2 = p1 + len (tag%name) - 1
  if (extract (string, p1, p2) /= tag%name) then
    call cstream%revert_record ("<" // string)
    success = .false.; return
  else

    ! Look for attributes
    string = extract (string, p2 + 1)
    READ_ATTRIBUTES: do
      call tag%read_attribute (string, done)
    end do
  end if
end if

```

```

        if (done) exit READ_ATTRIBUTES
    end do READ_ATTRIBUTES

    ! Look for closing >
    p1 = verify (string, WS); if (p1 == 0) call err_incomplete ()
    p2 = p1
    if (extract (string, p1, p1) == ">") then
        tag%has_content = .true.
    else

        ! Look for closing />
        p2 = p1 + 1
        if (extract (string, p1, p2) /= "/>") call err_incomplete ()
    end if

    ! Return trailing text to the stream
    string = extract (string, p2 + 1)
    if (string /= "") call cstream%revert_record (string)
    success = .true.

end if
end if

contains

subroutine err_io ()
    select case (iostat)
    case (:-1)
        call msg_fatal ("XML: Error reading tag '" // char (tag%name) &
            // "': end of file")
    case (1:)
        call msg_fatal ("XML: Error reading tag '" // char (tag%name) &
            // "': I/O error")
    end select
    success = .false.
end subroutine err_io

subroutine err_incomplete ()
    call msg_fatal ("XML: Error reading tag '" // char (tag%name) &
        // "': tag incomplete")
    success = .false.
end subroutine err_incomplete

end subroutine xml_tag_read

```

Read a single attribute. If the attribute is valid, assign the value. Setting a value twice should be an error, but is not detected. If the attribute is unknown, ignore it. If we reach the closing sign, report this.

```

<XML: tag: TBP>+≡
    procedure :: read_attribute => xml_tag_read_attribute

<XML: procedures>+≡
    subroutine xml_tag_read_attribute (tag, string, done)
        class(xml_tag_t), intent(inout) :: tag

```

```

type(string_t), intent(inout) :: string
logical, intent(out) :: done
character(2), parameter :: WS = BLANK // TAB
type(string_t) :: name, value
integer :: p1, p2, i

p1 = verify (string, WS); if (p1 == 0) call err ()
p2 = p1

! Look for first terminating '>' or '/>'
if (extract (string, p1, p2) == ">") then
    done = .true.
else
    p2 = p1 + 1
    if (extract (string, p1, p2) == "/>") then
        done = .true.
    else

        ! Look for '='
        p2 = scan (string, '=')
        if (p2 == 0) call err ()
        name = trim (extract (string, p1, p2 - 1))

        ! Look for '"'
        string = extract (string, p2 + 1)
        p1 = verify (string, WS); if (p1 == 0) call err ()
        p2 = p1
        if (extract (string, p1, p2) /= '"') call err ()

        ! Look for matching '"' and get value
        string = extract (string, p2 + 1)
        p1 = 1
        p2 = scan (string, '"')
        if (p2 == 0) call err ()
        value = extract (string, p1, p2 - 1)

        SCAN_KNOWN_ATTRIBUTES: do i = 1, size (tag%attribute)
            if (name == tag%attribute(i)%name) then
                call tag%attribute(i)%set_value (value)
                exit SCAN_KNOWN_ATTRIBUTES
            end if
        end do SCAN_KNOWN_ATTRIBUTES

        string = extract (string, p2 + 1)
        done = .false.
    end if
end if

contains

subroutine err ()
    call msg_fatal ("XML: Error reading attributes of '" // char (tag%name) &
        // "': syntax error")
end subroutine err

```

```
end subroutine xml_tag_read_attribute
```

Read the content string of a tag. We check for the appropriate closing tag and report it. If a closing tag does not match in name, ignore it.

Note: this assumes that no tag with the same name is embedded in the current content. Also, we do not check for XML validity inside the content.

<XML: tag: TBP>+≡

```
procedure :: read_content => xml_tag_read_content
```

<XML: procedures>+≡

```
subroutine xml_tag_read_content (tag, cstream, content, closing)
  class(xml_tag_t), intent(in) :: tag
  type(cstream_t), intent(inout) :: cstream
  type(string_t), intent(out) :: content
  type(string_t) :: string
  logical, intent(out) :: closing
  integer :: iostat
  integer :: p0, p1, p2
  character(2), parameter :: WS = BLANK // TAB
  call cstream%get_record (content, iostat)
  if (iostat /= 0) call err_io ()
  closing = .false.
  FIND_CLOSING: do p0 = 1, len (content) - 1

    ! Look for terminating </
    p1 = p0
    p2 = p1 + 1
    if (extract (content, p1, p2) == "</") then

      ! Look for closing tag name
      string = extract (content, p2 + 1)
      p1 = verify (string, WS); if (p1 == 0) call err_incomplete ()
      p2 = p1 + len (tag%name) - 1
      if (extract (string, p1, p2) == tag%name) then

        ! Tag name matches: look for final >
        string = extract (string, p2 + 1)
        p1 = verify (string, WS); if (p1 == 0) call err_incomplete ()
        p2 = p1
        if (extract (string, p1, p2) /= ">") call err_incomplete ()

        ! Return trailing text to the stream
        string = extract (string, p2 + 1)
        if (string /= "") call cstream%revert_record (string)
        content = extract (content, 1, p0 -1)
        closing = .true.
        exit FIND_CLOSING

      end if
    end if
  end do FIND_CLOSING
```

contains

```

subroutine err_io ()
  select case (iostat)
  case (:-1)
    call msg_fatal ("XML: Error reading content of '" // char (tag%name) &
      // "': end of file")
  case (1:)
    call msg_fatal ("XML: Error reading content of '" // char (tag%name) &
      // "': I/O error")
  end select
  closing = .false.
end subroutine err_io

subroutine err_incomplete ()
  call msg_fatal ("XML: Error reading content '" // char (tag%name) &
    // "': closing tag incomplete")
  closing = .false.
end subroutine err_incomplete

end subroutine xml_tag_read_content

```

7.5.4 Unit tests

Test module, followed by the corresponding implementation module.

<xml_ut.f90>≡
<File header>

```

module xml_ut
  use unit_tests
  use xml_uti

```

<Standard module head>

<XML: public test>

contains

<XML: test driver>

```

end module xml_ut

```

<xml_uti.f90>≡
<File header>

```

module xml_uti

```

<Use strings>

```

  use io_units

```

```

  use xml

```

<Standard module head>

```

    <XML: test declarations>

contains

    <XML: tests>

    <XML: test auxiliary>

end module xml_util

API: driver for the unit tests below.
<XML: public test>≡
    public :: xml_test
<XML: test driver>≡
    subroutine xml_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <XML: execute tests>
end subroutine xml_test

```

7.5.5 Auxiliary Routines

Show the contents of a temporary file, i.e., open unit.

```

<XML: test auxiliary>≡
    subroutine show (u_tmp, u)
        integer, intent(in) :: u_tmp, u
        character (80) :: buffer
        integer :: iostat
        write (u, "(A)") "File content:"
        rewind (u_tmp)
        do
            read (u_tmp, "(A)", iostat = iostat) buffer
            if (iostat /= 0) exit
            write (u, "(A)") trim (buffer)
        end do
        rewind (u_tmp)
    end subroutine show

```

7.5.6 Basic Tag I/O

Write a tag and read it again, using a temporary file.

```

<XML: execute tests>≡
    call test (xml_1, "xml_1", &
        "basic I/O", &
        u, results)
<XML: test declarations>≡
    public :: xml_1

```

```

<XML: tests>≡
subroutine xml_1 (u)
  integer, intent(in) :: u
  type(xml_tag_t), allocatable :: tag
  integer :: u_tmp
  type(cstream_t) :: cstream
  logical :: success

  write (u, "(A)")  "* Test output: xml_1"
  write (u, "(A)")  "* Purpose: write and read tag"
  write (u, "(A)")

  write (u, "(A)")  "* Empty tag"
  write (u, *)

  u_tmp = free_unit ()
  open (u_tmp, status = "scratch", action = "readwrite")

  allocate (tag)
  call tag%init (var_str ("tagname"))
  call tag%write (u_tmp)
  write (u_tmp, *)
  deallocate (tag)

  call show (u_tmp, u)

  write (u, *)
  write (u, "(A)")  "Result from read:"
  call cstream%init (u_tmp)
  allocate (tag)
  call tag%init (var_str ("tagname"))
  call tag%read (cstream, success)
  call tag%write (u)
  write (u, *)
  write (u, "(A,L1)")  "success = ", success
  deallocate (tag)
  close (u_tmp)
  call cstream%final ()

  write (u, *)
  write (u, "(A)")  "* Tag with preceding blank lines"
  write (u, *)

  u_tmp = free_unit ()
  open (u_tmp, status = "scratch", action = "readwrite")

  allocate (tag)
  call tag%init (var_str ("tagname"))
  write (u_tmp, *)
  write (u_tmp, "(A)")  "    "
  write (u_tmp, "(2x)", advance = "no")
  call tag%write (u_tmp)
  write (u_tmp, *)
  deallocate (tag)

```

```

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, *)
write (u, "(A)") "* Tag with preceding comments"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("tagname"))
write (u_tmp, "(A)") "<!-- comment -->"
write (u_tmp, *)
write (u_tmp, "(A)") "<!-- multiline"
write (u_tmp, "(A)") "      comment -->"
call tag%write (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
close (u_tmp)
deallocate (tag)

call cstream%final ()

write (u, *)
write (u, "(A)") "* Tag with name mismatch"
write (u, *)

u_tmp = free_unit ()

```



```

open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("wrongname"))
call tag%write (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: xml_1"

end subroutine xml_1

```

7.5.7 Optional Tag

Write and read two tags, one of them optional.

```

<XML: execute tests>+≡
  call test (xml_2, "xml_2", &
    "optional tag", &
    u, results)

<XML: test declarations>+≡
  public :: xml_2

<XML: tests>+≡
  subroutine xml_2 (u)
    integer, intent(in) :: u
    type(xml_tag_t), allocatable :: tag1, tag2
    integer :: u_tmp
    type(cstream_t) :: cstream
    logical :: success

    write (u, "(A)") "* Test output: xml_2"
    write (u, "(A)") "* Purpose: handle optional tag"
    write (u, "(A)")

    write (u, "(A)") "* Optional tag present"
    write (u, *)

```

```

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag1)
call tag1%init (var_str ("option"))
call tag1%write (u_tmp)
write (u_tmp, *)
allocate (tag2)
call tag2%init (var_str ("tagname"))
call tag2%write (u_tmp)
write (u_tmp, *)
deallocate (tag1, tag2)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag1)
call tag1%init (var_str ("option"))
call tag1%read (cstream, success)
call tag1%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
write (u, *)
allocate (tag2)
call tag2%init (var_str ("tagname"))
call tag2%read (cstream, success)
call tag2%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
deallocate (tag1, tag2)
close (u_tmp)
call cstream%final ()

write (u, *)
write (u, "(A)") "* Optional tag absent"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag2)
call tag2%init (var_str ("tagname"))
call tag2%write (u_tmp)
write (u_tmp, *)
deallocate (tag2)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)

```

```

allocate (tag1)
call tag1%init (var_str ("option"))
call tag1%read (cstream, success)
call tag1%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
write (u, *)
allocate (tag2)
call tag2%init (var_str ("tagname"))
call tag2%read (cstream, success)
call tag2%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
deallocate (tag1, tag2)
close (u_tmp)
call cstream%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: xml_2"

end subroutine xml_2

```

7.5.8 Optional Tag

Write and read a tag with single-line content.

```

<XML: execute tests>+≡
    call test (xml_3, "xml_3", &
               "content", &
               u, results)

<XML: test declarations>+≡
    public :: xml_3

<XML: tests>+≡
    subroutine xml_3 (u)
        integer, intent(in) :: u
        type(xml_tag_t), allocatable :: tag
        integer :: u_tmp
        type(cstream_t) :: cstream
        logical :: success, closing
        type(string_t) :: content

        write (u, "(A)")  "* Test output: xml_3"
        write (u, "(A)")  "* Purpose: handle tag with content"
        write (u, "(A)")

        write (u, "(A)")  "* Tag without content"
        write (u, *)

        u_tmp = free_unit ()
        open (u_tmp, status = "scratch", action = "readwrite")

        allocate (tag)

```

```

call tag%init (var_str ("tagname"))
call tag%write (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
write (u, "(A,L1)") "content = ", tag%has_content
write (u, *)
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, "(A)") "* Tag with content"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("tagname"), has_content = .true.)
call tag%write (var_str ("Content text"), u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)") "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%read_content (cstream, content, closing)
call tag%write (u)
write (u, "(A)", advance = "no") char (content)
call tag%close (u)
write (u, *)
write (u, "(A,L1)") "success = ", success
write (u, "(A,L1)") "content = ", tag%has_content
write (u, "(A,L1)") "closing = ", closing
deallocate (tag)
close (u_tmp)
call cstream%final ()

```

```

write (u, *)
write (u, "(A)")  "* Tag with multiline content"
write (u, *)

u_tmp = free_unit ()
open (u_tmp, status = "scratch", action = "readwrite")

allocate (tag)
call tag%init (var_str ("tagname"), has_content = .true.)
call tag%write (u_tmp)
write (u_tmp, *)
write (u_tmp, "(A)")  "Line 1"
write (u_tmp, "(A)")  "Line 2"
call tag%close (u_tmp)
write (u_tmp, *)
deallocate (tag)

call show (u_tmp, u)

write (u, *)
write (u, "(A)")  "Result from read:"
call cstream%init (u_tmp)
allocate (tag)
call tag%init (var_str ("tagname"))
call tag%read (cstream, success)
call tag%write (u)
write (u, *)
do
  call tag%read_content (cstream, content, closing)
  if (closing) exit
  write (u, "(A)")  char (content)
end do
call tag%close (u)
write (u, *)
write (u, "(A,L1)")  "success = ", success
write (u, "(A,L1)")  "content = ", tag%has_content
deallocate (tag)
close (u_tmp)
call cstream%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: xml_3"

end subroutine xml_3

```

7.5.9 Basic Tag I/O

Write a tag and read it again, using a temporary file.

```

<XML: execute tests>+≡
  call test (xml_4, "xml_4", &
    "attributes", &
    u, results)

```

```

<XML: test declarations>+≡
    public :: xml_4

<XML: tests>+≡
    subroutine xml_4 (u)
        integer, intent(in) :: u
        type(xml_tag_t), allocatable :: tag
        integer :: u_tmp
        type(cstream_t) :: cstream
        logical :: success

        write (u, "(A)")  "* Test output: xml_4"
        write (u, "(A)")  "*   Purpose: handle tag with attributes"
        write (u, "(A)")

        write (u, "(A)")  "* Tag with one mandatory and one optional attribute,"
        write (u, "(A)")  "* unknown attribute ignored"
        write (u, *)

        u_tmp = free_unit ()
        open (u_tmp, status = "scratch", action = "readwrite")

        allocate (tag)
        call tag%init (var_str ("tagname"), &
            [xml_attribute (var_str ("a1"), var_str ("foo")), &
             xml_attribute (var_str ("a3"), var_str ("gee"))])
        call tag%write (u_tmp)
        deallocate (tag)

        call show (u_tmp, u)

        write (u, *)
        write (u, "(A)")  "Result from read:"
        call cstream%init (u_tmp)
        allocate (tag)
        call tag%init (var_str ("tagname"), &
            [xml_attribute (var_str ("a1")), &
             xml_attribute (var_str ("a2"), var_str ("bar"))])
        call tag%read (cstream, success)
        call tag%write (u)
        write (u, *)
        deallocate (tag)
        close (u_tmp)
        call cstream%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: xml_4"

    end subroutine xml_4

```

Chapter 8

Random-Number Generator

These modules implement abstract types and tools for random-number generation.

rng_base Abstract random-number generator and factory

selectors Selection depending on weights and random numbers

Implementation of the RNG abstract types:

Module rng_tao: Interface to the TAO random number generator which the VAMP package provides. Note that VAMP explicitly requests this generator.

Module rngstream: Implementation of RNGstream proposed by L'Ecuyer. The RNGStream provides access to different streams and/or substream of random numbers.

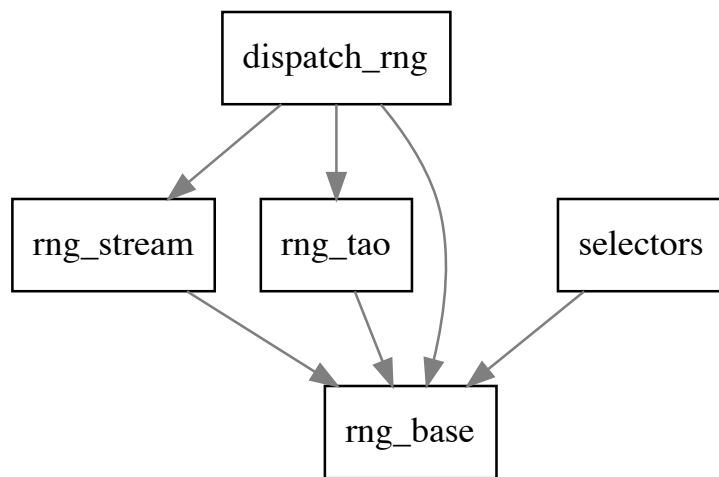


Figure 8.1: Module dependencies in `src/rng`.

8.1 Generic Random-Number Generator

For all generator implementations, we define a `rng` type which represents the state of a random-number generator with the associated methods that produce a random number. Furthermore, we define a `rng_factory` type. An object of this type is capable of allocating a sequence of `rng` objects. These generator states should be, if possible, statistically independent, so they can be used in parallel in different places of the event-generation chain.

```
<rng_base.f90>≡  
  <File header>  
  
  module rng_base  
  
    <Use kinds>  
    use kinds, only: i16  
    use constants, only: TWOPI  
  
    <Standard module head>  
  
    <RNG base: public>  
  
    <RNG base: types>  
  
    <RNG base: interfaces>  
  
    contains  
  
    <RNG base: procedures>  
  
  end module rng_base
```

8.1.1 Generator type

The `rng` object is actually the state of the random-number generator. The methods `initialize/reset` and `call` the generator for this state.

```
<RNG base: public>≡  
  public :: rng_t  
  
<RNG base: types>≡  
  type, abstract :: rng_t  
    contains  
    <RNG base: rng: TBP>  
  end type rng_t
```

The `init` method initializes the generator and sets a seed. We should implement the interface such that a single integer is sufficient for a seed.

The seed may be omitted. The behavior without seed is not defined, however.

```
<RNG base: rng: TBP>≡  
  procedure (rng_init), deferred :: init  
  
<RNG base: interfaces>≡  
  abstract interface  
    subroutine rng_init (rng, seed)
```

```

import
class(rng_t), intent(out) :: rng
integer, intent(in), optional :: seed
end subroutine rng_init
end interface

```

The `final` method deallocates memory where necessary and allows for another call of `init` to reset the generator.

```

<RNG base: rng: TBP>+≡
  procedure (rng_final), deferred :: final

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_final (rng)
      import
      class(rng_t), intent(inout) :: rng
    end subroutine rng_final
  end interface

```

Output. We should, at least, identify the generator.

```

<RNG base: rng: TBP>+≡
  procedure (rng_write), deferred :: write

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_write (rng, unit, indent)
      import
      class(rng_t), intent(in) :: rng
      integer, intent(in), optional :: unit, indent
    end subroutine rng_write
  end interface

```

These routines generate a single and an array of uniformly distributed default-precision random numbers, respectively.

```

<RNG base: rng: TBP>+≡
  generic :: generate => generate_single, generate_array
  procedure (rng_generate_single), deferred :: generate_single
  procedure (rng_generate_array), deferred :: generate_array

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_generate_single (rng, x)
      import
      class(rng_t), intent(inout) :: rng
      real(default), intent(out) :: x
    end subroutine rng_generate_single
  end interface

  abstract interface
    subroutine rng_generate_array (rng, x)
      import
      class(rng_t), intent(inout) :: rng
      real(default), dimension(:), intent(out) :: x
    end subroutine rng_generate_array
  end interface

```

```

    end subroutine rng_generate_array
end interface

```

These routines generate a single and an array of Gaussian (normal) distributed default-precision random numbers, respectively. Mean is 0 and $\sigma = 1$. Note that $z = \mu + \sigma x$ then distributes with mean μ and variance σ^2 .

The algorithm uses twice as much uniformly distributed random numbers, taken from the PDG review.

```

<RNG base: rng: TBP>+≡
  generic :: generate_gaussian => &
    rng_generate_gaussian_single, rng_generate_gaussian_array
  procedure, private :: rng_generate_gaussian_single
  procedure, private :: rng_generate_gaussian_array

<RNG base: procedures>≡
  subroutine rng_generate_gaussian_single (rng, x)
    class(rng_t), intent(inout) :: rng
    real(default), intent(out) :: x
    real(default), dimension(2) :: u
    call rng%generate (u)
    x = sin (twopi * u(1)) * sqrt (- 2 * log (u(2)))
  end subroutine rng_generate_gaussian_single

  subroutine rng_generate_gaussian_array (rng, x)
    class(rng_t), intent(inout) :: rng
    real(default), dimension(:), intent(out) :: x
    integer :: i
    do i = 1, size (x)
      call rng%generate_gaussian (x(i))
    end do
  end subroutine rng_generate_gaussian_array

```

8.1.2 RNG Factory

A factory object has a `make` method that allocates and initializes a new generator of appropriate type. It uses a 16-bit integer for initialization. For a real-life implementation, the factory should return a sequence of statistically independent generators, and for different seeds, the sequences should also be independent.

```

<RNG base: public>+≡
  public :: rng_factory_t

<RNG base: types>+≡
  type, abstract :: rng_factory_t
  contains
    <RNG base: rng factory: TBP>
  end type rng_factory_t

```

Output. Should be short, just report the seed and current state of the factory.

```

<RNG base: rng factory: TBP>≡
  procedure (rng_factory_write), deferred :: write

```

```

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_factory_write (object, unit)
      import
      class(rng_factory_t), intent(in) :: object
      integer, intent(in), optional :: unit
    end subroutine rng_factory_write
  end interface

```

Initialize. It should be possible to do this repeatedly, resetting the state. The default seed should be 0.

```

<RNG base: rng factory: TBP>+≡
  procedure (rng_factory_init), deferred :: init

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_factory_init (factory, seed)
      import
      class(rng_factory_t), intent(out) :: factory
      integer(i16), intent(in), optional :: seed
    end subroutine rng_factory_init
  end interface

```

Spawn a new generator.

```

<RNG base: rng factory: TBP>+≡
  procedure (rng_factory_make), deferred :: make

<RNG base: interfaces>+≡
  abstract interface
    subroutine rng_factory_make (factory, rng)
      import
      class(rng_factory_t), intent(inout) :: factory
      class(rng_t), intent(out), allocatable :: rng
    end subroutine rng_factory_make
  end interface

```

8.1.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<rng_base_ut.f90>≡
  <File header>

  module rng_base_ut
    use unit_tests
    use rng_base_uti

    <Standard module head>

    <RNG base: public test>

    <RNG base: public test auxiliary>

```

```

contains

  <RNG base: test driver>

end module rng_base_ut

<rng_base_util.f90>≡
  <File header>

module rng_base_util

  <Use kinds>
    use kinds, only: i16
    use format_utils, only: write_indent
    use io_units

    use rng_base

  <Standard module head>

  <RNG base: public test auxiliary>

  <RNG base: test declarations>

  <RNG base: test types>

contains

  <RNG base: tests>

  <RNG base: test auxiliary>

end module rng_base_util
API: driver for the unit tests below.
<RNG base: public test>≡
  public :: rng_base_test
<RNG base: test driver>≡
  subroutine rng_base_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <RNG base: execute tests>
  end subroutine rng_base_test

```

Test generator

The test 'mock' random generator generates a repeating series with the numbers 0.1, 0.3, 0.5, 0.7, 0.9. It has an integer stored as state. The integer must be one of 1, 3, 5, 7, 9.

```

<RNG base: public test auxiliary>≡
  public :: rng_test_t

```

```

<RNG base: test types>≡
type, extends (rng_t) :: rng_test_t
  integer :: state = 1
contains
  procedure :: write => rng_test_write
  procedure :: init => rng_test_init
  procedure :: final => rng_test_final
  procedure :: generate_single => rng_test_generate_single
  procedure :: generate_array => rng_test_generate_array
end type rng_test_t

```

Output. The state is a single number, so print it.

```

<RNG base: test auxiliary>≡
subroutine rng_test_write (rng, unit, indent)
  class(rng_test_t), intent(in) :: rng
  integer, intent(in), optional :: unit, indent
  integer :: u, ind
  u = given_output_unit (unit)
  ind = 0; if (present (indent)) ind = indent
  call write_indent (u, ind)
  write (u, "(A,IO,A)") "Random-number generator: &
    &test (state = ", rng%state, ")"
end subroutine rng_test_write

```

The default seed is 1.

```

<RNG base: test auxiliary>+≡
subroutine rng_test_init (rng, seed)
  class(rng_test_t), intent(out) :: rng
  integer, intent(in), optional :: seed
  if (present (seed)) rng%state = seed
end subroutine rng_test_init

```

Nothing to finalize:

```

<RNG base: test auxiliary>+≡
subroutine rng_test_final (rng)
  class(rng_test_t), intent(inout) :: rng
end subroutine rng_test_final

```

Generate a single number and advance the state.

```

<RNG base: test auxiliary>+≡
subroutine rng_test_generate_single (rng, x)
  class(rng_test_t), intent(inout) :: rng
  real(default), intent(out) :: x
  x = rng%state / 10._default
  rng%state = mod (rng%state + 2, 10)
end subroutine rng_test_generate_single

```

The array generator calls the single-item generator multiple times.

```

<RNG base: test auxiliary>+≡
subroutine rng_test_generate_array (rng, x)
  class(rng_test_t), intent(inout) :: rng

```

```

    real(default), dimension(:), intent(out) :: x
    integer :: i
    do i = 1, size (x)
        call rng%generate (x(i))
    end do
end subroutine rng_test_generate_array

```

Test Factory

This factory makes `rng_test_t` generators, initialized with integers 1, 3, 5, 7, 9 if given the input 0, 1, 2, 3, 4. The generators within one sequence are all identical, however.

```

<RNG base: public test auxiliary>+≡
    public :: rng_test_factory_t

<RNG base: test types>+≡
    type, extends (rng_factory_t) :: rng_test_factory_t
        integer :: seed = 1
    contains
        <RNG base: rng test factory: TBP>
    end type rng_test_factory_t

```

Output.

```

<RNG base: rng test factory: TBP>≡
    procedure :: write => rng_test_factory_write

<RNG base: test auxiliary>+≡
    subroutine rng_test_factory_write (object, unit)
        class(rng_test_factory_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A,I0,A)") "RNG factory: test (", object%seed, ")"
    end subroutine rng_test_factory_write

```

Initialize, translating the given seed.

```

<RNG base: rng test factory: TBP>+≡
    procedure :: init => rng_test_factory_init

<RNG base: test auxiliary>+≡
    subroutine rng_test_factory_init (factory, seed)
        class(rng_test_factory_t), intent(out) :: factory
        integer(i16), intent(in), optional :: seed
        if (present (seed)) factory%seed = mod (seed * 2 + 1, 10)
    end subroutine rng_test_factory_init

```

```

<RNG base: rng test factory: TBP>+≡
    procedure :: make => rng_test_factory_make

```

```

<RNG base: test auxiliary>+≡
  subroutine rng_test_factory_make (factory, rng)
    class(rng_test_factory_t), intent(inout) :: factory
    class(rng_t), intent(out), allocatable :: rng
    allocate (rng_test_t :: rng)
    select type (rng)
    type is (rng_test_t)
      call rng%init (int (factory%seed))
    end select
  end subroutine rng_test_factory_make

```

Generator check

Initialize the generator and draw random numbers.

```

<RNG base: execute tests>≡
  call test (rng_base_1, "rng_base_1", &
    "rng initialization and call", &
    u, results)

<RNG base: test declarations>≡
  public :: rng_base_1

<RNG base: tests>≡
  subroutine rng_base_1 (u)
    integer, intent(in) :: u
    class(rng_t), allocatable :: rng

    real(default) :: x
    real(default), dimension(2) :: x2

    write (u, "(A)")  "* Test output: rng_base_1"
    write (u, "(A)")  "* Purpose: initialize and call a test random-number &
      &generator"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize generator"
    write (u, "(A)")

    allocate (rng_test_t :: rng)
    call rng%init (3)

    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Get random number"
    write (u, "(A)")

    call rng%generate (x)
    write (u, "(A,2(1x,F9.7))")  "x =", x

    write (u, "(A)")
    write (u, "(A)")  "* Get random number pair"
    write (u, "(A)")

```



```

call rng%generate (x2)
write (u, "(A,2(1x,F9.7))")  "x =", x2

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_base_1"

end subroutine rng_base_1

```

Factory check

Set up a factory and spawn generators.

```

<RNG base: execute tests>+≡
  call test (rng_base_2, "rng_base_2", &
    "rng factory", &
    u, results)

<RNG base: test declarations>+≡
  public :: rng_base_2

<RNG base: tests>+≡
  subroutine rng_base_2 (u)
    integer, intent(in) :: u
    type(rng_test_factory_t) :: rng_factory
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: rng_base_2"
    write (u, "(A)")  "* Purpose: initialize and use a rng factory"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize factory"
    write (u, "(A)")

    call rng_factory%init ()
    call rng_factory%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Make a generator"
    write (u, "(A)")

    call rng_factory%make (rng)
    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call rng%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: rng_base_2"

```

```
end subroutine rng_base_2
```

8.2 Select from a weighted sample

```
<selectors.f90>≡  
  <File header>  
  
  module selectors  
  
    <Use kinds>  
    use io_units  
    use diagnostics  
    use format_defs, only: FMT_14, FMT_19  
    use rng_base  
  
    <Standard module head>  
  
    <Selectors: public>  
  
    <Selectors: types>  
  
    contains  
  
    <Selectors: procedures>  
  
  end module selectors
```

8.2.1 Selector type

The rng object is actually the state of the random-number generator. The methods initialize/reset and call the generator for this state.

```
<Selectors: public>≡  
  public :: selector_t  
  
<Selectors: types>≡  
  type :: selector_t  
    integer :: offset = 0  
    integer, dimension(:), allocatable :: map  
    real(default), dimension(:), allocatable :: weight  
    real(default), dimension(:), allocatable :: acc  
    contains  
    <Selectors: selector: TBP>  
  end type selector_t
```

Display contents.

```
<Selectors: selector: TBP>≡  
  procedure :: write => selector_write  
  
<Selectors: procedures>≡  
  subroutine selector_write (object, unit, testflag)  
    class(selector_t), intent(in) :: object  
    integer, intent(in), optional :: unit  
    logical, intent(in), optional :: testflag  
    integer :: u, i  
    logical :: truncate  
    u = given_output_unit (unit)
```

```

truncate = .false.; if (present (testflag)) truncate = testflag
write (u, "(1x,A)") "Selector: i, weight, acc. weight"
if (allocated (object%weight)) then
  do i = 1, size (object%weight)
    if (truncate) then
      write (u, "(3x,I0,2(1x," // FMT_14 // ")") &
        object%map(i), object%weight(i), object%acc(i)
    else
      write (u, "(3x,I0,2(1x," // FMT_19 // ")") &
        object%map(i), object%weight(i), object%acc(i)
    end if
  end do
else
  write (u, "(3x,A)") "[undefined]"
end if
end subroutine selector_write

```

We pack the input weight array such that zero-weight entries are removed. We also normalize it. This makes a `map` array for mapping the selected weight to the actual entry necessary.

We may encounter a case where all weights are zero. We do not reject this, but set up the selector so that it always returns the first entry.

```

⟨Selectors: selector: TBP⟩+≡
  procedure :: init => selector_init
⟨Selectors: procedures⟩+≡
  subroutine selector_init (selector, weight, negative_weights, offset)
    class(selector_t), intent(out) :: selector
    real(default), dimension(:), intent(in) :: weight
    logical, intent(in), optional :: negative_weights
    integer, intent(in), optional :: offset
    real(default) :: s
    integer :: n, i
    logical :: neg_wgt
    logical, dimension(:), allocatable :: mask
    if (present (offset)) selector%offset = offset
    if (size (weight) == 0) &
      call msg_bug ("Selector init: zero-size weight array")
    neg_wgt = .false.
    if (present (negative_weights)) neg_wgt = negative_weights
    if (.not. neg_wgt .and. any (weight < 0)) &
      call msg_fatal ("Selector init: negative weight encountered")
    s = sum (weight)
    allocate (mask (size (weight)), &
      source = weight /= 0)
    n = count (mask)
    if (n > 0) then
      allocate (selector%map (n), &
        source = pack ([i + selector%offset, i = 1, size (weight)], mask))
      allocate (selector%weight (n), &
        source = pack (abs (weight) / s, mask))
      allocate (selector%acc (n))
      selector%acc(1) = selector%weight(1)
      do i = 2, n - 1

```

```

        selector%acc(i) = selector%acc(i-1) + selector%weight(i)
    end do
    selector%acc(n) = 1
else
    allocate (selector%map (1), source = 1)
    allocate (selector%weight (1), source = 0._default)
    allocate (selector%acc (1), source = 1._default)
end if
end subroutine selector_init

```

Select an entry based upon the number x , which should be a uniformly distributed random number between 0 and 1.

```

⟨Selectors: selector: TBP⟩+≡
    procedure :: select => selector_select

⟨Selectors: procedures⟩+≡
    function selector_select (selector, x) result (n)
        class(selector_t), intent(in) :: selector
        real(default), intent(in) :: x
        integer :: n
        integer :: i
        if (x < 0 .or. x > 1) &
            call msg_bug ("Selector: random number out of range")
        do i = 1, size (selector%acc)
            if (x <= selector%acc(i)) exit
        end do
        n = selector%map(i)
    end function selector_select

```

Use the provided random-number generator to select an entry. (Unless there is only one entry.)

```

⟨Selectors: selector: TBP⟩+≡
    procedure :: generate => selector_generate

⟨Selectors: procedures⟩+≡
    subroutine selector_generate (selector, rng, n)
        class(selector_t), intent(in) :: selector
        class(rng_t), intent(inout) :: rng
        integer, intent(out) :: n
        real(default) :: x
        select case (size (selector%acc))
        case (1)
            n = selector%map(1)
        case default
            call rng%generate (x)
            n = selector%select (x)
        end select
    end subroutine selector_generate

```

Determine the normalized weight for a selected entry. We use a linear search for the inverse lookup, assuming that efficiency is not an issue for this function.

```

⟨Selectors: selector: TBP⟩+≡
    procedure :: get_weight => selector_get_weight

```

```

<Selectors: procedures>+≡
  function selector_get_weight (selector, n) result (weight)
    class(selector_t), intent(in) :: selector
    integer, intent(in) :: n
    real(default) :: weight
    integer :: i
    do i = 1, size (selector%weight)
      if (selector%map(i) == n) then
        weight = selector%weight(i)
        return
      end if
    end do
    weight = 0
  end function selector_get_weight

```

8.2.2 Unit tests

Test module, followed by the corresponding implementation module.

```

<selectors_ut.f90>≡
  <File header>

  module selectors_ut
    use unit_tests
    use selectors_uti

    <Standard module head>

    <Selectors: public test>

    contains

    <Selectors: test driver>

  end module selectors_ut

<selectors_uti.f90>≡
  <File header>

  module selectors_uti

    <Use kinds>
    use rng_base

    use selectors

    use rng_base_ut, only: rng_test_t

    <Standard module head>

    <Selectors: test declarations>

    contains

```

<Selectors: tests>

end module selectors_util

API: driver for the unit tests below.

<Selectors: public test>≡

public :: selectors_test

<Selectors: test driver>≡

subroutine selectors_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Selectors: execute tests>

end subroutine selectors_test

Basic check

Initialize the selector and draw random numbers.

<Selectors: execute tests>≡

call test (selectors_1, "selectors_1", &
"initialize, generate, query", &
u, results)

<Selectors: test declarations>≡

public :: selectors_1

<Selectors: tests>≡

subroutine selectors_1 (u)

integer, intent(in) :: u

type(selector_t) :: selector

class(rng_t), allocatable, target :: rng

integer :: i, n

write (u, "(A)") "* Test output: selectors_1"

write (u, "(A)") "* Purpose: initialize a selector and test it"

write (u, "(A)")

write (u, "(A)") "* Initialize selector"

write (u, "(A)")

call selector%init &

 ([2._default, 3.5_default, 0._default, &

 2._default, 0.5_default, 2._default])

call selector%write (u)

write (u, "(A)")

write (u, "(A)") "* Select numbers using predictable test generator"

write (u, "(A)")

allocate (rng_test_t :: rng)

call rng%init (1)

do i = 1, 5

 call selector%generate (rng, n)

 write (u, "(1x,I0)") n

```

end do

write (u, "(A)")
write (u, "(A)")  "* Select numbers using real input number"
write (u, "(A)")

write (u, "(1x,A,I0)") "select(0.00) = ", selector%select (0._default)
write (u, "(1x,A,I0)") "select(0.77) = ", selector%select (0.77_default)
write (u, "(1x,A,I0)") "select(1.00) = ", selector%select (1._default)

write (u, "(A)")
write (u, "(A)")  "* Get weight"
write (u, "(A)")

write (u, "(1x,A,ES19.12)") "weight(2) =", selector%get_weight(2)
write (u, "(1x,A,ES19.12)") "weight(3) =", selector%get_weight(3)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: selectors_1"

end subroutine selectors_1

```

Offset

Same tests with a -1 offset on all indices, i.e., counting from zero.

```

<Selectors: execute tests>+≡
  call test (selectors_2, "selectors_2", &
    "handle index offset", &
    u, results)

<Selectors: test declarations>+≡
  public :: selectors_2

<Selectors: tests>+≡
  subroutine selectors_2 (u)
    integer, intent(in) :: u
    type(selector_t) :: selector
    class(rng_t), allocatable, target :: rng
    integer :: i, n

    write (u, "(A)")  "* Test output: selectors_2"
    write (u, "(A)")  "* Purpose: initialize and use a selector &
      &with offset index"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize selector"
    write (u, "(A)")

    call selector%init &

```



```

        ([2._default, 3.5_default, 0._default, &
         2._default, 0.5_default, 2._default], &
         offset = -1)
    call selector%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Select numbers using predictable test generator"
    write (u, "(A)")

    allocate (rng_test_t :: rng)
    call rng%init (1)

    do i = 1, 5
        call selector%generate (rng, n)
        write (u, "(1x,I0)")  n
    end do

    write (u, "(A)")
    write (u, "(A)")  "* Select numbers using real input number"
    write (u, "(A)")

    write (u, "(1x,A,I0)")  "select(0.00) = ", selector%select (0._default)
    write (u, "(1x,A,I0)")  "select(0.77) = ", selector%select (0.77_default)
    write (u, "(1x,A,I0)")  "select(1.00) = ", selector%select (1._default)

    write (u, "(A)")
    write (u, "(A)")  "* Get weight"
    write (u, "(A)")

    write (u, "(1x,A,ES19.12)")  "weight(1) =", selector%get_weight(1)
    write (u, "(1x,A,ES19.12)")  "weight(2) =", selector%get_weight(2)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call rng%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: selectors_2"

end subroutine selectors_2

```

8.3 TAO Random-Number Generator

This module provides an implementation for the generic random-number generator. Actually, we interface the TAO random-number generator which is available via the VAMP package.

```

<rng_tao.f90>≡
  <File header>

```

```

module rng_tao

```

```

<Use kinds>
  use io_units
  use format_utils, only: write_indent
  use tao_random_numbers !NODEP!

  use rng_base

<Standard module head>

<RNG tao: public>

<RNG tao: types>

contains

<RNG tao: procedures>

end module rng_tao

```

8.3.1 Generator type

The rng object is actually the state of the random-number generator. The methods initialize/reset and call the generator for this state.

We keep the seed, in case we want to recover it later, and count the number of calls since seeding.

```

<RNG tao: public>≡
  public :: rng_tao_t

<RNG tao: types>≡
  type, extends (rng_t) :: rng_tao_t
    integer :: seed = 0
    integer :: n_calls = 0
    type(tao_random_state) :: state
  contains
    <RNG tao: rng tao: TBP>
  end type rng_tao_t

```

Output: Display seed and number of calls.

```

<RNG tao: rng tao: TBP>≡
  procedure :: write => rng_tao_write

<RNG tao: procedures>≡
  subroutine rng_tao_write (rng, unit, indent)
    class(rng_tao_t), intent(in) :: rng
    integer, intent(in), optional :: unit, indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(A)") "TA0 random-number generator:"
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") "seed = ", rng%seed
  end subroutine rng_tao_write

```

```

    call write_indent (u, ind)
    write (u, "(2x,A,I0)") "calls = ", rng%n_calls
end subroutine rng_tao_write

```

The `init` method initializes the generator and sets a seed. We should implement the interface such that a single integer is sufficient for a seed.

The seed may be omitted. The default seed is 0.

```

(RNG tao: rng tao: TBP)+≡
  procedure :: init => rng_tao_init

(RNG tao: procedures)+≡
  subroutine rng_tao_init (rng, seed)
    class(rng_tao_t), intent(out) :: rng
    integer, intent(in), optional :: seed
    if (present (seed)) rng%seed = seed
    call tao_random_create (rng%state, rng%seed)
  end subroutine rng_tao_init

```

The `final` method deallocates memory where necessary and allows for another call of `init` to reset the generator.

```

(RNG tao: rng tao: TBP)+≡
  procedure :: final => rng_tao_final

(RNG tao: procedures)+≡
  subroutine rng_tao_final (rng)
    class(rng_tao_t), intent(inout) :: rng
    call tao_random_destroy (rng%state)
  end subroutine rng_tao_final

```

These routines generate a single and an array of default-precision random numbers, respectively.

We have to convert from explicit double to abstract default precision. Under normal conditions, both are equivalent, however. Unless, someone decides to do single precision, there is always an interface for `tao_random_numbers`.

```

(RNG tao: rng tao: TBP)+≡
  procedure :: generate_single => rng_tao_generate_single
  procedure :: generate_array => rng_tao_generate_array

(RNG tao: procedures)+≡
  subroutine rng_tao_generate_single (rng, x)
    class(rng_tao_t), intent(inout) :: rng
    real(default), intent(out) :: x
    real(default) :: r
    call tao_random_number (rng%state, r)
    x = r
    rng%n_calls = rng%n_calls + 1
  end subroutine rng_tao_generate_single

  subroutine rng_tao_generate_array (rng, x)
    class(rng_tao_t), intent(inout) :: rng
    real(default), dimension(:), intent(out) :: x
    real(default) :: r
    integer :: i

```

```

do i = 1, size (x)
  call tao_random_number (rng%state, r)
  x(i) = r
end do
rng%n_calls = rng%n_calls + size (x)
end subroutine rng_tao_generate_array

```

Factory

This factory makes `rng_tao_t` generators, initialized with the seeds

$$s_i = s_0 * 2^{16} + i \quad (8.1)$$

where s_0 is the seed (a 16-bit integer) given to the factory object, and i is the index in the generated sequence of generators, starting with zero.

```

<RNG tao: public>+≡
  public :: rng_tao_factory_t

<RNG tao: types>+≡
  type, extends (rng_factory_t) :: rng_tao_factory_t
    integer(i16) :: s = 0
    integer(i16) :: i = 0
  contains
    <RNG tao: rng tao factory: TBP>
  end type rng_tao_factory_t

```

Output.

```

<RNG tao: rng tao factory: TBP>≡
  procedure :: write => rng_tao_factory_write

<RNG tao: procedures>+≡
  subroutine rng_tao_factory_write (object, unit)
    class(rng_tao_factory_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,2(IO,A))") &
      "RNG factory: tao (", object%s, ",", object%i, ")"
  end subroutine rng_tao_factory_write

```

Initialize, translating the given seed.

```

<RNG tao: rng tao factory: TBP>+≡
  procedure :: init => rng_tao_factory_init

<RNG tao: procedures>+≡
  subroutine rng_tao_factory_init (factory, seed)
    class(rng_tao_factory_t), intent(out) :: factory
    integer(i16), intent(in), optional :: seed
    if (present (seed)) factory%s = seed
  end subroutine rng_tao_factory_init

```

```

<RNG tao: rng tao factory: TBP>+≡
  procedure :: make => rng_tao_factory_make

```

```

⟨RNG tao: procedures⟩+=
  subroutine rng_tao_factory_make (factory, rng)
    class(rng_tao_factory_t), intent(inout) :: factory
    class(rng_t), intent(out), allocatable :: rng
    allocate (rng_tao_t :: rng)
    select type (rng)
    type is (rng_tao_t)
      call rng%init (factory%s * 65536 + factory%i)
      factory%i = int (factory%i + 1, kind = i16)
    end select
  end subroutine rng_tao_factory_make

```

8.3.2 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨rng_tao.ut.f90⟩≡
  ⟨File header⟩

  module rng_tao_ut
    use unit_tests
    use rng_tao_uti

    ⟨Standard module head⟩

    ⟨RNG tao: public test⟩

    contains

    ⟨RNG tao: test driver⟩

  end module rng_tao_ut

⟨rng_tao.uti.f90⟩≡
  ⟨File header⟩

  module rng_tao_uti

    ⟨Use kinds⟩
    use kinds, only: i16
    use rng_base

    use rng_tao

    ⟨Standard module head⟩

    ⟨RNG tao: test declarations⟩

    contains

    ⟨RNG tao: tests⟩

  end module rng_tao_uti

```

API: driver for the unit tests below.

```
<RNG tao: public test>≡  
  public :: rng_tao_test  
  
<RNG tao: test driver>≡  
  subroutine rng_tao_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <RNG tao: execute tests>  
  end subroutine rng_tao_test
```

Generator check

Initialize the generator and draw random numbers.

```
<RNG tao: execute tests>≡  
  call test (rng_tao_1, "rng_tao_1", &  
    "rng initialization and call", &  
    u, results)  
  
<RNG tao: test declarations>≡  
  public :: rng_tao_1  
  
<RNG tao: tests>≡  
  subroutine rng_tao_1 (u)  
    integer, intent(in) :: u  
    class(rng_t), allocatable, target :: rng  
  
    real(default) :: x  
    real(default), dimension(2) :: x2  
  
    write (u, "(A)")  "* Test output: rng_tao_1"  
    write (u, "(A)")  "* Purpose: initialize and call the TAO random-number &  
      &generator"  
    write (u, "(A)")  
  
    write (u, "(A)")  "* Initialize generator (default seed)"  
    write (u, "(A)")  
  
    allocate (rng_tao_t :: rng)  
    call rng%init ()  
  
    call rng%write (u)  
  
    write (u, "(A)")  
    write (u, "(A)")  "* Get random number"  
    write (u, "(A)")  
  
    call rng%generate (x)  
    write (u, "(A,2(1x,F9.7))")  "x =", x  
  
    write (u, "(A)")  
    write (u, "(A)")  "* Get random number pair"  
    write (u, "(A)")
```

```

call rng%generate (x2)
write (u, "(A,2(1x,F9.7))") "x =", x2

write (u, "(A)")
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_tao_1"

end subroutine rng_tao_1

```

Factory check

Set up a factory and spawn generators.

```

<RNG tao: execute tests>+≡
  call test (rng_tao_2, "rng_tao_2", &
    "rng factory", &
    u, results)

<RNG tao: test declarations>+≡
  public :: rng_tao_2

<RNG tao: tests>+≡
  subroutine rng_tao_2 (u)
    integer, intent(in) :: u
    type(rng_tao_factory_t) :: rng_factory
    class(rng_t), allocatable :: rng
    real(default) :: x

    write (u, "(A)")  "* Test output: rng_tao_2"
    write (u, "(A)")  "* Purpose: initialize and use a rng factory"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize factory"
    write (u, "(A)")

    call rng_factory%init ()
    call rng_factory%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Make a generator"
    write (u, "(A)")

    call rng_factory%make (rng)
    call rng%write (u)
    call rng%generate (x)
    write (u, *)
    write (u, "(1x,A,F7.5)") "x = ", x
    call rng%final ()

```

```

deallocate (rng)

write (u, "(A)")
write (u, "(A)")  "* Repeat"
write (u, "(A)")

call rng_factory%make (rng)
call rng%write (u)
call rng%generate (x)
write (u, *)
write (u, "(1x,A,F7.5)")  "x = ", x
call rng%final ()
deallocate (rng)

write (u, *)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize factory with different seed"
write (u, "(A)")

call rng_factory%init (1_i16)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Make a generator"
write (u, "(A)")

call rng_factory%make (rng)
call rng%write (u)
call rng%generate (x)
write (u, *)
write (u, "(1x,A,F7.5)")  "x = ", x
call rng%final ()
deallocate (rng)

write (u, *)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_tao_2"

end subroutine rng_tao_2

```

8.4 RNG Stream

We implement the RNGstream proposed and implemented in C++, C and Java by L'Ecuyer et al. (L'Ecuyer, Pierre, Richard Simard, E. Jack Chen, and W. David Kelton. "An Object-Oriented Random-Number Package with Many Long Streams and Substreams." *Operations Research* 50, no. 6 (December 2002): 1073–1075. doi:10.1287/opre.50.6.1073.358.). RNGstream allows us to access

multiple independent streams of random numbers.

```

<rng_stream.f90>≡
  <File header>

  module rng_stream

    <Use kinds>
    use kinds, only: i16
    use io_units
    use format_utils, only: write_indent
    use diagnostics

    use rng_base

    <Standard module head>

    <RNG stream: parameters>

    <RNG stream: public>

    <RNG stream: types>

    contains

    <RNG stream: procedures>

  end module rng_stream

```

We store the current position in the stream of random numbers. Furthermore, we store the beginning of the (latest) substream and the initial starting point of the stream, which corresponds to the “seed”. The default seed is 1234.

```

<RNG stream: public>≡
  public :: rng_stream_t

<RNG stream: types>≡
  type, extends(rng_t) :: rng_stream_t
    private
    logical :: antithetic = .false.
    logical :: increased_precision = .false.
    real(default), dimension(3, 2) :: current_position = 1234._default
    real(default), dimension(3, 2) :: beginning_substream = 1234._default
    real(default), dimension(3, 2) :: initial_stream = 1234._default
  contains
    <RNG stream: rng stream: TBP>
  end type rng_stream_t

```

Output. Display current position and the (sub-)stream positions.

```

<RNG stream: rng stream: TBP>≡
  procedure, public :: write => rng_stream_write

<RNG stream: procedures>≡
  subroutine rng_stream_write (rng, unit, indent)
    class(rng_stream_t), intent(in) :: rng
    integer, intent(in), optional :: unit

```

```

integer, intent(in), optional :: indent
integer :: j, u, ind
u = given_output_unit (unit)
ind = 0; if (present (indent)) ind = indent
call write_indent (u, ind)
write (u, "(A)") "RNG Stream generator"
call write_indent (u, ind)
write (u, "(A)") "Current position = [ "
call write_indent (u, ind)
write (u, "(3(F20.1,' ',1X))") rng%current_position(:, 1)
call write_indent (u, ind)
write (u, "(3(F20.1,' ',1X))") rng%current_position(:, 2)
call write_indent (u, ind)
write (u, "(A)") "]"
call write_indent (u, ind)
write (u, "(A)") "Beginning substream = [ "
call write_indent (u, ind)
write (u, "(3(F20.1,' ',1X))") rng%beginning_substream(:, 1)
call write_indent (u, ind)
write (u, "(3(F20.1,' ',1X))") rng%beginning_substream(:, 2)
call write_indent (u, ind)
write (u, "(A)") "]"
call write_indent (u, ind)
write (u, "(A)") "Initial stream = [ "
call write_indent (u, ind)
write (u, "(3(F20.1,' ',1X))") rng%initial_stream(:, 1)
call write_indent (u, ind)
write (u, "(3(F20.1,' ',1X))") rng%initial_stream(:, 2)
call write_indent (u, ind)
write (u, "(A)") "]"
end subroutine rng_stream_write

```

Initialise the generator. Set the states to the (optional) seed.

```

<RNG stream: rng stream: TBP>+≡
  procedure, public :: init => rng_stream_init

<RNG stream: procedures>+≡
  subroutine rng_stream_init (rng, seed)
    class(rng_stream_t), intent(out) :: rng
    integer, intent(in), optional :: seed
    real(default), dimension(3, 2) :: real_seed
    if (present (seed)) then
      real_seed = real(seed, default)
      call rng%set_initial_stream (real_seed)
    end if
  end subroutine rng_stream_init

```

Finalize. Nothing to do.

```

<RNG stream: rng stream: TBP>+≡
  procedure, public :: final => rng_stream_final

<RNG stream: procedures>+≡
  subroutine rng_stream_final (rng)
    class(rng_stream_t), intent(inout) :: rng

```

```
end subroutine rng_stream_final
```

Set the initial stream, but test the seed before. They are not allowed to be 0 or larger than m_1 or m_2 .

```
<RNG stream: rng stream: TBP>+≡
  procedure, public :: set_initial_stream => rng_stream_set_initial_stream

<RNG stream: procedures>+≡
  subroutine rng_stream_set_initial_stream (rng, seed)
    class(rng_stream_t), intent(inout) :: rng
    real(default), dimension(3, 2), intent(in) :: seed
    if (any (seed(:, 1) > m1)) then
      write (msg_buffer, "(A, F20.1, 1X, A)") "ERROR: seed(:, 1) >= ", m1, ",&
        & Seed is not set."
      call msg_fatal ()
    end if
    if (any (seed(:, 2) > m2)) then
      write (msg_buffer, "(A, F20.1, 1X, A)") "ERROR: seed(:, 2) >= ", m2, ",&
        & Seed is not set."
      call msg_fatal ()
    end if
    if (any (seed(:, 1) == 0)) then
      write (msg_buffer, "(A, F20.1, 1X, A)") "ERROR: First 3 seed = 0."
      call msg_fatal ()
    end if
    if (any (seed(:, 2) == 0)) then
      write (msg_buffer, "(A, F20.1, 1X, A)") "ERROR: Last 3 seed = 0."
      call msg_fatal ()
    end if
    rng%initial_stream = seed
    call rng%reset_stream ()
  end subroutine rng_stream_set_initial_stream
```

Generate a single real random number from the current state of (sub-)stream.

The machine representation of the result can lead to negative numbers. We add m_1 or m_2 to the respective number to ensure they are all positive and are still congruent to $\text{mod } m_1$ or $\text{mod } m_2$.

The final formula $x = y(3, 1) - y(3, 2) \pmod{m_1}$ can lead to negative random numbers. Instead of directly calculating the modulo, we check whether $y(3, 1)$ is larger than $y(3, 2)$, or not. If $x(3, 1) > y(3, 2)$, then $y(3, 1) - y(3, 2)$ is congruent to $y(3, 1) - y(3, 2) \pmod{m_1}$. If $y(3, 1) < y(3, 2)$, then $y(3, 1) - y(3, 2) + m_1$ is congruent to $y(3, 1) - y(3, 2) \pmod{m_1}$.

```
<RNG stream: parameters>≡
  real(default), parameter :: &
    m1 = 4294967087.0_default, &
    m2 = 4294944443.0_default, &
    norm = 1.0_default / (m1 + 1.0_default)
  real(default), dimension(3, 3), parameter :: A1p0 = reshape (&
    [0.0_default, 1.0_default, 0.0_default, &
    0.0_default, 0.0_default, 1.0_default, &
    -810728.0_default, 1403580.0_default, 0.0_default], &
    shape (A1p0), order = [2, 1])
```

```

real(default), dimension(3, 3), parameter :: A2p0 = reshape (&
    [0.0_default, 1.0_default, 0.0_default, &
    0.0_default, 0.0_default, 1.0_default, &
    -1370589.0_default, 0.0_default, 527612.0_default], &
    shape (A2p0), order = [2, 1])

<RNG stream: rng stream: TBP>+≡
    procedure, public :: generate_single => rng_stream_generate_single

<RNG stream: procedures>+≡
    subroutine rng_stream_generate_single (rng, x)
        class(rng_stream_t), intent(inout) :: rng
        real(default), intent(out) :: x
        associate (y => rng%current_position)
            y(:, 1) = mod (matmul (A1p0, y(:, 1)), m1)
            if (y(3, 1) < 0.) y(3, 1) = y(3, 1) + m1
            y(:, 2) = mod (matmul (A2p0, y(:, 2)), m2)
            if (y(3, 2) < 0.) y(3, 2) = y(3, 2) + m2
            x = y(3, 1) - y(3, 2)
            if (x < 0.) x = x + m1
            x = x * norm
        end associate
        if (rng%antithetic) x = 1. - x
    end subroutine rng_stream_generate_single

```

Generate an array of real random numbers.

```

<RNG stream: rng stream: TBP>+≡
    procedure, public :: generate_array => rng_stream_generate_array

<RNG stream: procedures>+≡
    subroutine rng_stream_generate_array (rng, x)
        class(rng_stream_t), intent(inout) :: rng
        real(default), dimension(:), intent(out) :: x
        integer :: j
        do j = 1, size (x)
            call rng%generate_single(x(j))
        end do
    end subroutine rng_stream_generate_array

```

Reset to initial stream.

```

<RNG stream: rng stream: TBP>+≡
    procedure, public :: reset_stream => rng_stream_reset_stream

<RNG stream: procedures>+≡
    subroutine rng_stream_reset_stream (rng)
        class(rng_stream_t), intent(inout) :: rng
        rng%current_position = rng%initial_stream
        rng%beginning_substream = rng%initial_stream
    end subroutine rng_stream_reset_stream

```

Reset to beginning of substream.

```

<RNG stream: rng stream: TBP>+≡
    procedure, public :: reset_substream => rng_stream_reset_substream

```

```

(RNG stream: procedures)+≡
  subroutine rng_stream_reset_substream (rng)
    class(rng_stream_t), intent(inout) :: rng
    rng%current_position = rng%beginning_substream
  end subroutine rng_stream_reset_substream

```

Advance to next substream.

```

(RNG stream: parameters)+≡
  real(default), dimension(3, 3), parameter :: A1p76 = reshape (&
    [82758667.0_default, 1871391091.0_default, 4127413238.0_default, &
    3672831523.0_default, 69195019.0_default, 1871391091.0_default, &
    3672091415.0_default, 352874325.0_default, 69195019.0_default], &
    shape(A1p76), order = [2, 1])
  real(default), dimension(3, 3), parameter :: A2p76 = reshape (&
    [1511326704.0_default, 3759209742.0_default, 1610795712.0_default, &
    4292754251.0_default, 1511326704.0_default, 3889917532.0_default, &
    3859662829.0_default, 4292754251.0_default, 3708466080.0_default], &
    shape(A2p76), order = [2, 1])

```

```

(RNG stream: rng stream: TBP)+≡
  procedure, public :: next_substream => rng_stream_next_substream

```

```

(RNG stream: procedures)+≡
  subroutine rng_stream_next_substream (rng)
    class(rng_stream_t), intent(inout) :: rng
    associate (x => rng%beginning_substream)
      x(:,1) = matmul_mod (A1p76, x(:,1), m1)
      x(:,2) = matmul_mod (A2p76, x(:,2), m2)
    end associate
    call rng%reset_substream ()
  end subroutine rng_stream_next_substream

```

Advance state of the current stream by n steps. We do not touch the beginning of the substream nor the initial stream. The purpose of the procedure is to reproduce the same random number (streams) among multiple workers without additional communication cost. E.g. worker 1 needs the first 5000 random numbers and the second one needs the next 5000 random numbers. In such a way we can exactly reproduce results (upon numerical noise) in single or parallel runs with the RngStream. The procedure must only be used with care! Misuse can lead to wrong results!

```

(RNG stream: parameter)+≡
  real(default), dimension(3, 3), parameter :: A1p0 = reshape (&
    [0.0_default, 1.0_default, 0.0_default, &
    0.0_default, 0.0_default, 1.0_default, &
    -810728.0_default, 1403580.0_default, 0.0_default], &
    shape(A1p0), order = [2, 1])
  real(default), dimension(3, 3), parameter :: A2p0 = reshape (&
    [0.0_default, 1.0_default, 0.0_default, &
    0.0_default, 0.0_default, 1.0_default, &
    -1370589.0_default, 0.0_default, 527612.0_default], &
    shape(A2p0), order = [2, 1])

```

```

(RNG stream: rng stream: TBP)+≡
  procedure, public :: advance_state => rng_stream_advance_state

```

```

<RNG stream: procedures>+≡
subroutine rng_stream_advance_state (rng, n)
  class(rng_stream_t), intent(inout) :: rng
  integer, intent(in) :: n
  real(default), dimension(3, 3) :: A1pn, A2pn
  associate (x => rng%current_position)
    A1pn = matpow_mod (A1p0, m1, n)
    A2pn = matpow_mod (A2p0, m2, n)
    x(:,1) = matmul_mod (A1pn, x(:,1), m1)
    x(:,2) = matmul_mod (A2pn, x(:,2), m2)
  end associate
end subroutine rng_stream_advance_state

```

A divide and conquer algorithm is applied to calculate $A^n \bmod m$. We refer to the original paper from L'Ecuyer for further reading.

```

<RNG stream: procedures>+≡
function matpow_mod (a, m, n) result (c)
  real(default), dimension(3, 3), intent(in) :: a
  real(default), intent(in) :: m
  integer, intent(in) :: n
  real(default), dimension(3, 3) :: c
  real(default), dimension(3, 3) :: w
  integer :: i
  w = a
  c = 0.; forall (i = 1:3) c(i, i) = 1.
  i = n
  do while (i > 0)
    if (mod(i, 2) /= 0) c = matmat_mod (w, c, m)
    w = matmat_mod (w, w, m)
    i = i / 2
  end do
end function matpow_mod

function matmat_mod (a, b, m) result (c)
  real(default), dimension(3, 3), intent(in) :: a
  real(default), dimension(3, 3), intent(in) :: b
  real(default), dimension(3, 3) :: c
  real(default), intent(in) :: m
  integer :: i
  do i = 1, 3
    c(:, i) = matmul_mod (a, b(:, i), m)
  end do
end function matmat_mod

```

8.4.1 Factory

We utilize the streams proposed by L'Ecuyer where we use precalculated transition matrices to jump between different (sub-)streams.

The random generator has the period ρ and the transition function $T : s_n \rightarrow s_{n+1}$ whereas s_n is the generator's state after n steps. Furthermore, it is $T^\rho(s) = s$. The stream of random number then is disjoint into streams and

substreams. The length of the streams, which divide the overall stream, should be $Z = 2^z$ and partition those streams again in $V = 2^v$ substreams of length $W = 2^w$.

We store the seed and the initial stream, also, the beginning of the substream.

```

<RNG stream: public>+≡
  public :: rng_stream_factory_t

<RNG stream: types>+≡
  type, extends(rng_factory_t) :: rng_stream_factory_t
    real(default), dimension(3, 2) :: seed = 1234._default
    contains
    <RNG stream: rng stream factory: TBP>
  end type rng_stream_factory_t

```

Output.

```

<RNG stream: rng stream factory: TBP>≡
  procedure, public :: write => rng_stream_factory_write

<RNG stream: procedures>+≡
  subroutine rng_stream_factory_write (object, unit)
    class(rng_stream_factory_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "RNG Stream factory"
    write (u, "(1x,A,6(F20.1,' ',1X),A)") "Next seed = [ "
    write (u, "(1x,3(F20.1,' ',1X))") object%seed(:, 1)
    write (u, "(1x,3(F20.1,' ',1X))") object%seed(:, 2)
    write (u, "(1x,A)") "]"
  end subroutine rng_stream_factory_write

```

Initialize. Default seed is 1234. We do not check whether the seed is valid, this is later done in `rng_stream_init`.

Additionally, we have to explicitly convert from `integer` to `real` because we are using floating-point arithmetic and not integer arithmetic due to a larger set of number in the representation of real numbers.

```

<RNG stream: rng stream factory: TBP>+≡
  procedure, public :: init => rng_stream_factory_init

<RNG stream: procedures>+≡
  subroutine rng_stream_factory_init (factory, seed)
    class(rng_stream_factory_t), intent(out) :: factory
    integer(i16), intent(in), optional :: seed
    real(default), dimension(3, 2) :: real_seed
    if (present (seed)) then
      factory%seed = real(seed, default)
    end if
  end subroutine rng_stream_factory_init

```

Allocate a new RNG and different stream states, accordingly.

```

<RNG stream: rng stream factory: TBP>+≡
  procedure, public :: make => rng_stream_factory_make

```

```

(RNG stream: procedures)+≡
subroutine rng_stream_factory_make (factory, rng)
  class(rng_stream_factory_t), intent(inout) :: factory
  class(rng_t), intent(out), allocatable :: rng
  allocate (rng_stream_t :: rng)
  select type (rng)
  type is (rng_stream_t)
    call rng%init ()
    call rng%set_initial_stream (factory%seed)
  end select
  call factory%advance_seed ()
end subroutine rng_stream_factory_make

```

Advance seed. Use the precalculated transistion matrices for the streams.

```

(RNG stream: parameters)+≡
real(default), dimension(3,3), parameter :: A1p127 = reshape (&
  [2427906178.0_default, 3580155704.0_default, 949770784.0_default, &
  226153695.0_default, 1230515664.0_default, 3580155704.0_default, &
  1988835001.0_default, 986791581.0_default, 1230515664.0_default], &
  shape(A1p127), order = [2, 1])
real(default), dimension(3,3), parameter :: A2p127 = reshape (&
  [1464411153.0_default, 277697599.0_default, 1610723613.0_default, &
  32183930.0_default, 1464411153.0_default, 1022607788.0_default, &
  2824425944.0_default, 32183930.0_default, 2093834863.0_default], &
  shape(A2p127), order = [2, 1])

```

```

(RNG stream: rng stream factory: TBP)+≡
procedure, private :: advance_seed => rng_stream_factory_advance_seed

```

```

(RNG stream: procedures)+≡
subroutine rng_stream_factory_advance_seed (factory)
  class(rng_stream_factory_t), intent(inout) :: factory
  factory%seed(:,1) = matmul_mod (A1p127, factory%seed(:,1), m1)
  factory%seed(:,2) = matmul_mod (A2p127, factory%seed(:,2), m2)
end subroutine rng_stream_factory_advance_seed

```

Matrix modulo calculation optimized for 2^{53} representation of floating numbers. Speed efficiency is not a requirement, because the streams should not be advanced that often.

```

(RNG stream: public)+≡
private :: matmul_mod

(RNG stream: procedures)+≡
function matmul_mod (a, u, m) result (v)
  real(default), dimension(:, :), intent(in) :: a
  real(default), dimension(:), intent(in) :: u
  real(default), intent(in) :: m
  real(default), dimension(size (u)) :: v
  integer :: i
  do i = 1, 3
    v(i) = mult_mod (a(i, 1), u(1), 0.0_default, m)
    v(i) = mult_mod (a(i, 2), u(2), v(i), m)
    v(i) = mult_mod (a(i, 3), u(3), v(i), m)
  end do

```



```
end function matmul_mod
```

Decompose.

Decomposition to ensure exact accuracy for the case v exceeds 2^{53} .

$$a \cdot smodm = ((a1 \cdot s \bmod m) * 2^{17} + a2 \cdot s) \bmod m.$$

```

⟨RNG stream: parameters⟩+≡
  real(default), parameter :: &
    a12 = 1403580.0_default, &
    a13n = 810728.0_default, &
    a21 = 527612.0_default, &
    a23n = 1370589.0_default, &
    two53 = 9007199254740992.0_default, &
    two17 = 131072.0_default

⟨RNG stream: public⟩+≡
  private :: mult_mod

⟨RNG stream: procedures⟩+≡
  function mult_mod (a, b, c, m) result (v)
    real(default), intent(in) :: a
    real(default), intent(in) :: b
    real(default), intent(in) :: c
    real(default), intent(in) :: m
    real(default) :: v
    integer :: a1
    real(default) :: a2
    v = a * b + c
    if (v >= two53 .or. v <= -two53) then
      a1 = int (a / two17)
      a2 = a - a1 * two17
      v = mod (a1 * b, m)
      v = v * two17 + a2 * b + c
    end if
    v = mod (v, m)
    if (v < 0.0) v = v + m
  end function mult_mod

```

8.4.2 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨rng_stream_ut.f90⟩≡
  ⟨File header⟩

  module rng_stream_ut
    use unit_tests
    use rng_stream_uti

    ⟨Standard module head⟩

    ⟨RNG stream: public test⟩

```

```

contains

  <RNG stream: test driver>

  end module rng_stream_ut

  <rng_stream_util.f90>≡
  <File header>

  module rng_stream_util

    <Use kinds>
    use kinds, only: i16
    use rng_base

    use rng_stream

    <Standard module head>

    <RNG stream: test declarations>

    contains

    <RNG stream: tests>

  end module rng_stream_util
API: driver for the unit tests below.
  <RNG stream: public test>≡
    public :: rng_stream_test
  <RNG stream: test driver>≡
    subroutine rng_stream_test (u, results)
      integer, intent(in) :: u
      type(test_results_t), intent(inout) :: results
    <RNG stream: execute tests>
    end subroutine rng_stream_test

```

Generator check

Initialize the generator and draw random numbers.

```

  <RNG stream: execute tests>≡
    call test (rng_stream_1, "rng_stream_1", &
      "rng initialization and call", &
      u, results)
  <RNG stream: test declarations>≡
    public :: rng_stream_1
  <RNG stream: tests>≡
    subroutine rng_stream_1 (u)
      integer, intent(in) :: u
      class(rng_t), allocatable, target :: rng

      real(default) :: x

```

```

real(default), dimension(2) :: x2

write (u, "(A)")  "* Test output: rng_stream_1"
write (u, "(A)")  "* Purpose: initialize and call the RNGstream random-number &
    &generator"
write (u, "(A)")

write (u, "(A)")  "* Initialize generator (default seed)"
write (u, "(A)")

allocate (rng_stream_t :: rng)
call rng%init ()

call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Get random number"
write (u, "(A)")

call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
write (u, "(A)")  "* Get random number pair"
write (u, "(A)")

call rng%generate (x2)
write (u, "(A,2(1x,F9.7))")  "x =", x2

write (u, "(A)")
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Jump to next substream and get random number"
write (u, "(A)")

select type (rng)
type is (rng_stream_t)
    call rng%next_substream ()
end select
call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_stream_1"

```

```
end subroutine rng_stream_1
```

Factory check

Set up a factory and spawn generators.

```
<RNG stream: execute tests>+≡
  call test (rng_stream_2, "rng_stream_2", &
    "rng_factory", &
    u, results)

<RNG stream: test declarations>+≡
  public :: rng_stream_2

<RNG stream: tests>+≡
  subroutine rng_stream_2 (u)
    integer, intent(in) :: u
    type(rng_stream_factory_t) :: rng_factory
    class(rng_t), allocatable :: rng
    real(default) :: x

    write (u, "(A)")  "* Test output: rng_stream_2"
    write (u, "(A)")  "* Purpose: initialize and use a rng factory"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize factory"
    write (u, "(A)")

    call rng_factory%init ()
    call rng_factory%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Make a generator"
    write (u, "(A)")

    call rng_factory%make (rng)
    call rng%write (u)
    call rng%generate (x)
    write (u, *)
    write (u, "(1x,A,F7.5)")  "x = ", x
    call rng%final ()
    deallocate (rng)

    write (u, "(A)")
    write (u, "(A)")  "* Repeat"
    write (u, "(A)")

    call rng_factory%make (rng)
    call rng%write (u)
    call rng%generate (x)
    write (u, *)
    write (u, "(1x,A,F7.5)")  "x = ", x
    call rng%final ()
    deallocate (rng)
```

```

write (u, *)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize factory with different seed"
write (u, "(A)")

call rng_factory%init (1_i16)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Make a generator"
write (u, "(A)")

call rng_factory%make (rng)
call rng%write (u)
call rng%generate (x)
write (u, *)
write (u, "(1x,A,F7.5)")  "x = ", x
call rng%final ()
deallocate (rng)

write (u, *)
call rng_factory%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_stream_2"

end subroutine rng_stream_2

```

RNG Stream extension

Initialize the generator and advance state by 15389 steps and compare with regular advanced stream position.

```

<RNG stream: execute tests>+≡
  call test (rng_stream_3, "rng_stream_3", &
    "rng initialization and advance state", &
    u, results)

<RNG stream: test declarations>+≡
  public :: rng_stream_3

<RNG stream: tests>+≡
  subroutine rng_stream_3 (u)
    integer, intent(in) :: u
    class(rng_t), allocatable, target :: rng

    integer :: i
    real(default) :: x
    real(default), dimension(2) :: x2

    write (u, "(A)")  "* Test output: rng_stream_3"
    write (u, "(A)")  "* Purpose: initialize and advance the state of the random-number &

```

```

        &generator"
write (u, "(A)")

write (u, "(A)")  "* Initialize generator (default seed)"
write (u, "(A)")

allocate (rng_stream_t :: rng)
call rng%init ()

call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Advance state by 15389 by iteration"
write (u, "(A)")

do i = 1, 15389
    call rng%generate (x)
end do

call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Get random number"
write (u, "(A)")

call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
write (u, "(A)")  "* Advance state by 15389 by procedure"
write (u, "(A)")

select type (rng)
type is (rng_stream_t)
    call rng%reset_substream ()
    call rng%advance_state (15389)
end select

call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Get random number"
write (u, "(A)")

call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
write (u, "(A)")  "* Get random number pair"
write (u, "(A)")

call rng%generate (x2)
write (u, "(A,2(1x,F9.7))")  "x =", x2

```

```

write (u, "(A)")
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Jump to next substream and get random number"
write (u, "(A)")

select type (rng)
type is (rng_stream_t)
  call rng%next_substream ()
end select
call rng%generate (x)
write (u, "(A,2(1x,F9.7))")  "x =", x

write (u, "(A)")
call rng%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call rng%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rng_stream_3"

end subroutine rng_stream_3

```

8.5 Dispatch

```

⟨dispatch_rng.f90⟩≡
  ⟨File header⟩

  module dispatch_rng

    use kinds, only: i16
    ⟨Use strings⟩
    use diagnostics
    use variables

    use rng_base
    use rng_tao
    use rng_stream

    ⟨Standard module head⟩

    ⟨Dispatch rng: public⟩

    ⟨Dispatch rng: variables⟩

    contains

```

<Dispatch rng: procedures>

end module dispatch_rng

Allocate a random-number generator factory according to the variable `$rng_method`, using the current seed in the global record. (If the variable does not exist, the lookup will return the value 0.) We take only the lower 15 bits of the seed, so the actual value fits into a positive 16-bit signed integer.

Since we want to guarantee that all random-number generators in a run are independent, we increment the global seed by one after creating the rng factory and return it to the caller. If the user wants to have identical sequences, he can always set the seed manually, before it is used.

<Dispatch rng: public>≡

public :: dispatch_rng_factory

<Dispatch rng: procedures>≡

```
subroutine dispatch_rng_factory (rng_factory, var_list, next_rng_seed)
  class(rng_factory_t), allocatable, intent(inout) :: rng_factory
  type(var_list_t), intent(in) :: var_list
  integer, intent(out) :: next_rng_seed
  type(var_list_t) :: local
  type(string_t) :: rng_method
  integer :: seed
  character(30) :: buffer
  integer(i16) :: s
  rng_method = var_list%get_sval (var_str ("rng_method"))
  seed = var_list%get_ival (var_str ("seed"))
  s = int (mod (seed, 32768), i16)
  select case (char (rng_method))
  case ("tao")
    allocate (rng_tao_factory_t :: rng_factory)
    call msg_message ("RNG: Initializing TAO random-number generator")
    next_rng_seed = seed + 1
  case ("rng_stream")
    allocate (rng_stream_factory_t :: rng_factory)
    call msg_message ("RNG: Initializing RNG Stream random-number generator")
    next_rng_seed = seed + 1
  case default
    if (associated (dispatch_rng_factory_fallback)) then
      call dispatch_rng_factory_fallback &
        (rng_factory, var_list, next_rng_seed)
    end if
    if (.not. allocated (rng_factory)) then
      call msg_fatal ("Random-number generator '" &
        // char (rng_method) // "' not implemented")
    end if
  end select
  write (buffer, "(I0)") s
  call msg_message ("RNG: Setting seed for random-number generator to " &
    // trim (buffer))
  call rng_factory%init (s)
end subroutine dispatch_rng_factory
```

This is a hook that allows us to inject further handlers for RNG factory objects,

in particular a test RNG.

```

<Dispatch rng: public>+≡
    public :: dispatch_rng_factory_fallback

<Dispatch rng: variables>≡
    procedure (dispatch_rng_factory), pointer :: &
        dispatch_rng_factory_fallback => null ()

```

If the RNG factory dispatcher has used up a seed, we should reset it in the variable list. Separate subroutine with optional argument for more flexibility.

```

<Dispatch rng: public>+≡
    public :: update_rng_seed_in_var_list

<Dispatch rng: procedures>+≡
    subroutine update_rng_seed_in_var_list (var_list, next_rng_seed)
        type(var_list_t), intent(inout), optional :: var_list
        integer, intent(in) :: next_rng_seed
        if (present (var_list)) then
            call var_list%set_int (var_str ("seed"), next_rng_seed, is_known=.true.)
        end if
    end subroutine update_rng_seed_in_var_list

```

8.5.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<dispatch_rng_ut.f90>≡
    <File header>

    module dispatch_rng_ut
        use unit_tests
        use dispatch_rng_uti

    <Standard module head>

    <Dispatch rng: public test>

    <Dispatch rng: public test auxiliary>

    contains

    <Dispatch rng: test driver>

    end module dispatch_rng_ut

<dispatch_rng_uti.f90>≡
    <File header>

    module dispatch_rng_uti

    <Use strings>
        use variables
        use diagnostics
        use rng_base
        use dispatch_rng

```

```

    <Standard module head>

    <Dispatch rng: public test auxiliary>

    <Dispatch rng: test declarations>

contains

    <Dispatch rng: tests>

    <Dispatch rng: test auxiliary>

end module dispatch_rng_util
API: driver for the unit tests below.
<Dispatch rng: public test>≡
    public :: dispatch_rng_test
<Dispatch rng: test driver>≡
    subroutine dispatch_rng_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Dispatch rng: execute tests>
    end subroutine dispatch_rng_test

```

Select type: random number generator

This is an extra dispatcher that enables the test RNG. This procedure should be assigned to the `dispatch_rng_factory_fallback` hook before any tests are executed.

The test generator does not use the seed at all, but it does increment it to be consistent with the other implementations.

```

<Dispatch rng: public test auxiliary>≡
    public :: dispatch_rng_factory_test
<Dispatch rng: test auxiliary>≡
    subroutine dispatch_rng_factory_test (rng_factory, var_list, next_rng_seed)
        use rng_base
        use rng_base_util, only: rng_test_factory_t
        class(rng_factory_t), allocatable, intent(inout) :: rng_factory
        type(var_list_t), intent(in) :: var_list
        integer, intent(out) :: next_rng_seed
        type(string_t) :: rng_method
        if (var_list%contains (var_str ("rng_method"))) then
            rng_method = var_list%get_sval (var_str ("rng_method"))
        else
            rng_method = "unit_test"
        end if
        next_rng_seed = &
            var_list%get_ival (var_str ("seed")) + 1
        select case (char (rng_method))

```

```

        case ("unit_test")
            allocate (rng_test_factory_t :: rng_factory)
            call msg_message ("RNG: Initializing Test random-number generator")
        end select
    end subroutine dispatch_rng_factory_test

```

This is the analog for the TAO RNG, for the unit tests we need a full generator.
(The seed is to be zero or a small integer.)

```

<Dispatch rng: public test auxiliary>+≡
    public :: dispatch_rng_factory_tao

<Dispatch rng: test auxiliary>+≡
    subroutine dispatch_rng_factory_tao (rng_factory, var_list, next_rng_seed)
        use kinds, only: i16
        use rng_base
        use rng_tao, only: rng_tao_factory_t
        class(rng_factory_t), allocatable, intent(inout) :: rng_factory
        type(var_list_t), intent(in) :: var_list
        integer, intent(out) :: next_rng_seed
        type(string_t) :: rng_method
        integer(i16) :: s
        if (var_list%contains (var_str ("rng_method"))) then
            rng_method = var_list%get_sval (var_str ("rng_method"))
        else
            rng_method = "tao"
        end if
        s = var_list%get_ival (var_str ("seed"))
        select case (char (rng_method))
        case ("tao")
            allocate (rng_tao_factory_t :: rng_factory)
            call rng_factory%init (s)
        end select
        next_rng_seed = s + 1
    end subroutine dispatch_rng_factory_tao

```

Create RNG factories for different algorithms. Note that the seed is updated after each rng factory call.

```

<Dispatch rng: execute tests>≡
    call test (dispatch_rng_1, "dispatch_rng_1", &
        "random-number generator", &
        u, results)

<Dispatch rng: test declarations>≡
    public :: dispatch_rng_1

<Dispatch rng: tests>≡
    subroutine dispatch_rng_1 (u)
        integer, intent(in) :: u
        type(var_list_t) :: var_list
        integer :: next_rng_seed
        class(rng_factory_t), allocatable :: rng_factory

        write (u, "(A)")  "* Test output: dispatch_rng_1"
        write (u, "(A)")  "* Purpose: select random-number generator"
    end subroutine dispatch_rng_1

```

```

write (u, "(A)")

call var_list%init_defaults (0)

write (u, "(A)")  "* Allocate RNG factory as rng_test_factory_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("rng_method"), &
    var_str ("unit_test"), is_known = .true.)
call var_list%set_int (&
    var_str ("seed"), 1, is_known = .true.)

call dispatch_rng_factory (rng_factory, var_list, next_rng_seed)

call rng_factory%write (u)
deallocate (rng_factory)

write (u, "(A)")
write (u, "(A)")  "* Allocate RNG factory as rng_tao_factory_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("rng_method"), &
    var_str ("tao"), is_known = .true.)
call update_rng_seed_in_var_list (var_list, next_rng_seed)
call dispatch_rng_factory (rng_factory, var_list, next_rng_seed)

call rng_factory%write (u)
deallocate (rng_factory)

write (u, "(A)")
write (u, "(A)")  "* Allocate RNG factory as rng_stream_factory_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("rng_method"), &
    var_str ("rng_stream"), is_known = .true.)
call update_rng_seed_in_var_list (var_list, next_rng_seed)
call dispatch_rng_factory (rng_factory, var_list, next_rng_seed)

call rng_factory%write (u)
deallocate (rng_factory)

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_rng_1"

end subroutine dispatch_rng_1

```

Chapter 9

Physics

Here we collect definitions and functions that we need for (particle) physics in general, to make them available for the more specific needs of WHIZARD.

physics_defs Physical constants.

c_particles A simple data type for particles which is C compatible.

lorentz Define three-vectors, four-vectors and Lorentz transformations and common operations for them.

phs_point Collections of Lorentz vectors.

sm_physics Here, running functions are stored for special kinematical setup like running coupling constants, Catani-Seymour dipoles, or Sudakov factors.

sm_qcd Definitions and methods for dealing with the running QCD coupling.

shower_algorithms Algorithms typically used in Parton Showers as well as in their matching to NLO computations, e.g. with the POWHEG method.

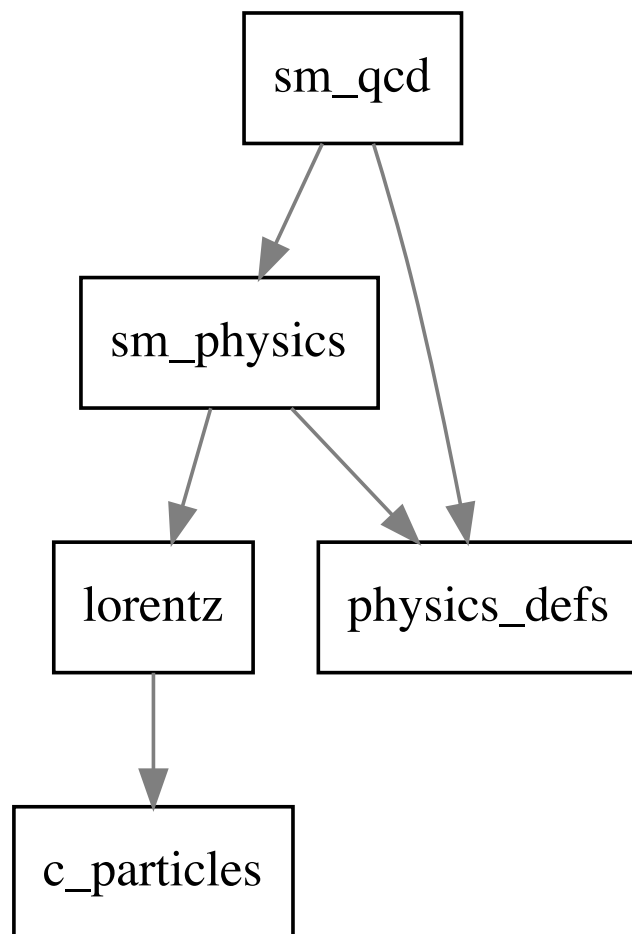


Figure 9.1: Module dependencies in `src/physics`.

9.1 Physics Constants

There is also the generic `constants` module. The constants listed here are more specific for particle physics.

```
<physics_defs.f90>≡  
<File header>  
  
module physics_defs  
  
  <Use kinds>  
  <Use strings>  
  use constants, only: one, two, three  
  
  <Standard module head>  
  
  <Physics defs: public parameters>  
  
  <Physics defs: public>  
  
  <Physics defs: interfaces>  
  
contains  
  
  <Physics defs: procedures>  
  
end module physics_defs
```

9.1.1 Units

Conversion from energy units to cross-section units.

```
<Physics defs: public parameters>≡  
  real(default), parameter, public :: &  
    conv = 0.38937966e12_default
```

Conversion from millimeter to nanoseconds for lifetimes.

```
<Physics defs: public parameters>+≡  
  real(default), parameter, public :: &  
    ns_per_mm = 1.e6_default / 299792458._default
```

Rescaling factor.

```
<Physics defs: public parameters>+≡  
  real(default), parameter, public :: &  
    pb_per_fb = 1.e-3_default
```

String for the default energy and cross-section units.

```
<Physics defs: public parameters>+≡  
  character(*), parameter, public :: &  
    energy_unit = "GeV"  
  character(*), parameter, public :: &  
    cross_section_unit = "fb"
```

9.1.2 SM and QCD constants

```
<Physics defs: public parameters>+≡
  real(default), parameter, public :: &
    NC = three, &
    CF = (NC**2 - one) / two / NC, &
    CA = NC, &
    TR = one / two
```

9.1.3 Parameter Reference values

These are used exclusively in the context of running QCD parameters. In other contexts, we rely on the uniform parameter set as provided by the model definition, modifiable by the user.

```
<Physics defs: public parameters>+≡
  real(default), public, parameter :: MZ_REF = 91.188_default
  real(default), public, parameter :: ALPHA_QCD_MZ_REF = 0.1178_default
  real(default), public, parameter :: LAMBDA_QCD_REF = 200.e-3_default
```

9.1.4 Particle codes

Let us define a few particle codes independent of the model.

We need an UNDEFINED value:

```
<Physics defs: public parameters>+≡
  integer, parameter, public :: UNDEFINED = 0
```

SM fermions:

```
<Physics defs: public parameters>+≡
  integer, parameter, public :: DOWN_Q = 1
  integer, parameter, public :: UP_Q = 2
  integer, parameter, public :: STRANGE_Q = 3
  integer, parameter, public :: CHARM_Q = 4
  integer, parameter, public :: BOTTOM_Q = 5
  integer, parameter, public :: TOP_Q = 6
  integer, parameter, public :: ELECTRON = 11
  integer, parameter, public :: ELECTRON_NEUTRINO = 12
  integer, parameter, public :: MUON = 13
  integer, parameter, public :: MUON_NEUTRINO = 14
  integer, parameter, public :: TAU = 15
  integer, parameter, public :: TAU_NEUTRINO = 16
```

Gauge bosons:

```
<Physics defs: public parameters>+≡
  integer, parameter, public :: GLUON = 21
  integer, parameter, public :: PHOTON = 22
  integer, parameter, public :: PHOTON_OFFSHELL = -2002
  integer, parameter, public :: PHOTON_ONSHELL = 2002
  integer, parameter, public :: Z_BOSON = 23
  integer, parameter, public :: W_BOSON = 24
```


Light mesons:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: PION = 111  
  integer, parameter, public :: PIPLUS = 211  
  integer, parameter, public :: PIMINUS = - PIPLUS
```

Di-Quarks:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: UD0 = 2101  
  integer, parameter, public :: UD1 = 2103  
  integer, parameter, public :: UU1 = 2203
```

Mesons:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: KOL = 130  
  integer, parameter, public :: KOS = 310  
  integer, parameter, public :: K0 = 311  
  integer, parameter, public :: KPLUS = 321  
  integer, parameter, public :: DPLUS = 411  
  integer, parameter, public :: D0 = 421  
  integer, parameter, public :: B0 = 511  
  integer, parameter, public :: BPLUS = 521
```

Light baryons:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: PROTON = 2212  
  integer, parameter, public :: NEUTRON = 2112  
  integer, parameter, public :: DELTAPLUSPLUS = 2224  
  integer, parameter, public :: DELTAPLUS = 2214  
  integer, parameter, public :: DELTA0 = 2114  
  integer, parameter, public :: DELTAMINUS = 1114
```

Strange baryons:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: SIGMAPLUS = 3222  
  integer, parameter, public :: SIGMA0 = 3212  
  integer, parameter, public :: SIGMAMINUS = 3112
```

Charmed baryons:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: SIGMACPLUSPLUS = 4222  
  integer, parameter, public :: SIGMACPLUS = 4212  
  integer, parameter, public :: SIGMAC0 = 4112
```

Bottom baryons:

```
(Physics defs: public parameters)+≡  
  integer, parameter, public :: SIGMAB0 = 5212  
  integer, parameter, public :: SIGMABPLUS = 5222
```

81-100 are reserved for internal codes. Hadron and beam remnants:

```
(Physics defs: public parameters)+≡
integer, parameter, public :: BEAM_REMNANT = 9999
integer, parameter, public :: HADRON_REMNANT = 90
integer, parameter, public :: HADRON_REMNANT_SINGLET = 91
integer, parameter, public :: HADRON_REMNANT_TRIPLET = 92
integer, parameter, public :: HADRON_REMNANT_OCTET = 93
```

Further particle codes for internal use:

```
(Physics defs: public parameters)+≡
integer, parameter, public :: INTERNAL = 94
integer, parameter, public :: INVALID = 97

integer, parameter, public :: COMPOSITE = 99
```

9.1.5 Spin codes

Somewhat redundant, but for better readability we define named constants for spin types. If the mass is nonzero, this is equal to the number of degrees of freedom.

```
(Physics defs: public parameters)+≡
integer, parameter, public :: UNKNOWN = 0
integer, parameter, public :: SCALAR = 1, SPINOR = 2, VECTOR = 3, &
VECTORSPINOR = 4, TENSOR = 5
```

Isospin types and charge types are counted in an analogous way, where charge type 1 is charge 0, 2 is charge 1/3, and so on. Zero always means unknown. Note that charge and isospin types have an explicit sign.

Color types are defined as the dimension of the representation.

9.1.6 NLO status codes

Used to specify whether a `term_instance_t` of a `process_instance_t` is associated with a Born, real-subtracted, virtual-subtracted or subtraction-dummy matrix element.

```
(Physics defs: public parameters)+≡
integer, parameter, public :: BORN = 0
integer, parameter, public :: NLO_REAL = 1
integer, parameter, public :: NLO_VIRTUAL = 2
integer, parameter, public :: NLO_MISMATCH = 3
integer, parameter, public :: NLO_DGLAP = 4
integer, parameter, public :: NLO_SUBTRACTION = 5
integer, parameter, public :: NLO_FULL = 6
integer, parameter, public :: GKS = 7
integer, parameter, public :: COMPONENT_UNDEFINED = 99
```

NLO_FULL is not strictly a component status code but having it is convenient. We define the number of additional subtractions for beam-involved NLO calculations. Each subtraction refers to a rescaling of one of two beams. Obviously,

this approach is not flexible enough to support setups with just a single beam described by a structure function.

```

<Physics defs: public parameters>+=
    integer, parameter, public :: n_beams_rescaled = 2

<Physics defs: public>=
    public :: component_status

<Physics defs: interfaces>=
    interface component_status
        module procedure component_status_of_string
        module procedure component_status_to_string
    end interface

<Physics defs: procedures>=
    elemental function component_status_of_string (string) result (i)
        integer :: i
        type(string_t), intent(in) :: string
        select case (char(string))
            case ("born")
                i = BORN
            case ("real")
                i = NLO_REAL
            case ("virtual")
                i = NLO_VIRTUAL
            case ("mismatch")
                i = NLO_MISMATCH
            case ("dglap")
                i = NLO_DGLAP
            case ("subtraction")
                i = NLO_SUBTRACTION
            case ("full")
                i = NLO_FULL
            case ("GKS")
                i = GKS
            case default
                i = COMPONENT_UNDEFINED
        end select
    end function component_status_of_string

    elemental function component_status_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
        select case (i)
            case (BORN)
                string = "born"
            case (NLO_REAL)
                string = "real"
            case (NLO_VIRTUAL)
                string = "virtual"
            case (NLO_MISMATCH)
                string = "mismatch"
            case (NLO_DGLAP)
                string = "dglap"
            case (NLO_SUBTRACTION)

```

```

        string = "subtraction"
    case (NLO_FULL)
        string = "full"
    case (GKS)
        string = "GKS"
    case default
        string = "undefined"
    end select
end function component_status_to_string

```

```

<Physics defs: public>+=
    public :: is_nlo_component

```

```

<Physics defs: procedures>+=
    elemental function is_nlo_component (comp) result (is_nlo)
        logical :: is_nlo
        integer, intent(in) :: comp
        select case (comp)
        case (BORN : GKS)
            is_nlo = .true.
        case default
            is_nlo = .false.
        end select
    end function is_nlo_component

```

```

<Physics defs: public>+=
    public :: is_subtraction_component

```

```

<Physics defs: procedures>+=
    function is_subtraction_component (emitter, nlo_type) result (is_subtraction)
        logical :: is_subtraction
        integer, intent(in) :: emitter, nlo_type
        is_subtraction = nlo_type == NLO_REAL .and. emitter < 0
    end function is_subtraction_component

```

9.1.7 Threshold

Some commonly used variables for the threshold computation

```

<Physics defs: public parameters>+=
    integer, parameter, public :: THR_POS_WP = 3
    integer, parameter, public :: THR_POS_WM = 4
    integer, parameter, public :: THR_POS_B = 5
    integer, parameter, public :: THR_POS_BBAR = 6
    integer, parameter, public :: THR_POS_GLUON = 7

    integer, parameter, public :: THR_EMITTER_OFFSET = 4

    integer, parameter, public :: NO_FACTORIZATION = 0
    integer, parameter, public :: FACTORIZATION_THRESHOLD = 1

    integer, dimension(2), parameter, public :: ass_quark = [5, 6]
    integer, dimension(2), parameter, public :: ass_boson = [3, 4]

```

```

integer, parameter, public :: PROC_MODE_UNDEFINED = 0
integer, parameter, public :: PROC_MODE_TT = 1
integer, parameter, public :: PROC_MODE_WBWB = 2

<Physics defs: public>+≡
    public :: thr_leg

<Physics defs: procedures>+≡
    function thr_leg (emitter) result (leg)
        integer :: leg
        integer, intent(in) :: emitter
        leg = emitter - THR_EMITTER_OFFSET
    end function thr_leg

```

9.2 C-compatible Particle Type

For easy communication with C code, we introduce a simple C-compatible type for particles. The components are either default C integers or default C doubles.

The `c_prt` type is transparent, and its contents should be regarded as part of the interface.

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

  module c_particles

    use, intrinsic :: iso_c_binding !NODEP!

    use io_units
    use format_defs, only: FMT_14, FMT_19

    <Standard module head>

    <C Particles: public>

    <C Particles: types>

    contains

    <C Particles: procedures>
    end module c_particles

  <C Particles: public>≡
    public :: c_prt_t

  <C Particles: types>≡
    type, bind(C) :: c_prt_t
      integer(c_int) :: type = 0
      integer(c_int) :: pdg = 0
      integer(c_int) :: polarized = 0
      integer(c_int) :: h = 0
      real(c_double) :: pe = 0
      real(c_double) :: px = 0
      real(c_double) :: py = 0
      real(c_double) :: pz = 0
      real(c_double) :: p2 = 0
    end type c_prt_t
```

This is for debugging only, there is no C binding. It is a simplified version of `prt_write`.

```
<C Particles: public>+≡
  public :: c_prt_write

  <C Particles: procedures>≡
    subroutine c_prt_write (prt, unit)
      type(c_prt_t), intent(in) :: prt
      integer, intent(in), optional :: unit
      integer :: u
      u = given_output_unit (unit); if (u < 0) return
```

```

write (u, "(1x,A)", advance="no")  prt("
write (u, "(I0,':')", advance="no")  prt%type
if (prt%polarized /= 0) then
    write (u, "(I0,'/',I0,'|')", advance="no")  prt%pdg, prt%h
else
    write (u, "(I0,'|')", advance="no")  prt%pdg
end if
write (u, "(" // FMT_14 // ",',';" // FMT_14 // ",','," // &
    FMT_14 // ",','," // FMT_14 // ")", advance="no") &
    prt%pe, prt%px, prt%py, prt%pz
write (u, "( '|'," // FMT_19 // ")", advance="no")  prt%p2
write (u, "(A)"  ") "
end subroutine c_prt_write

```

9.3 Lorentz algebra

Define Lorentz vectors, three-vectors, boosts, and some functions to manipulate them.

To make maximum use of this, all functions, if possible, are declared elemental (or pure, if this is not possible).

```
<lorentz.f90>≡  
  <File header>  
  
  module lorentz  
  
    <Use kinds with double>  
    use numeric_utils  
    use io_units  
    use constants, only: pi, twopi, degree, zero, one, two, eps0, tiny_07  
    use format_defs, only: FMT_11, FMT_13, FMT_15, FMT_19  
    use format_utils, only: pac_fmt  
    use diagnostics  
    use c_particles  
  
    <Standard module head>  
  
    <Lorentz: public>  
  
    <Lorentz: public operators>  
  
    <Lorentz: public functions>  
  
    <Lorentz: types>  
  
    <Lorentz: parameters>  
  
    <Lorentz: interfaces>  
  
    contains  
  
    <Lorentz: procedures>  
  end module lorentz
```

9.3.1 Three-vectors

First of all, let us introduce three-vectors in a trivial way. The functions and overloaded elementary operations clearly are too much overhead, but we like to keep the interface for three-vectors and four-vectors exactly parallel. By the way, we might attach a label to a vector by extending the type definition later.

```
<Lorentz: public>≡  
  public :: vector3_t  
  
<Lorentz: types>≡  
  type :: vector3_t  
    real(default), dimension(3) :: p  
  end type vector3_t
```


Output a vector

```

(Lorentz: public)+≡
    public :: vector3_write

(Lorentz: procedures)≡
    subroutine vector3_write (p, unit, testflag)
        type(vector3_t), intent(in) :: p
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        character(len=7) :: fmt
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call pac_fmt (fmt, FMT_19, FMT_15, testflag)
        write(u, "(1x,A,3(1x," // fmt // "))" 'P = ', p%p
    end subroutine vector3_write

```

This is a three-vector with zero components

```

(Lorentz: public)+≡
    public :: vector3_null

(Lorentz: parameters)≡
    type(vector3_t), parameter :: vector3_null = &
        vector3_t ([ zero, zero, zero ])

```

Canonical three-vector:

```

(Lorentz: public)+≡
    public :: vector3_canonical

(Lorentz: procedures)+≡
    elemental function vector3_canonical (k) result (p)
        type(vector3_t) :: p
        integer, intent(in) :: k
        p = vector3_null
        p%p(k) = 1
    end function vector3_canonical

```

A moving particle (k -axis, or arbitrary axis). Note that the function for the generic momentum cannot be elemental.

```

(Lorentz: public)+≡
    public :: vector3_moving

(Lorentz: interfaces)≡
    interface vector3_moving
        module procedure vector3_moving_canonical
        module procedure vector3_moving_generic
    end interface

(Lorentz: procedures)+≡
    elemental function vector3_moving_canonical (p, k) result(q)
        type(vector3_t) :: q
        real(default), intent(in) :: p
        integer, intent(in) :: k
        q = vector3_null
        q%p(k) = p

```

```

end function vector3_moving_canonical
pure function vector3_moving_generic (p) result(q)
  real(default), dimension(3), intent(in) :: p
  type(vector3_t) :: q
  q%p = p
end function vector3_moving_generic

```

Equality and inequality

```

<Lorentz: public operators>≡
  public :: operator(==), operator(/=)

<Lorentz: interfaces>+≡
  interface operator(==)
    module procedure vector3_eq
  end interface
  interface operator(/=)
    module procedure vector3_neq
  end interface

<Lorentz: procedures>+≡
  elemental function vector3_eq (p, q) result (r)
    logical :: r
    type(vector3_t), intent(in) :: p,q
    r = all (abs (p%p - q%p) < eps0)
  end function vector3_eq
  elemental function vector3_neq (p, q) result (r)
    logical :: r
    type(vector3_t), intent(in) :: p,q
    r = any (abs(p%p - q%p) > eps0)
  end function vector3_neq

```

Define addition and subtraction

```

<Lorentz: public operators>+≡
  public :: operator(+), operator(-)

<Lorentz: interfaces>+≡
  interface operator(+)
    module procedure add_vector3
  end interface
  interface operator(-)
    module procedure sub_vector3
  end interface

<Lorentz: procedures>+≡
  elemental function add_vector3 (p, q) result (r)
    type(vector3_t) :: r
    type(vector3_t), intent(in) :: p,q
    r%p = p%p + q%p
  end function add_vector3
  elemental function sub_vector3 (p, q) result (r)
    type(vector3_t) :: r
    type(vector3_t), intent(in) :: p,q
    r%p = p%p - q%p
  end function sub_vector3

```

The multiplication sign is overloaded with scalar multiplication; similarly division:

```

(Lorentz: public operators)+≡
    public :: operator(*), operator(/)

(Lorentz: interfaces)+≡
    interface operator(*)
        module procedure prod_integer_vector3, prod_vector3_integer
        module procedure prod_real_vector3, prod_vector3_real
    end interface
    interface operator(/)
        module procedure div_vector3_real, div_vector3_integer
    end interface

(Lorentz: procedures)+≡
    elemental function prod_real_vector3 (s, p) result (q)
        type(vector3_t) :: q
        real(default), intent(in) :: s
        type(vector3_t), intent(in) :: p
        q%p = s * p%p
    end function prod_real_vector3
    elemental function prod_vector3_real (p, s) result (q)
        type(vector3_t) :: q
        real(default), intent(in) :: s
        type(vector3_t), intent(in) :: p
        q%p = s * p%p
    end function prod_vector3_real
    elemental function div_vector3_real (p, s) result (q)
        type(vector3_t) :: q
        real(default), intent(in) :: s
        type(vector3_t), intent(in) :: p
        q%p = p%p/s
    end function div_vector3_real
    elemental function prod_integer_vector3 (s, p) result (q)
        type(vector3_t) :: q
        integer, intent(in) :: s
        type(vector3_t), intent(in) :: p
        q%p = s * p%p
    end function prod_integer_vector3
    elemental function prod_vector3_integer (p, s) result (q)
        type(vector3_t) :: q
        integer, intent(in) :: s
        type(vector3_t), intent(in) :: p
        q%p = s * p%p
    end function prod_vector3_integer
    elemental function div_vector3_integer (p, s) result (q)
        type(vector3_t) :: q
        integer, intent(in) :: s
        type(vector3_t), intent(in) :: p
        q%p = p%p/s
    end function div_vector3_integer

```

The multiplication sign can also indicate scalar products:

```

(Lorentz: interfaces)+≡

```

```

interface operator(*)
  module procedure prod_vector3
end interface

<Lorentz: procedures>+≡
  elemental function prod_vector3 (p, q) result (s)
    real(default) :: s
    type(vector3_t), intent(in) :: p,q
    s = dot_product (p%p, q%p)
  end function prod_vector3

<Lorentz: public functions>≡
  public :: cross_product

<Lorentz: interfaces>+≡
  interface cross_product
    module procedure vector3_cross_product
  end interface

<Lorentz: procedures>+≡
  elemental function vector3_cross_product (p, q) result (r)
    type(vector3_t) :: r
    type(vector3_t), intent(in) :: p,q
    integer :: i
    do i=1,3
      r%p(i) = dot_product (p%p, matmul(epsilon_three(i,:,:), q%p))
    end do
  end function vector3_cross_product

```

Exponentiation is defined only for integer powers. Odd powers mean take the square root; so `p**1` is the length of `p`.

```

<Lorentz: public operators>+≡
  public :: operator(**)

<Lorentz: interfaces>+≡
  interface operator(**)
    module procedure power_vector3
  end interface

<Lorentz: procedures>+≡
  elemental function power_vector3 (p, e) result (s)
    real(default) :: s
    type(vector3_t), intent(in) :: p
    integer, intent(in) :: e
    s = dot_product (p%p, p%p)
    if (e/=2) then
      if (mod(e,2)==0) then
        s = s**(e/2)
      else
        s = sqrt(s)**e
      end if
    end if
  end function power_vector3

```

Finally, we need a negation.

```

<Lorentz: interfaces>+≡
    interface operator(-)
        module procedure negate_vector3
    end interface

<Lorentz: procedures>+≡
    elemental function negate_vector3 (p) result (q)
        type(vector3_t) :: q
        type(vector3_t), intent(in) :: p
        integer :: i
        do i = 1, 3
            if (abs (p%p(i)) < eps0) then
                q%p(i) = 0
            else
                q%p(i) = -p%p(i)
            end if
        end do
    end function negate_vector3

```

The sum function can be useful:

```

<Lorentz: public functions>+≡
    public :: sum

<Lorentz: interfaces>+≡
    interface sum
        module procedure sum_vector3
    end interface

<Lorentz: public>+≡
    public :: vector3_set_component

<Lorentz: procedures>+≡
    subroutine vector3_set_component (p, i, value)
        type(vector3_t), intent(inout) :: p
        integer, intent(in) :: i
        real(default), intent(in) :: value
        p%p(i) = value
    end subroutine vector3_set_component

<Lorentz: procedures>+≡
    pure function sum_vector3 (p) result (q)
        type(vector3_t) :: q
        type(vector3_t), dimension(:), intent(in) :: p
        integer :: i
        do i=1, 3
            q%p(i) = sum (p%p(i))
        end do
    end function sum_vector3

```

Any component:

```

<Lorentz: public>+≡
    public :: vector3_get_component

```

```

⟨Lorentz: procedures⟩+≡
  elemental function vector3_get_component (p, k) result (c)
    type(vector3_t), intent(in) :: p
    integer, intent(in) :: k
    real(default) :: c
    c = p%p(k)
  end function vector3_get_component

```

Extract all components. This is not elemental.

```

⟨Lorentz: public⟩+≡
  public :: vector3_get_components

⟨Lorentz: procedures⟩+≡
  pure function vector3_get_components (p) result (a)
    type(vector3_t), intent(in) :: p
    real(default), dimension(3) :: a
    a = p%p
  end function vector3_get_components

```

This function returns the direction of a three-vector, i.e., a normalized three-vector. If the vector is null, we return a null vector.

```

⟨Lorentz: public functions⟩+≡
  public :: direction

⟨Lorentz: interfaces⟩+≡
  interface direction
    module procedure vector3_get_direction
  end interface

⟨Lorentz: procedures⟩+≡
  elemental function vector3_get_direction (p) result (q)
    type(vector3_t) :: q
    type(vector3_t), intent(in) :: p
    real(default) :: pp
    pp = p**1
    if (pp > eps0) then
      q%p = p%p / pp
    else
      q%p = 0
    end if
  end function vector3_get_direction

```

9.3.2 Four-vectors

In four-vectors the zero-component needs special treatment, therefore we do not use the standard operations. Sure, we pay for the extra layer of abstraction by losing efficiency; so we have to assume that the time-critical applications do not involve four-vector operations.

```

⟨Lorentz: public⟩+≡
  public :: vector4_t

```

```

<Lorentz: types>+≡
  type :: vector4_t
    real(default), dimension(0:3) :: p = &
      [zero, zero, zero, zero]
  contains
    <Lorentz: vector4: TBP>
  end type vector4_t

```

Output a vector

```

<Lorentz: public>+≡
  public :: vector4_write

<Lorentz: vector4: TBP>≡
  procedure :: write => vector4_write

<Lorentz: procedures>+≡
  subroutine vector4_write &
    (p, unit, show_mass, testflag, compressed, ultra)
    class(vector4_t), intent(in) :: p
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_mass, testflag, compressed, ultra
    logical :: comp, sm, tf, extreme
    integer :: u
    character(len=7) :: fmt
    real(default) :: m
    comp = .false.; if (present (compressed)) comp = compressed
    sm = .false.; if (present (show_mass)) sm = show_mass
    tf = .false.; if (present (testflag)) tf = testflag
    extreme = .false.; if (present (ultra)) extreme = ultra
    if (extreme) then
      call pac_fmt (fmt, FMT_19, FMT_11, testflag)
    else
      call pac_fmt (fmt, FMT_19, FMT_13, testflag)
    end if
    u = given_output_unit (unit); if (u < 0) return
    if (comp) then
      write (u, "(4(F12.3,1X))", advance="no") p%p(0:3)
    else
      write (u, "(1x,A,1x," // fmt // ")") 'E = ', p%p(0)
      write (u, "(1x,A,3(1x," // fmt // ")") 'P = ', p%p(1:)
      if (sm) then
        m = p**1
        if (tf) call pacify (m, tolerance = 1E-6_default)
        write (u, "(1x,A,1x," // fmt // ")") 'M = ', m
      end if
    end if
  end subroutine vector4_write

```

Binary I/O

```

<Lorentz: public>+≡
  public :: vector4_write_raw
  public :: vector4_read_raw

<Lorentz: procedures>+≡
  subroutine vector4_write_raw (p, u)

```

```

        type(vector4_t), intent(in) :: p
        integer, intent(in) :: u
        write (u) p%p
    end subroutine vector4_write_raw

    subroutine vector4_read_raw (p, u, iostat)
        type(vector4_t), intent(out) :: p
        integer, intent(in) :: u
        integer, intent(out), optional :: iostat
        read (u, iostat=iostat) p%p
    end subroutine vector4_read_raw

```

This is a four-vector with zero components

```

<Lorentz: public>+≡
    public :: vector4_null

<Lorentz: parameters>+≡
    type(vector4_t), parameter :: vector4_null = &
        vector4_t ([ zero, zero, zero, zero ])

```

Canonical four-vector:

```

<Lorentz: public>+≡
    public :: vector4_canonical

<Lorentz: procedures>+≡
    elemental function vector4_canonical (k) result (p)
        type(vector4_t) :: p
        integer, intent(in) :: k
        p = vector4_null
        p%p(k) = 1
    end function vector4_canonical

```

A particle at rest:

```

<Lorentz: public>+≡
    public :: vector4_at_rest

<Lorentz: procedures>+≡
    elemental function vector4_at_rest (m) result (p)
        type(vector4_t) :: p
        real(default), intent(in) :: m
        p = vector4_t ([ m, zero, zero, zero ])
    end function vector4_at_rest

```

A moving particle (k -axis, or arbitrary axis)

```

<Lorentz: public>+≡
    public :: vector4_moving

<Lorentz: interfaces>+≡
    interface vector4_moving
        module procedure vector4_moving_canonical
        module procedure vector4_moving_generic
    end interface

```



```

(Lorentz: procedures)+≡
  elemental function vector4_moving_canonical (E, p, k) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: E, p
    integer, intent(in) :: k
    q = vector4_at_rest(E)
    q%p(k) = p
  end function vector4_moving_canonical
  elemental function vector4_moving_generic (E, p) result (q)
    type(vector4_t) :: q
    real(default), intent(in) :: E
    type(vector3_t), intent(in) :: p
    q%p(0) = E
    q%p(1:) = p%p
  end function vector4_moving_generic

```

Equality and inequality

```

(Lorentz: interfaces)+≡
  interface operator(==)
    module procedure vector4_eq
  end interface
  interface operator(/=)
    module procedure vector4_neq
  end interface

(Lorentz: procedures)+≡
  elemental function vector4_eq (p, q) result (r)
    logical :: r
    type(vector4_t), intent(in) :: p,q
    r = all (abs (p%p - q%p) < eps0)
  end function vector4_eq
  elemental function vector4_neq (p, q) result (r)
    logical :: r
    type(vector4_t), intent(in) :: p,q
    r = any (abs (p%p - q%p) > eps0)
  end function vector4_neq

```

Addition and subtraction:

```

(Lorentz: interfaces)+≡
  interface operator(+)
    module procedure add_vector4
  end interface
  interface operator(-)
    module procedure sub_vector4
  end interface

(Lorentz: procedures)+≡
  elemental function add_vector4 (p,q) result (r)
    type(vector4_t) :: r
    type(vector4_t), intent(in) :: p,q
    r%p = p%p + q%p
  end function add_vector4
  elemental function sub_vector4 (p,q) result (r)
    type(vector4_t) :: r

```

```

    type(vector4_t), intent(in) :: p,q
    r%p = p%p - q%p
end function sub_vector4

```

We also need scalar multiplication and division:

```

(Lorentz: interfaces)+≡
    interface operator(*)
        module procedure prod_real_vector4, prod_vector4_real
        module procedure prod_integer_vector4, prod_vector4_integer
    end interface
    interface operator(/)
        module procedure div_vector4_real
        module procedure div_vector4_integer
    end interface

(Lorentz: procedures)+≡
    elemental function prod_real_vector4 (s, p) result (q)
        type(vector4_t) :: q
        real(default), intent(in) :: s
        type(vector4_t), intent(in) :: p
        q%p = s * p%p
    end function prod_real_vector4
    elemental function prod_vector4_real (p, s) result (q)
        type(vector4_t) :: q
        real(default), intent(in) :: s
        type(vector4_t), intent(in) :: p
        q%p = s * p%p
    end function prod_vector4_real
    elemental function div_vector4_real (p, s) result (q)
        type(vector4_t) :: q
        real(default), intent(in) :: s
        type(vector4_t), intent(in) :: p
        q%p = p%p/s
    end function div_vector4_real
    elemental function prod_integer_vector4 (s, p) result (q)
        type(vector4_t) :: q
        integer, intent(in) :: s
        type(vector4_t), intent(in) :: p
        q%p = s * p%p
    end function prod_integer_vector4
    elemental function prod_vector4_integer (p, s) result (q)
        type(vector4_t) :: q
        integer, intent(in) :: s
        type(vector4_t), intent(in) :: p
        q%p = s * p%p
    end function prod_vector4_integer
    elemental function div_vector4_integer (p, s) result (q)
        type(vector4_t) :: q
        integer, intent(in) :: s
        type(vector4_t), intent(in) :: p
        q%p = p%p/s
    end function div_vector4_integer

```

Scalar products and squares in the Minkowski sense:

```

(Lorentz: interfaces)+≡
  interface operator(*)
    module procedure prod_vector4
  end interface
  interface operator(**)
    module procedure power_vector4
  end interface
(Lorentz: procedures)+≡
  elemental function prod_vector4 (p, q) result (s)
    real(default) :: s
    type(vector4_t), intent(in) :: p,q
    s = p%p(0)*q%p(0) - dot_product(p%p(1:), q%p(1:))
  end function prod_vector4

```

The power operation for four-vectors is signed, i.e., p^{**1} is positive for timelike and negative for spacelike vectors. Note that $(p^{**1})^{**2}$ is not necessarily equal to p^{**2} .

```

(Lorentz: procedures)+≡
  elemental function power_vector4 (p, e) result (s)
    real(default) :: s
    type(vector4_t), intent(in) :: p
    integer, intent(in) :: e
    s = p * p
    if (e /= 2) then
      if (mod(e, 2) == 0) then
        s = s**(e / 2)
      else if (s >= 0) then
        s = sqrt(s)**e
      else
        s = -(sqrt(abs(s))**e)
      end if
    end if
  end function power_vector4

```

Finally, we introduce a negation

```

(Lorentz: interfaces)+≡
  interface operator(-)
    module procedure negate_vector4
  end interface
(Lorentz: procedures)+≡
  elemental function negate_vector4 (p) result (q)
    type(vector4_t) :: q
    type(vector4_t), intent(in) :: p
    integer :: i
    do i = 0, 3
      if (abs (p%p(i)) < eps0) then
        q%p(i) = 0
      else
        q%p(i) = -p%p(i)
      end if
    end do
  end function negate_vector4

```

```

        end do
    end function negate_vector4

```

The sum function can be useful:

```

<Lorentz: interfaces>+≡
    interface sum
        module procedure sum_vector4, sum_vector4_mask
    end interface

<Lorentz: procedures>+≡
    pure function sum_vector4 (p) result (q)
        type(vector4_t) :: q
        type(vector4_t), dimension(:), intent(in) :: p
        integer :: i
        do i = 0, 3
            q%p(i) = sum (p%p(i))
        end do
    end function sum_vector4

    pure function sum_vector4_mask (p, mask) result (q)
        type(vector4_t) :: q
        type(vector4_t), dimension(:), intent(in) :: p
        logical, dimension(:), intent(in) :: mask
        integer :: i
        do i = 0, 3
            q%p(i) = sum (p%p(i), mask=mask)
        end do
    end function sum_vector4_mask

```

9.3.3 Conversions

Manually set a component of the four-vector:

```

<Lorentz: public>+≡
    public :: vector4_set_component

<Lorentz: procedures>+≡
    subroutine vector4_set_component (p, k, c)
        type(vector4_t), intent(inout) :: p
        integer, intent(in) :: k
        real(default), intent(in) :: c
        p%p(k) = c
    end subroutine vector4_set_component

```

Any component:

```

<Lorentz: public>+≡
    public :: vector4_get_component

<Lorentz: procedures>+≡
    elemental function vector4_get_component (p, k) result (c)
        real(default) :: c
        type(vector4_t), intent(in) :: p
        integer, intent(in) :: k

```

```

        c = p%p(k)
    end function vector4_get_component

```

Extract all components. This is not elemental.

```

<Lorentz: public>+≡
    public :: vector4_get_components

<Lorentz: procedures>+≡
    pure function vector4_get_components (p) result (a)
        real(default), dimension(0:3) :: a
        type(vector4_t), intent(in) :: p
        a = p%p
    end function vector4_get_components

```

This function returns the space part of a four-vector, such that we can apply three-vector operations on it:

```

<Lorentz: public functions>+≡
    public :: space_part

<Lorentz: interfaces>+≡
    interface space_part
        module procedure vector4_get_space_part
    end interface

<Lorentz: procedures>+≡
    elemental function vector4_get_space_part (p) result (q)
        type(vector3_t) :: q
        type(vector4_t), intent(in) :: p
        q%p = p%p(1:)
    end function vector4_get_space_part

```

This function returns the direction of a four-vector, i.e., a normalized three-vector. If the four-vector has zero space part, we return a null vector.

```

<Lorentz: interfaces>+≡
    interface direction
        module procedure vector4_get_direction
    end interface

<Lorentz: procedures>+≡
    elemental function vector4_get_direction (p) result (q)
        type(vector3_t) :: q
        type(vector4_t), intent(in) :: p
        real(default) :: qq
        q%p = p%p(1:)
        qq = q**1
        if (abs(qq) > eps0) then
            q%p = q%p / qq
        else
            q%p = 0
        end if
    end function vector4_get_direction

```

Change the sign of the spatial part of a four-vector

```

(Lorentz: public)+≡
    public :: vector4_invert_direction

(Lorentz: procedures)+≡
    elemental subroutine vector4_invert_direction (p)
        type(vector4_t), intent(inout) :: p
        p%p(1:3) = -p%p(1:3)
    end subroutine vector4_invert_direction

```

This function returns the four-vector as an ordinary array. A second version for an array of four-vectors.

```

(Lorentz: public)+≡
    public :: assignment (=)

(Lorentz: interfaces)+≡
    interface assignment (=)
        module procedure array_from_vector4_1, array_from_vector4_2, &
            array_from_vector3_1, array_from_vector3_2, &
            vector4_from_array, vector3_from_array
    end interface

(Lorentz: procedures)+≡
    pure subroutine array_from_vector4_1 (a, p)
        real(default), dimension(:), intent(out) :: a
        type(vector4_t), intent(in) :: p
        a = p%p
    end subroutine array_from_vector4_1

    pure subroutine array_from_vector4_2 (a, p)
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), dimension(:,:), intent(out) :: a
        integer :: i
        forall (i=1:size(p))
            a(:,i) = p(i)%p
        end forall
    end subroutine array_from_vector4_2

    pure subroutine array_from_vector3_1 (a, p)
        real(default), dimension(:), intent(out) :: a
        type(vector3_t), intent(in) :: p
        a = p%p
    end subroutine array_from_vector3_1

    pure subroutine array_from_vector3_2 (a, p)
        type(vector3_t), dimension(:), intent(in) :: p
        real(default), dimension(:,:), intent(out) :: a
        integer :: i
        forall (i=1:size(p))
            a(:,i) = p(i)%p
        end forall
    end subroutine array_from_vector3_2

    pure subroutine vector4_from_array (p, a)
        type(vector4_t), intent(out) :: p

```

```

        real(default), dimension(:), intent(in) :: a
        p%p(0:3) = a
    end subroutine vector4_from_array

    pure subroutine vector3_from_array (p, a)
        type(vector3_t), intent(out) :: p
        real(default), dimension(:), intent(in) :: a
        p%p(1:3) = a
    end subroutine vector3_from_array

<Lorentz: public>+≡
    public :: vector4

<Lorentz: procedures>+≡
    pure function vector4 (a) result (p)
        type(vector4_t) :: p
        real(default), intent(in), dimension(4) :: a
        p%p = a
    end function vector4

<Lorentz: vector4: TBP>+≡
    procedure :: to_pythia6 => vector4_to_pythia6

<Lorentz: procedures>+≡
    pure function vector4_to_pythia6 (vector4, m) result (p)
        real(double), dimension(1:5) :: p
        class(vector4_t), intent(in) :: vector4
        real(default), intent(in), optional :: m
        p(1:3) = vector4%p(1:3)
        p(4) = vector4%p(0)
        if (present (m)) then
            p(5) = m
        else
            p(5) = vector4 ** 1
        end if
    end function vector4_to_pythia6

```

9.3.4 Interface to c_prt

Transform the momentum of a c_prt object into a four-vector and vice versa:

```

<Lorentz: interfaces>+≡
    interface assignment (=)
        module procedure vector4_from_c_prt, c_prt_from_vector4
    end interface

<Lorentz: procedures>+≡
    pure subroutine vector4_from_c_prt (p, c_prt)
        type(vector4_t), intent(out) :: p
        type(c_prt_t), intent(in) :: c_prt
        p%p(0) = c_prt%pe
        p%p(1) = c_prt%px
        p%p(2) = c_prt%py
        p%p(3) = c_prt%pz
    end subroutine vector4_from_c_prt

```

```

end subroutine vector4_from_c_prt

pure subroutine c_prt_from_vector4 (c_prt, p)
  type(c_prt_t), intent(out) :: c_prt
  type(vector4_t), intent(in) :: p
  c_prt%pe = p%p(0)
  c_prt%px = p%p(1)
  c_prt%py = p%p(2)
  c_prt%pz = p%p(3)
  c_prt%p2 = p ** 2
end subroutine c_prt_from_vector4

```

Initialize a `c_prt_t` object with the components of a four-vector as its kinematical entries. Compute the invariant mass, or use the optional mass-squared value instead.

```

<Lorentz: public>+≡
  public :: vector4_to_c_prt

<Lorentz: procedures>+≡
  elemental function vector4_to_c_prt (p, p2) result (c_prt)
    type(c_prt_t) :: c_prt
    type(vector4_t), intent(in) :: p
    real(default), intent(in), optional :: p2
    c_prt%pe = p%p(0)
    c_prt%px = p%p(1)
    c_prt%py = p%p(2)
    c_prt%pz = p%p(3)
    if (present (p2)) then
      c_prt%p2 = p2
    else
      c_prt%p2 = p ** 2
    end if
  end function vector4_to_c_prt

```

9.3.5 Angles

Return the angles in a canonical system. The angle ϕ is defined between $0 \leq \phi < 2\pi$. In degenerate cases, return zero.

```

<Lorentz: public functions>+≡
  public :: azimuthal_angle

<Lorentz: interfaces>+≡
  interface azimuthal_angle
    module procedure vector3_azimuthal_angle
    module procedure vector4_azimuthal_angle
  end interface

<Lorentz: procedures>+≡
  elemental function vector3_azimuthal_angle (p) result (phi)
    real(default) :: phi
    type(vector3_t), intent(in) :: p
    if (any (abs (p%p(1:2)) > 0)) then
      phi = atan2(p%p(2), p%p(1))
    end if
  end function vector3_azimuthal_angle

```



```

        if (phi < 0) phi = phi + twopi
    else
        phi = 0
    end if
end function vector3_azimuthal_angle
elemental function vector4_azimuthal_angle (p) result (phi)
    real(default) :: phi
    type(vector4_t), intent(in) :: p
    phi = vector3_azimuthal_angle (space_part (p))
end function vector4_azimuthal_angle

```

Azimuthal angle in degrees

```

<Lorentz: public functions>+≡
    public :: azimuthal_angle_deg

<Lorentz: interfaces>+≡
    interface azimuthal_angle_deg
        module procedure vector3_azimuthal_angle_deg
        module procedure vector4_azimuthal_angle_deg
    end interface

<Lorentz: procedures>+≡
    elemental function vector3_azimuthal_angle_deg (p) result (phi)
        real(default) :: phi
        type(vector3_t), intent(in) :: p
        phi = vector3_azimuthal_angle (p) / degree
    end function vector3_azimuthal_angle_deg
    elemental function vector4_azimuthal_angle_deg (p) result (phi)
        real(default) :: phi
        type(vector4_t), intent(in) :: p
        phi = vector4_azimuthal_angle (p) / degree
    end function vector4_azimuthal_angle_deg

```

The azimuthal distance of two vectors. This is the difference of the azimuthal angles, but cannot be larger than π : The result is between $-\pi < \Delta\phi \leq \pi$.

```

<Lorentz: public functions>+≡
    public :: azimuthal_distance

<Lorentz: interfaces>+≡
    interface azimuthal_distance
        module procedure vector3_azimuthal_distance
        module procedure vector4_azimuthal_distance
    end interface

<Lorentz: procedures>+≡
    elemental function vector3_azimuthal_distance (p, q) result (dphi)
        real(default) :: dphi
        type(vector3_t), intent(in) :: p,q
        dphi = vector3_azimuthal_angle (q) - vector3_azimuthal_angle (p)
        if (dphi <= -pi) then
            dphi = dphi + twopi
        else if (dphi > pi) then
            dphi = dphi - twopi
        end if
    end function vector3_azimuthal_distance

```

```

elemental function vector4_azimuthal_distance (p, q) result (dphi)
  real(default) :: dphi
  type(vector4_t), intent(in) :: p,q
  dphi = vector3_azimuthal_distance &
    (space_part (p), space_part (q))
end function vector4_azimuthal_distance

```

The same in degrees:

```

<Lorentz: public functions>+≡
  public :: azimuthal_distance_deg

<Lorentz: interfaces>+≡
  interface azimuthal_distance_deg
    module procedure vector3_azimuthal_distance_deg
    module procedure vector4_azimuthal_distance_deg
  end interface

<Lorentz: procedures>+≡
  elemental function vector3_azimuthal_distance_deg (p, q) result (dphi)
    real(default) :: dphi
    type(vector3_t), intent(in) :: p,q
    dphi = vector3_azimuthal_distance (p, q) / degree
  end function vector3_azimuthal_distance_deg
  elemental function vector4_azimuthal_distance_deg (p, q) result (dphi)
    real(default) :: dphi
    type(vector4_t), intent(in) :: p,q
    dphi = vector4_azimuthal_distance (p, q) / degree
  end function vector4_azimuthal_distance_deg

```

The polar angle is defined $0 \leq \theta \leq \pi$. Note that ATAN2 has the reversed order of arguments: ATAN2(Y,X). Here, x is the 3-component while y is the transverse momentum which is always nonnegative. Therefore, the result is nonnegative as well.

```

<Lorentz: public functions>+≡
  public :: polar_angle

<Lorentz: interfaces>+≡
  interface polar_angle
    module procedure polar_angle_vector3
    module procedure polar_angle_vector4
  end interface

<Lorentz: procedures>+≡
  elemental function polar_angle_vector3 (p) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p
    if (any (abs (p%p) > 0)) then
      theta = atan2 (sqrt(p%p(1)**2 + p%p(2)**2), p%p(3))
    else
      theta = 0
    end if
  end function polar_angle_vector3
  elemental function polar_angle_vector4 (p) result (theta)
    real(default) :: theta
    type(vector4_t), intent(in) :: p

```

```

        theta = polar_angle (space_part (p))
    end function polar_angle_vector4

```

This is the cosine of the polar angle: $-1 \leq \cos \theta \leq 1$.

```

<Lorentz: public functions>+≡
    public :: polar_angle_ct

<Lorentz: interfaces>+≡
    interface polar_angle_ct
        module procedure polar_angle_ct_vector3
        module procedure polar_angle_ct_vector4
    end interface

<Lorentz: procedures>+≡
    elemental function polar_angle_ct_vector3 (p) result (ct)
        real(default) :: ct
        type(vector3_t), intent(in) :: p
        if (any (abs (p%p) > 0)) then
            ct = p%p(3) / p**1
        else
            ct = 1
        end if
    end function polar_angle_ct_vector3
    elemental function polar_angle_ct_vector4 (p) result (ct)
        real(default) :: ct
        type(vector4_t), intent(in) :: p
        ct = polar_angle_ct (space_part (p))
    end function polar_angle_ct_vector4

```

The polar angle in degrees.

```

<Lorentz: public functions>+≡
    public :: polar_angle_deg

<Lorentz: interfaces>+≡
    interface polar_angle_deg
        module procedure polar_angle_deg_vector3
        module procedure polar_angle_deg_vector4
    end interface

<Lorentz: procedures>+≡
    elemental function polar_angle_deg_vector3 (p) result (theta)
        real(default) :: theta
        type(vector3_t), intent(in) :: p
        theta = polar_angle (p) / degree
    end function polar_angle_deg_vector3
    elemental function polar_angle_deg_vector4 (p) result (theta)
        real(default) :: theta
        type(vector4_t), intent(in) :: p
        theta = polar_angle (p) / degree
    end function polar_angle_deg_vector4

```

This is the angle enclosed between two three-momenta. If one of the momenta is zero, we return an angle of zero. The range of the result is $0 \leq \theta \leq \pi$. If there is only one argument, take the positive z axis as reference.

```

<Lorentz: public functions>+≡

```

```

    public :: enclosed_angle
<Lorentz: interfaces>+≡
    interface enclosed_angle
        module procedure enclosed_angle_vector3
        module procedure enclosed_angle_vector4
    end interface
<Lorentz: procedures>+≡
    elemental function enclosed_angle_vector3 (p, q) result (theta)
        real(default) :: theta
        type(vector3_t), intent(in) :: p, q
        theta = acos (enclosed_angle_ct (p, q))
    end function enclosed_angle_vector3
    elemental function enclosed_angle_vector4 (p, q) result (theta)
        real(default) :: theta
        type(vector4_t), intent(in) :: p, q
        theta = enclosed_angle (space_part (p), space_part (q))
    end function enclosed_angle_vector4

```

The cosine of the enclosed angle.

```

<Lorentz: public functions>+≡
    public :: enclosed_angle_ct
<Lorentz: interfaces>+≡
    interface enclosed_angle_ct
        module procedure enclosed_angle_ct_vector3
        module procedure enclosed_angle_ct_vector4
    end interface
<Lorentz: procedures>+≡
    elemental function enclosed_angle_ct_vector3 (p, q) result (ct)
        real(default) :: ct
        type(vector3_t), intent(in) :: p, q
        if (any (abs (p%p) > 0) .and. any (abs (q%p) > 0)) then
            ct = p*q / (p**1 * q**1)
            if (ct>1) then
                ct = 1
            else if (ct<-1) then
                ct = -1
            end if
        else
            ct = 1
        end if
    end function enclosed_angle_ct_vector3
    elemental function enclosed_angle_ct_vector4 (p, q) result (ct)
        real(default) :: ct
        type(vector4_t), intent(in) :: p, q
        ct = enclosed_angle_ct (space_part (p), space_part (q))
    end function enclosed_angle_ct_vector4

```

The enclosed angle in degrees.

```

<Lorentz: public functions>+≡
    public :: enclosed_angle_deg

```

```

<Lorentz: interfaces>+≡
  interface enclosed_angle_deg
    module procedure enclosed_angle_deg_vector3
    module procedure enclosed_angle_deg_vector4
  end interface

<Lorentz: procedures>+≡
  elemental function enclosed_angle_deg_vector3 (p, q) result (theta)
    real(default) :: theta
    type(vector3_t), intent(in) :: p, q
    theta = enclosed_angle (p, q) / degree
  end function enclosed_angle_deg_vector3
  elemental function enclosed_angle_deg_vector4 (p, q) result (theta)
    real(default) :: theta
    type(vector4_t), intent(in) :: p, q
    theta = enclosed_angle (p, q) / degree
  end function enclosed_angle_deg_vector4

```

The polar angle of the first momentum w.r.t. the second momentum, evaluated in the rest frame of the second momentum. If the second four-momentum is not timelike, return zero.

```

<Lorentz: public functions>+≡
  public :: enclosed_angle_rest_frame
  public :: enclosed_angle_ct_rest_frame
  public :: enclosed_angle_deg_rest_frame

<Lorentz: interfaces>+≡
  interface enclosed_angle_rest_frame
    module procedure enclosed_angle_rest_frame_vector4
  end interface
  interface enclosed_angle_ct_rest_frame
    module procedure enclosed_angle_ct_rest_frame_vector4
  end interface
  interface enclosed_angle_deg_rest_frame
    module procedure enclosed_angle_deg_rest_frame_vector4
  end interface

<Lorentz: procedures>+≡
  elemental function enclosed_angle_rest_frame_vector4 (p, q) result (theta)
    type(vector4_t), intent(in) :: p, q
    real(default) :: theta
    theta = acos (enclosed_angle_ct_rest_frame (p, q))
  end function enclosed_angle_rest_frame_vector4
  elemental function enclosed_angle_ct_rest_frame_vector4 (p, q) result (ct)
    type(vector4_t), intent(in) :: p, q
    real(default) :: ct
    if (invariant_mass(q) > 0) then
      ct = enclosed_angle_ct ( &
        space_part (boost(-q, invariant_mass (q)) * p), &
        space_part (q))
    else
      ct = 1
    end if
  end function enclosed_angle_ct_rest_frame_vector4
  elemental function enclosed_angle_deg_rest_frame_vector4 (p, q) &

```

```

        result (theta)
    type(vector4_t), intent(in) :: p, q
    real(default) :: theta
    theta = enclosed_angle_rest_frame (p, q) / degree
end function enclosed_angle_deg_rest_frame_vector4

```

9.3.6 More kinematical functions (some redundant)

The scalar transverse momentum (assuming the z axis is longitudinal)

```

<Lorentz: public functions>+≡
    public :: transverse_part

<Lorentz: interfaces>+≡
    interface transverse_part
        module procedure transverse_part_vector4_beam_axis
        module procedure transverse_part_vector4_vector4
    end interface

<Lorentz: procedures>+≡
    elemental function transverse_part_vector4_beam_axis (p) result (pT)
        real(default) :: pT
        type(vector4_t), intent(in) :: p
        pT = sqrt(p%p(1)**2 + p%p(2)**2)
    end function transverse_part_vector4_beam_axis

    elemental function transverse_part_vector4_vector4 (p1, p2) result (pT)
        real(default) :: pT
        type(vector4_t), intent(in) :: p1, p2
        real(default) :: p1_norm, p2_norm, p1p2, pT2
        p1_norm = space_part_norm(p1)**2
        p2_norm = space_part_norm(p2)**2
        ! p1p2 = p1%p(1:3)*p2%p(1:3)
        p1p2 = vector4_get_space_part(p1) * vector4_get_space_part(p2)
        pT2 = (p1_norm*p2_norm - p1p2)/p1_norm
        pT = sqrt (pT2)
    end function transverse_part_vector4_vector4

```

The scalar longitudinal momentum (assuming the z axis is longitudinal). Identical to `momentum_z_component`.

```

<Lorentz: public functions>+≡
    public :: longitudinal_part

<Lorentz: interfaces>+≡
    interface longitudinal_part
        module procedure longitudinal_part_vector4
    end interface

<Lorentz: procedures>+≡
    elemental function longitudinal_part_vector4 (p) result (pL)
        real(default) :: pL
        type(vector4_t), intent(in) :: p
        pL = p%p(3)
    end function longitudinal_part_vector4

```

Absolute value of three-momentum

```

<Lorentz: public functions>+≡
    public :: space_part_norm

<Lorentz: interfaces>+≡
    interface space_part_norm
        module procedure space_part_norm_vector4
    end interface

<Lorentz: procedures>+≡
    elemental function space_part_norm_vector4 (p) result (p3)
        real(default) :: p3
        type(vector4_t), intent(in) :: p
        p3 = sqrt (p%p(1)**2 + p%p(2)**2 + p%p(3)**2)
    end function space_part_norm_vector4

```

The energy (the zeroth component)

```

<Lorentz: public functions>+≡
    public :: energy

<Lorentz: interfaces>+≡
    interface energy
        module procedure energy_vector4
        module procedure energy_vector3
        module procedure energy_real
    end interface

<Lorentz: procedures>+≡
    elemental function energy_vector4 (p) result (E)
        real(default) :: E
        type(vector4_t), intent(in) :: p
        E = p%p(0)
    end function energy_vector4

```

Alternative: The energy corresponding to a given momentum and mass. If the mass is omitted, it is zero

```

<Lorentz: procedures>+≡
    elemental function energy_vector3 (p, mass) result (E)
        real(default) :: E
        type(vector3_t), intent(in) :: p
        real(default), intent(in), optional :: mass
        if (present (mass)) then
            E = sqrt (p**2 + mass**2)
        else
            E = p**1
        end if
    end function energy_vector3

    elemental function energy_real (p, mass) result (E)
        real(default) :: E
        real(default), intent(in) :: p
        real(default), intent(in), optional :: mass
        if (present (mass)) then
            E = sqrt (p**2 + mass**2)
        else

```

```

        E = abs (p)
    end if
end function energy_real

```

The invariant mass of four-momenta. Zero for lightlike, negative for spacelike momenta.

```

<Lorentz: public functions>+≡
    public :: invariant_mass

<Lorentz: interfaces>+≡
    interface invariant_mass
        module procedure invariant_mass_vector4
    end interface

<Lorentz: procedures>+≡
    elemental function invariant_mass_vector4 (p) result (m)
        real(default) :: m
        type(vector4_t), intent(in) :: p
        real(default) :: msq
        msq = p*p
        if (msq >= 0) then
            m = sqrt (msq)
        else
            m = - sqrt (abs (msq))
        end if
    end function invariant_mass_vector4

```

The invariant mass squared. Zero for lightlike, negative for spacelike momenta.

```

<Lorentz: public functions>+≡
    public :: invariant_mass_squared

<Lorentz: interfaces>+≡
    interface invariant_mass_squared
        module procedure invariant_mass_squared_vector4
    end interface

<Lorentz: procedures>+≡
    elemental function invariant_mass_squared_vector4 (p) result (msq)
        real(default) :: msq
        type(vector4_t), intent(in) :: p
        msq = p*p
    end function invariant_mass_squared_vector4

```

The transverse mass. If the mass squared is negative, this value also is negative.

```

<Lorentz: public functions>+≡
    public :: transverse_mass

<Lorentz: interfaces>+≡
    interface transverse_mass
        module procedure transverse_mass_vector4
    end interface

<Lorentz: procedures>+≡
    elemental function transverse_mass_vector4 (p) result (m)
        real(default) :: m
        type(vector4_t), intent(in) :: p

```



```

real(default) :: msq
msq = p%p(0)**2 - p%p(1)**2 - p%p(2)**2
if (msq >= 0) then
    m = sqrt (msq)
else
    m = - sqrt (abs (msq))
end if
end function transverse_mass_vector4

```

The rapidity (defined if particle is massive or $p_{\perp} > 0$)

```

<Lorentz: public functions>+≡
public :: rapidity

<Lorentz: interfaces>+≡
interface rapidity
    module procedure rapidity_vector4
end interface

<Lorentz: procedures>+≡
elemental function rapidity_vector4 (p) result (y)
    real(default) :: y
    type(vector4_t), intent(in) :: p
    y = .5 * log( (energy (p) + longitudinal_part (p)) &
        &          /(energy (p) - longitudinal_part (p)))
end function rapidity_vector4

```

The pseudorapidity (defined if $p_{\perp} > 0$)

```

<Lorentz: public functions>+≡
public :: pseudorapidity

<Lorentz: interfaces>+≡
interface pseudorapidity
    module procedure pseudorapidity_vector4
end interface

<Lorentz: procedures>+≡
elemental function pseudorapidity_vector4 (p) result (eta)
    real(default) :: eta
    type(vector4_t), intent(in) :: p
    eta = -log( tan (.5 * polar_angle (p)))
end function pseudorapidity_vector4

```

The rapidity distance (defined if both $p_{\perp} > 0$)

```

<Lorentz: public functions>+≡
public :: rapidity_distance

<Lorentz: interfaces>+≡
interface rapidity_distance
    module procedure rapidity_distance_vector4
end interface

<Lorentz: procedures>+≡
elemental function rapidity_distance_vector4 (p, q) result (dy)
    type(vector4_t), intent(in) :: p, q
    real(default) :: dy

```

```

dy = rapidity (q) - rapidity (p)
end function rapidity_distance_vector4

```

The pseudorapidity distance (defined if both $p_{\perp} > 0$)

```

<Lorentz: public functions>+≡
public :: pseudorapidity_distance

<Lorentz: interfaces>+≡
interface pseudorapidity_distance
  module procedure pseudorapidity_distance_vector4
end interface

<Lorentz: procedures>+≡
elemental function pseudorapidity_distance_vector4 (p, q) result (deta)
  real(default) :: deta
  type(vector4_t), intent(in) :: p, q
  deta = pseudorapidity (q) - pseudorapidity (p)
end function pseudorapidity_distance_vector4

```

The distance on the $\eta - \phi$ cylinder:

```

<Lorentz: public functions>+≡
public :: eta_phi_distance

<Lorentz: interfaces>+≡
interface eta_phi_distance
  module procedure eta_phi_distance_vector4
end interface

<Lorentz: procedures>+≡
elemental function eta_phi_distance_vector4 (p, q) result (dr)
  type(vector4_t), intent(in) :: p, q
  real(default) :: dr
  dr = sqrt ( &
    pseudorapidity_distance (p, q)**2 &
    + azimuthal_distance (p, q)**2)
end function eta_phi_distance_vector4

```

9.3.7 Lorentz transformations

```

<Lorentz: public>+≡
public :: lorentz_transformation_t

<Lorentz: types>+≡
type :: lorentz_transformation_t
  private
  real(default), dimension(0:3, 0:3) :: L
  contains
  <Lorentz: lorentz_transformation: TBP>
end type lorentz_transformation_t

```

Output:

```

<Lorentz: public>+≡
public :: lorentz_transformation_write

```

```

⟨Lorentz: lorentz transformation: TBP⟩≡
  procedure :: write => lorentz_transformation_write

⟨Lorentz: procedures⟩+≡
  subroutine lorentz_transformation_write (L, unit, testflag, ultra)
    class(lorentz_transformation_t), intent(in) :: L
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag, ultra
    integer :: u, i
    logical :: ult
    character(len=7) :: fmt
    ult = .false.; if (present (ultra)) ult = ultra
    if (ult) then
      call pac_fmt (fmt, FMT_19, FMT_11, ultra)
    else
      call pac_fmt (fmt, FMT_19, FMT_13, testflag)
    end if
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A,3(1x," // fmt // ")))" "L00 = ", L%L(0,0)
    write (u, "(1x,A,3(1x," // fmt // ")))" "L0j = ", L%L(0,1:3)
    do i = 1, 3
      write (u, "(1x,A,I0,A,3(1x," // fmt // ")))" &
        "L", i, "0 = ", L%L(i,0)
      write (u, "(1x,A,I0,A,3(1x," // fmt // ")))" &
        "L", i, "j = ", L%L(i,1:3)
    end do
  end subroutine lorentz_transformation_write

```

Extract all components:

```

⟨Lorentz: public⟩+≡
  public :: lorentz_transformation_get_components

⟨Lorentz: procedures⟩+≡
  pure function lorentz_transformation_get_components (L) result (a)
    type(lorentz_transformation_t), intent(in) :: L
    real(default), dimension(0:3,0:3) :: a
    a = L%L
  end function lorentz_transformation_get_components

```

9.3.8 Functions of Lorentz transformations

For the inverse, we make use of the fact that $\Lambda^{\mu\nu}\Lambda_{\mu\rho} = \delta_{\rho}^{\nu}$. So, lowering the indices and transposing is sufficient.

```

⟨Lorentz: public functions⟩+≡
  public :: inverse

⟨Lorentz: interfaces⟩+≡
  interface inverse
    module procedure lorentz_transformation_inverse
  end interface

```

```

<Lorentz: procedures>+≡
  elemental function lorentz_transformation_inverse (L) result (IL)
    type(lorentz_transformation_t) :: IL
    type(lorentz_transformation_t), intent(in) :: L
    IL%L(0,0) = L%L(0,0)
    IL%L(0,1:) = -L%L(1:,0)
    IL%L(1:,0) = -L%L(0,1:)
    IL%L(1:,1:) = transpose(L%L(1:,1:))
  end function lorentz_transformation_inverse

```

9.3.9 Invariants

These are used below. The first array index is varying fastest in FORTRAN; therefore the extra minus in the odd-rank tensor epsilon.

```

<Lorentz: parameters>+≡
  integer, dimension(3,3), parameter :: delta_three = &
    & reshape( source = [ 1,0,0, 0,1,0, 0,0,1 ], &
    &          shape = [3,3] )
  integer, dimension(3,3,3), parameter :: epsilon_three = &
    & reshape( source = [ 0, 0,0, 0,0,-1, 0,1,0, &
    &                    0, 0,1, 0,0, 0, -1,0,0, &
    &                    0,-1,0, 1,0, 0, 0,0,0 ],&
    &          shape = [3,3,3] )

```

This could be of some use:

```

<Lorentz: public>+≡
  public :: identity

<Lorentz: parameters>+≡
  type(lorentz_transformation_t), parameter :: &
    & identity = &
    & lorentz_transformation_t ( &
    & reshape( source = [ one, zero, zero, zero, &
    &                    zero, one, zero, zero, &
    &                    zero, zero, one, zero, &
    &                    zero, zero, zero, one ],&
    &          shape = [4,4] ) )

<Lorentz: public>+≡
  public :: space_reflection

<Lorentz: parameters>+≡
  type(lorentz_transformation_t), parameter :: &
    & space_reflection = &
    & lorentz_transformation_t ( &
    & reshape( source = [ one, zero, zero, zero, &
    &                    zero,-one, zero, zero, &
    &                    zero, zero,-one, zero, &
    &                    zero, zero, zero,-one ],&
    &          shape = [4,4] ) )

```

Builds a unit vector orthogonal to the input vector in the xy-plane.

```

<Lorentz: public functions>+≡
  public :: create_orthogonal

```

```

(Lorentz: procedures)+≡
function create_orthogonal (p_in) result (p_out)
  type(vector3_t), intent(in) :: p_in
  type(vector3_t) :: p_out
  real(default) :: ab
  ab = sqrt (p_in%p(1)**2 + p_in%p(2)**2)
  if (abs (ab) < eps0) then
    p_out%p(1) = 1
    p_out%p(2) = 0
    p_out%p(3) = 0
  else
    p_out%p(1) = p_in%p(2)
    p_out%p(2) = -p_in%p(1)
    p_out%p(3) = 0
    p_out = p_out / ab
  end if
end function create_orthogonal

```

```

(Lorentz: public functions)+≡
public :: create_unit_vector

```

```

(Lorentz: procedures)+≡
function create_unit_vector (p_in) result (p_out)
  type(vector4_t), intent(in) :: p_in
  type(vector3_t) :: p_out
  p_out%p = p_in%p(1:3) / space_part_norm (p_in)
end function create_unit_vector

```

```

(Lorentz: public functions)+≡
public :: normalize

```

```

(Lorentz: procedures)+≡
function normalize(p) result (p_norm)
  type(vector3_t) :: p_norm
  type(vector3_t), intent(in) :: p
  real(default) :: abs
  abs = sqrt (p%p(1)**2 + p%p(2)**2 + p%p(3)**2)
  p_norm = p / abs
end function normalize

```

Computes the invariant mass of the momenta sum given by the indices in `i_res_born` and the optional argument `i_emitter`.

```

(Lorentz: public)+≡
public :: compute_resonance_mass

(Lorentz: procedures)+≡
pure function compute_resonance_mass (p, i_res_born, i_gluon) result (m)
  real(default) :: m
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in), dimension(:) :: i_res_born
  integer, intent(in), optional :: i_gluon
  type(vector4_t) :: p_res
  p_res = get_resonance_momentum (p, i_res_born, i_gluon)
  m = p_res**1

```

```

end function compute_resonance_mass

<Lorentz: public>+≡
public :: get_resonance_momentum

<Lorentz: procedures>+≡
pure function get_resonance_momentum (p, i_res_born, i_gluon) result (p_res)
  type(vector4_t) :: p_res
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in), dimension(:) :: i_res_born
  integer, intent(in), optional :: i_gluon
  integer :: i
  p_res = vector4_null
  do i = 1, size (i_res_born)
    p_res = p_res + p (i_res_born(i))
  end do
  if (present (i_gluon)) p_res = p_res + p (i_gluon)
end function get_resonance_momentum

<Lorentz: public>+≡
public :: create_two_particle_decay

<Lorentz: procedures>+≡
function create_two_particle_decay (s, p1, p2) result (p_rest)
  type(vector4_t), dimension(3) :: p_rest
  real(default), intent(in) :: s
  type(vector4_t), intent(in) :: p1, p2
  real(default) :: m1_sq, m2_sq
  real(default) :: E1, E2, p
  m1_sq = p1**2; m2_sq = p2**2
  p = sqrt (lambda (s, m1_sq, m2_sq)) / (two * sqrt (s))
  E1 = sqrt (m1_sq + p**2); E2 = sqrt (m2_sq + p**2)
  p_rest(1)%p = [sqrt (s), zero, zero, zero]
  p_rest(2)%p(0) = E1
  p_rest(2)%p(1:3) = p * p1%p(1:3) / space_part_norm (p1)
  p_rest(3)%p(0) = E2; p_rest(3)%p(1:3) = -p_rest(2)%p(1:3)
end function create_two_particle_decay

```

This function creates a phase-space point for a $1 \rightarrow 3$ decay in the decaying particle's rest frame. There are three rest frames for this system, corresponding to s -, t -, and u -channel momentum exchange, also referred to as Gottfried-Jackson frames. Below, we choose the momentum with index 1 to be aligned along the z -axis. We then have

$$\begin{aligned}
s_1 &= (p_1 + p_2)^2, \\
s_2 &= (p_2 + p_3)^2, \\
s_3 &= (p_1 + p_3)^2, \\
s_1 + s_2 + s_3 &= s + m_1^2 + m_2^2 + m_3^2.
\end{aligned}$$

From these we can construct

$$\begin{aligned} E_1^{R23} &= \frac{s - s_2 - m_1^2}{2\sqrt{s_2}} & P_1^{R23} &= \frac{\lambda^{1/2}(s, s_2, m_1^2)}{2\sqrt{s_2}}, \\ E_2^{R23} &= \frac{s_2 + m_2^2 - m_3^2}{2\sqrt{s_2}} & P_2^{R23} &= \frac{\lambda^{1/2}(s_2, m_2^2, m_3^2)}{2\sqrt{s_2}}, \\ E_3^{R23} &= \frac{s_2 + m_3^2 - m_2^2}{2\sqrt{s_2}} & P_3^{R23} &= P_2^{R23}, \end{aligned}$$

where $R23$ denotes the Gottfried-Jackson frame of our choice. Finally, the scattering angle θ_{12}^{R23} between momentum 1 and 2 can be determined to be

$$\cos \theta_{12}^{R23} = \frac{(s - s_2 - m_1^2)(s_2 + m_2^2 - m_3^2) + 2s_2(m_1^2 + m_2^2 - s_1)}{\lambda^{1/2}(s, s_2, m_1^2)\lambda^{1/2}(s_2, m_2^2, m_3^2)}$$

(Lorentz: public)+≡

`public :: create_three_particle_decay`

(Lorentz: procedures)+≡

```
function create_three_particle_decay (p1, p2, p3) result (p_rest)
  type(vector4_t), dimension(4) :: p_rest
  type(vector4_t), intent(in) :: p1, p2, p3
  real(default) :: E1, E2, E3
  real(default) :: pr1, pr2, pr3
  real(default) :: s, s1, s2, s3
  real(default) :: m1_sq, m2_sq, m3_sq
  real(default) :: cos_theta_12
  type(vector3_t) :: v3_unit
  type(lorentz_transformation_t) :: rot
  m1_sq = p1**2
  m2_sq = p2**2
  m3_sq = p3**2
  s1 = (p1 + p2)**2
  s2 = (p2 + p3)**2
  s3 = (p3 + p1)**2
  s = s1 + s2 + s3 - m1_sq - m2_sq - m3_sq
  E1 = (s - s2 - m1_sq) / (two * sqrt (s2))
  E2 = (s2 + m2_sq - m3_sq) / (two * sqrt (s2))
  E3 = (s2 + m3_sq - m2_sq) / (two * sqrt (s2))
  pr1 = sqrt (lambda (s, s2, m1_sq)) / (two * sqrt (s2))
  pr2 = sqrt (lambda (s2, m2_sq, m3_sq)) / (two * sqrt(s2))
  pr3 = pr2
  cos_theta_12 = ((s - s2 - m1_sq) * (s2 + m2_sq - m3_sq) + two * s2 * (m1_sq + m2_sq - s1)) / &
    sqrt (lambda (s, s2, m1_sq) * lambda (s2, m2_sq, m3_sq))
  v3_unit%p = [zero, zero, one]
  p_rest(1)%p(0) = E1
  p_rest(1)%p(1:3) = v3_unit%p * pr1
  p_rest(2)%p(0) = E2
  p_rest(2)%p(1:3) = v3_unit%p * pr2
  p_rest(3)%p(0) = E3
  p_rest(3)%p(1:3) = v3_unit%p * pr3
  p_rest(4)%p(0) = (s + s2 - m1_sq) / (2 * sqrt (s2))
  p_rest(4)%p(1:3) = - p_rest(1)%p(1:3)
  rot = rotation (cos_theta_12, sqrt (one - cos_theta_12**2), 2)
```

```

    p_rest(2) = rot * p_rest(2)
    p_rest(3)%p(1:3) = - p_rest(2)%p(1:3)
end function create_three_particle_decay

```

<Lorentz: public>+≡

```

    public :: evaluate_one_to_two_splitting_special

```

<Lorentz: interfaces>+≡

```

    abstract interface
        subroutine evaluate_one_to_two_splitting_special (p_origin, &
            p1_in, p2_in, p1_out, p2_out, msq_in, jac)
            import
            type(vector4_t), intent(in) :: p_origin
            type(vector4_t), intent(in) :: p1_in, p2_in
            type(vector4_t), intent(inout) :: p1_out, p2_out
            real(default), intent(in), optional :: msq_in
            real(default), intent(inout), optional :: jac
        end subroutine evaluate_one_to_two_splitting_special
    end interface

```

<Lorentz: public>+≡

```

    public :: generate_on_shell_decay

```

<Lorentz: procedures>+≡

```

    recursive subroutine generate_on_shell_decay (p_dec, &
        p_in, p_out, i_real, msq_in, jac, evaluate_special)
        type(vector4_t), intent(in) :: p_dec
        type(vector4_t), intent(in), dimension(:) :: p_in
        type(vector4_t), intent(inout), dimension(:) :: p_out
        integer, intent(in) :: i_real
        real(default), intent(in), optional :: msq_in
        real(default), intent(inout), optional :: jac
        procedure(evaluate_one_to_two_splitting_special), intent(in), &
            pointer, optional :: evaluate_special
        type(vector4_t) :: p_dec_new
        integer :: n_recoil
        n_recoil = size (p_in) - 1
        if (n_recoil > 1) then
            if (present (evaluate_special)) then
                call evaluate_special (p_dec, p_in(1), sum (p_in (2 : n_recoil + 1)), &
                    p_out(i_real), p_dec_new)
                call generate_on_shell_decay (p_dec_new, p_in (2 : ), p_out, &
                    i_real + 1, msq_in, jac, evaluate_special)
            else
                call evaluate_one_to_two_splitting (p_dec, p_in(1), &
                    sum (p_in (2 : n_recoil + 1)), p_out(i_real), p_dec_new, msq_in, jac)
                call generate_on_shell_decay (p_dec_new, p_in (2 : ), p_out, &
                    i_real + 1, msq_in, jac)
            end if
        else
            call evaluate_one_to_two_splitting (p_dec, p_in(1), p_in(2), &
                p_out(i_real), p_out(i_real + 1), msq_in, jac)
        end if
    end if

```



```

end subroutine generate_on_shell_decay

subroutine evaluate_one_to_two_splitting (p_origin, &
    p1_in, p2_in, p1_out, p2_out, msq_in, jac)
    type(vector4_t), intent(in) :: p_origin
    type(vector4_t), intent(in) :: p1_in, p2_in
    type(vector4_t), intent(inout) :: p1_out, p2_out
    real(default), intent(in), optional :: msq_in
    real(default), intent(inout), optional :: jac
    type(lorentz_transformation_t) :: L
    type(vector4_t) :: p1_rest, p2_rest
    real(default) :: m, msq, msq1, msq2
    real(default) :: E1, E2, p
    real(default) :: lda, rlda_soft

    call get_rest_frame (p1_in, p2_in, p1_rest, p2_rest)

    msq = p_origin**2; m = sqrt(msq)
    msq1 = p1_in**2; msq2 = p2_in**2

    lda = lambda (msq, msq1, msq2)
    if (lda < zero) then
        print *, 'Encountered lambda < 0 in 1 -> 2 splitting! '
        print *, 'lda: ', lda
        print *, 'm: ', m, 'msq: ', msq
        print *, 'm1: ', sqrt (msq1), 'msq1: ', msq1
        print *, 'm2: ', sqrt (msq2), 'msq2: ', msq2
        stop
    end if
    p = sqrt (lda) / (two * m)

    E1 = sqrt (msq1 + p**2)
    E2 = sqrt (msq2 + p**2)

    p1_out = shift_momentum (p1_rest, E1, p)
    p2_out = shift_momentum (p2_rest, E2, p)

    L = boost (p_origin, p_origin**1)
    p1_out = L * p1_out
    p2_out = L * p2_out

    if (present (jac) .and. present (msq_in)) then
        jac = jac * sqrt(lda) / msq
        rlda_soft = sqrt (lambda (msq_in, msq1, msq2))
        !!! We have to undo the Jacobian which has already been
        !!! supplied by the Born phase space.
        jac = jac * msq_in / rlda_soft
    end if

contains

subroutine get_rest_frame (p1_in, p2_in, p1_out, p2_out)
    type(vector4_t), intent(in) :: p1_in, p2_in
    type(vector4_t), intent(out) :: p1_out, p2_out

```

```

    type(lorentz_transformation_t) :: L
    L = inverse (boost (p1_in + p2_in, (p1_in + p2_in)**1))
    p1_out = L * p1_in; p2_out = L * p2_in
end subroutine get_rest_frame

function shift_momentum (p_in, E, p) result (p_out)
    type(vector4_t) :: p_out
    type(vector4_t), intent(in) :: p_in
    real(default), intent(in) :: E, p
    type(vector3_t) :: vec
    vec = p_in%p(1:3) / space_part_norm (p_in)
    p_out = vector4_moving (E, p * vec)
end function shift_momentum

end subroutine evaluate_one_to_two_splitting

```

9.3.10 Boosts

We build Lorentz transformations from boosts and rotations. In both cases we can supply a three-vector which defines the axis and (hyperbolic) angle. For a boost, this is the vector $\vec{\beta} = \vec{p}/E$, such that a particle at rest with mass m is boosted to a particle with three-vector \vec{p} . Here, we have

$$\beta = \tanh \chi = p/E, \quad \gamma = \cosh \chi = E/m, \quad \beta\gamma = \sinh \chi = p/m \quad (9.1)$$

```

<Lorentz: public functions>+≡
    public :: boost

<Lorentz: interfaces>+≡
    interface boost
        module procedure boost_from_rest_frame
        module procedure boost_from_rest_frame_vector3
        module procedure boost_generic
        module procedure boost_canonical
    end interface

```

In the first form, the argument is some four-momentum, the space part of which determines a direction, and the associated mass (which is not checked against the four-momentum). The boost vector $\gamma\vec{\beta}$ is then given by \vec{p}/m . This boosts from the rest frame of a particle to the current frame. To be explicit, if \vec{p} is the momentum of a particle and m its mass, $L(\vec{p}/m)$ is the transformation that turns $(m; \vec{0})$ into $(E; \vec{p})$. Conversely, the inverse transformation boosts a vector *into* the rest frame of a particle, in particular $(E; \vec{p})$ into $(m; \vec{0})$.

```

<Lorentz: procedures>+≡
    elemental function boost_from_rest_frame (p, m) result (L)
        type(lorentz_transformation_t) :: L
        type(vector4_t), intent(in) :: p
        real(default), intent(in) :: m
        L = boost_from_rest_frame_vector3 (space_part (p), m)
    end function boost_from_rest_frame
    elemental function boost_from_rest_frame_vector3 (p, m) result (L)
        type(lorentz_transformation_t) :: L
        type(vector3_t), intent(in) :: p

```

```

real(default), intent(in) :: m
type(vector3_t) :: beta_gamma
real(default) :: bg2, g, c
integer :: i,j
if (m > eps0) then
    beta_gamma = p / m
    bg2 = beta_gamma**2
else
    bg2 = 0
    L = identity
    return
end if
if (bg2 > eps0) then
    g = sqrt(1 + bg2); c = (g-1)/bg2
else
    g = one + bg2 / two
    c = one / two
end if
L%L(0,0) = g
L%L(0,1:) = beta_gamma%p
L%L(1:,0) = L%L(0,1:)
do i=1,3
    do j=1,3
        L%L(i,j) = delta_three(i,j) + c*beta_gamma%p(i)*beta_gamma%p(j)
    end do
end do
end function boost_from_rest_frame_vector3

```

A canonical boost is a boost along one of the coordinate axes, which we may supply as an integer argument. Here, $\gamma\beta$ is scalar.

(Lorentz: procedures) + \equiv

```

elemental function boost_canonical (beta_gamma, k) result (L)
type(lorentz_transformation_t) :: L
real(default), intent(in) :: beta_gamma
integer, intent(in) :: k
real(default) :: g
g = sqrt(1 + beta_gamma**2)
L = identity
L%L(0,0) = g
L%L(0,k) = beta_gamma
L%L(k,0) = L%L(0,k)
L%L(k,k) = L%L(0,0)
end function boost_canonical

```

Instead of a canonical axis, we can supply an arbitrary axis which need not be normalized. If it is zero, return the unit matrix.

(Lorentz: procedures) + \equiv

```

elemental function boost_generic (beta_gamma, axis) result (L)
type(lorentz_transformation_t) :: L
real(default), intent(in) :: beta_gamma
type(vector3_t), intent(in) :: axis
if (any (abs (axis%p) > 0)) then
    L = boost_from_rest_frame_vector3 (beta_gamma * axis, axis**1)
else
    L = identity

```

```

end if
end function boost_generic

```

9.3.11 Rotations

For a rotation, the vector defines the rotation axis, and its length the rotation angle. All of these rotations rotate counterclockwise in a right-handed coordinate system.

```

(Lorentz: public functions)+≡
public :: rotation

(Lorentz: interfaces)+≡
interface rotation
  module procedure rotation_generic
  module procedure rotation_canonical
  module procedure rotation_generic_cs
  module procedure rotation_canonical_cs
end interface

```

If $\cos \phi$ and $\sin \phi$ is already known, we do not have to calculate them. Of course, the user has to ensure that $\cos^2 \phi + \sin^2 \phi = 1$, and that the given axis \mathbf{n} is normalized to one. In the second form, the length of `axis` is the rotation angle.

```

(Lorentz: procedures)+≡
elemental function rotation_generic_cs (cp, sp, axis) result (R)
  type(lorentz_transformation_t) :: R
  real(default), intent(in) :: cp, sp
  type(vector3_t), intent(in) :: axis
  integer :: i,j
  R = identity
  do i=1,3
    do j=1,3
      R%L(i,j) = cp*delta_three(i,j) + (1-cp)*axis%p(i)*axis%p(j) &
        & - sp*dot_product(epsilon_three(i,j,:), axis%p)
    end do
  end do
end function rotation_generic_cs
elemental function rotation_generic (axis) result (R)
  type(lorentz_transformation_t) :: R
  type(vector3_t), intent(in) :: axis
  real(default) :: phi
  if (any (abs(axis%p) > 0)) then
    phi = abs(axis**1)
    R = rotation_generic_cs (cos(phi), sin(phi), axis/phi)
  else
    R = identity
  end if
end function rotation_generic

```

Alternatively, give just the angle and label the coordinate axis by an integer.

```

(Lorentz: procedures)+≡
elemental function rotation_canonical_cs (cp, sp, k) result (R)
  type(lorentz_transformation_t) :: R

```

```

real(default), intent(in) :: cp, sp
integer, intent(in) :: k
integer :: i,j
R = identity
do i=1,3
  do j=1,3
    R%L(i,j) = -sp*epsilon_three(i,j,k)
  end do
  R%L(i,i) = cp
end do
R%L(k,k) = 1
end function rotation_canonical_cs
elemental function rotation_canonical (phi, k) result (R)
  type(lorentz_transformation_t) :: R
  real(default), intent(in) :: phi
  integer, intent(in) :: k
  R = rotation_canonical_cs(cos(phi), sin(phi), k)
end function rotation_canonical

```

This is viewed as a method for the first argument (three-vector): Reconstruct the rotation that rotates it into the second three-vector.

```

<Lorentz: public functions>+≡
  public :: rotation_to_2nd

<Lorentz: interfaces>+≡
  interface rotation_to_2nd
    module procedure rotation_to_2nd_generic
    module procedure rotation_to_2nd_canonical
  end interface

<Lorentz: procedures>+≡
  elemental function rotation_to_2nd_generic (p, q) result (R)
    type(lorentz_transformation_t) :: R
    type(vector3_t), intent(in) :: p, q
    type(vector3_t) :: a, b, ab
    real(default) :: ct, st
    if (any (abs (p%p) > 0) .and. any (abs (q%p) > 0)) then
      a = direction (p)
      b = direction (q)
      ab = cross_product(a,b)
      ct = a * b;  st = ab**1
      if (abs(st) > eps0) then
        R = rotation_generic_cs (ct, st, ab / st)
      else if (ct < 0) then
        R = space_reflection
      else
        R = identity
      end if
    else
      R = identity
    end if
  end function rotation_to_2nd_generic

```

The same for a canonical axis: The function returns the transformation that rotates the k -axis into the direction of p .

```

<Lorentz: procedures>+≡

```

```

elemental function rotation_to_2nd_canonical (k, p) result (R)
  type(lorentz_transformation_t) :: R
  integer, intent(in) :: k
  type(vector3_t), intent(in) :: p
  type(vector3_t) :: b, ab
  real(default) :: ct, st
  integer :: i, j
  if (any (abs (p%p) > 0)) then
    b = direction (p)
    ab%p = 0
    do i = 1, 3
      do j = 1, 3
        ab%p(j) = ab%p(j) + b%p(i) * epsilon_three(i,j,k)
      end do
    end do
    ct = b%p(k); st = ab**1
    if (abs(st) > eps0) then
      R = rotation_generic_cs (ct, st, ab / st)
    else if (ct < 0) then
      R = space_reflection
    else
      R = identity
    end if
  else
    R = identity
  end if
end function rotation_to_2nd_canonical

```

9.3.12 Composite Lorentz transformations

This function returns the transformation that, given a pair of vectors $p_{1,2}$, (a) boosts from the rest frame of the c.m. system (with invariant mass m) into the lab frame where p_i are defined, and (b) turns the given axis (or the canonical vectors $\pm e_k$) in the rest frame into the directions of $p_{1,2}$ in the lab frame. Note that the energy components are not used; for a consistent result one should have $(p_1 + p_2)^2 = m^2$.

```

<Lorentz: public functions>+≡
  public :: transformation

<Lorentz: interfaces>+≡
  interface transformation
    module procedure transformation_rec_generic
    module procedure transformation_rec_canonical
  end interface

<Lorentz: procedures>+≡
  elemental function transformation_rec_generic (axis, p1, p2, m) result (L)
    type(vector3_t), intent(in) :: axis
    type(vector4_t), intent(in) :: p1, p2
    real(default), intent(in) :: m
    type(lorentz_transformation_t) :: L
    L = boost (p1 + p2, m)
    L = L * rotation_to_2nd (axis, space_part (inverse (L) * p1))

```

```

end function transformation_rec_generic
elemental function transformation_rec_canonical (k, p1, p2, m) result (L)
  integer, intent(in) :: k
  type(vector4_t), intent(in) :: p1, p2
  real(default), intent(in) :: m
  type(lorentz_transformation_t) :: L
  L = boost (p1 + p2, m)
  L = L * rotation_to_2nd (k, space_part (inverse (L) * p1))
end function transformation_rec_canonical

```

9.3.13 Applying Lorentz transformations

Multiplying vectors and Lorentz transformations is straightforward.

```

<Lorentz: interfaces>+≡
  interface operator(*)
    module procedure prod_LT_vector4
    module procedure prod_LT_LT
    module procedure prod_vector4_LT
  end interface

<Lorentz: procedures>+≡
  elemental function prod_LT_vector4 (L, p) result (np)
    type(vector4_t) :: np
    type(lorentz_transformation_t), intent(in) :: L
    type(vector4_t), intent(in) :: p
    np%p = matmul (L%L, p%p)
  end function prod_LT_vector4
  elemental function prod_LT_LT (L1, L2) result (NL)
    type(lorentz_transformation_t) :: NL
    type(lorentz_transformation_t), intent(in) :: L1, L2
    NL%L = matmul (L1%L, L2%L)
  end function prod_LT_LT
  elemental function prod_vector4_LT (p, L) result (np)
    type(vector4_t) :: np
    type(vector4_t), intent(in) :: p
    type(lorentz_transformation_t), intent(in) :: L
    np%p = matmul (p%p, L%L)
  end function prod_vector4_LT

```

9.3.14 Special Lorentz transformations

These routines have their application in the generation and extraction of angles in the phase-space sampling routine. Since this part of the program is time-critical, we calculate the composition of transformations directly instead of multiplying rotations and boosts.

This Lorentz transformation is the composition of a rotation by ϕ around the 3 axis, a rotation by θ around the 2 axis, and a boost along the 3 axis:

$$L = B_3(\beta\gamma) R_2(\theta) R_3(\phi) \quad (9.2)$$

Instead of the angles we provide sine and cosine.

```

<Lorentz: public functions>+≡
  public :: LT_compose_r3_r2_b3

```

```

(Lorentz: procedures)+≡
elemental function LT_compose_r3_r2_b3 &
  (cp, sp, ct, st, beta_gamma) result (L)
  type(lorentz_transformation_t) :: L
  real(default), intent(in) :: cp, sp, ct, st, beta_gamma
  real(default) :: gamma
  if (abs(beta_gamma) < eps0) then
    L%L(0,0) = 1
    L%L(1:,0) = 0
    L%L(0,1:) = 0
    L%L(1,1:) = [ ct*cp, -ct*sp, st ]
    L%L(2,1:) = [      sp,      cp, zero ]
    L%L(3,1:) = [ -st*cp, st*sp, ct ]
  else
    gamma = sqrt(1 + beta_gamma**2)
    L%L(0,0) = gamma
    L%L(1,0) = 0
    L%L(2,0) = 0
    L%L(3,0) = beta_gamma
    L%L(0,1:) = beta_gamma * [ -st*cp, st*sp, ct ]
    L%L(1,1:) = [ ct*cp, -ct*sp, st ]
    L%L(2,1:) = [      sp,      cp, zero ]
    L%L(3,1:) = gamma * [ -st*cp, st*sp, ct ]
  end if
end function LT_compose_r3_r2_b3

```

Different ordering:

$$L = B_3(\beta\gamma) R_3(\phi) R_2(\theta) \quad (9.3)$$

```

(Lorentz: public functions)+≡
public :: LT_compose_r2_r3_b3

(Lorentz: procedures)+≡
elemental function LT_compose_r2_r3_b3 &
  (ct, st, cp, sp, beta_gamma) result (L)
  type(lorentz_transformation_t) :: L
  real(default), intent(in) :: ct, st, cp, sp, beta_gamma
  real(default) :: gamma
  if (abs(beta_gamma) < eps0) then
    L%L(0,0) = 1
    L%L(1:,0) = 0
    L%L(0,1:) = 0
    L%L(1,1:) = [ ct*cp, -sp, st*cp ]
    L%L(2,1:) = [ ct*sp, cp, st*sp ]
    L%L(3,1:) = [ -st, zero, ct ]
  else
    gamma = sqrt(1 + beta_gamma**2)
    L%L(0,0) = gamma
    L%L(1,0) = 0
    L%L(2,0) = 0
    L%L(3,0) = beta_gamma
    L%L(0,1:) = beta_gamma * [ -st, zero, ct ]
    L%L(1,1:) = [ ct*cp, -sp, st*cp ]
    L%L(2,1:) = [ ct*sp, cp, st*sp ]
    L%L(3,1:) = gamma * [ -st, zero, ct ]
  end if
end function LT_compose_r2_r3_b3

```



```

end if
end function LT_compose_r2_r3_b3

```

This function returns the previous Lorentz transformation applied to an arbitrary four-momentum and extracts the space part of the result:

$$\vec{n} = [B_3(\beta\gamma) R_2(\theta) R_3(\phi) p]_{\text{space part}} \quad (9.4)$$

The second variant applies if there is no rotation

```

<Lorentz: public functions>+≡
  public :: axis_from_p_r3_r2_b3, axis_from_p_b3

<Lorentz: procedures>+≡
  elemental function axis_from_p_r3_r2_b3 &
    (p, cp, sp, ct, st, beta_gamma) result (n)
    type(vector3_t) :: n
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: cp, sp, ct, st, beta_gamma
    real(default) :: gamma, px, py
    px = cp * p%p(1) - sp * p%p(2)
    py = sp * p%p(1) + cp * p%p(2)
    n%p(1) = ct * px + st * p%p(3)
    n%p(2) = py
    n%p(3) = -st * px + ct * p%p(3)
    if (abs(beta_gamma) > eps0) then
      gamma = sqrt(1 + beta_gamma**2)
      n%p(3) = n%p(3) * gamma + p%p(0) * beta_gamma
    end if
  end function axis_from_p_r3_r2_b3

  elemental function axis_from_p_b3 (p, beta_gamma) result (n)
    type(vector3_t) :: n
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: beta_gamma
    real(default) :: gamma
    n%p = p%p(1:3)
    if (abs(beta_gamma) > eps0) then
      gamma = sqrt(1 + beta_gamma**2)
      n%p(3) = n%p(3) * gamma + p%p(0) * beta_gamma
    end if
  end function axis_from_p_b3

```

9.3.15 Special functions

The Källén function, mostly used for the phase space. This is equivalent to $\lambda(x, y, z) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz$.

```

<Lorentz: public functions>+≡
  public :: lambda

<Lorentz: procedures>+≡
  elemental function lambda (m1sq, m2sq, m3sq)
    real(default) :: lambda
    real(default), intent(in) :: m1sq, m2sq, m3sq

```

```

        lambda = (m1sq - m2sq - m3sq)**2 - 4*m2sq*m3sq
    end function lambda

```

Return a pair of head-to-head colliding momenta, given the collider energy, particle masses, and optionally the momentum of the c.m. system.

```

(Lorentz: public functions)+≡
    public :: colliding_momenta

(Lorentz: procedures)+≡
    function colliding_momenta (sqrts, m, p_cm) result (p)
        type(vector4_t), dimension(2) :: p
        real(default), intent(in) :: sqrts
        real(default), dimension(2), intent(in), optional :: m
        real(default), intent(in), optional :: p_cm
        real(default), dimension(2) :: dmsq
        real(default) :: ch, sh
        real(default), dimension(2) :: E0, p0
        integer, dimension(2), parameter :: sgn = [1, -1]
        if (abs(sqrts) < eps0) then
            call msg_fatal (" Colliding beams: sqrts is zero (please set sqrts)")
            p = vector4_null; return
        else if (sqrts <= 0) then
            call msg_fatal (" Colliding beams: sqrts is negative")
            p = vector4_null; return
        end if
        if (present (m)) then
            dmsq = sgn * (m(1)**2-m(2)**2)
            E0 = (sqrts + dmsq/sqrts) / 2
            if (any (E0 < m)) then
                call msg_fatal &
                    (" Colliding beams: beam energy is less than particle mass")
                p = vector4_null; return
            end if
            p0 = sgn * sqrt (E0**2 - m**2)
        else
            E0 = sqrts / 2
            p0 = sgn * E0
        end if
        if (present (p_cm)) then
            sh = p_cm / sqrts
            ch = sqrt (1 + sh**2)
            p = vector4_moving (E0 * ch + p0 * sh, E0 * sh + p0 * ch, 3)
        else
            p = vector4_moving (E0, p0, 3)
        end if
    end function colliding_momenta

```

This subroutine is for the purpose of numerical checks and comparisons. The idea is to set a number to zero if it is numerically equivalent with zero. The equivalence is established by comparing with a **tolerance** argument. We implement this for vectors and transformations.

```

(Lorentz: public functions)+≡
    public :: pacify

```

```

<Lorentz: interfaces>+≡
  interface pacify
    module procedure pacify_vector3
    module procedure pacify_vector4
    module procedure pacify_LT
  end interface pacify

<Lorentz: procedures>+≡
  elemental subroutine pacify_vector3 (p, tolerance)
    type(vector3_t), intent(inout) :: p
    real(default), intent(in) :: tolerance
    where (abs (p%p) < tolerance) p%p = zero
  end subroutine pacify_vector3

  elemental subroutine pacify_vector4 (p, tolerance)
    type(vector4_t), intent(inout) :: p
    real(default), intent(in) :: tolerance
    where (abs (p%p) < tolerance) p%p = zero
  end subroutine pacify_vector4

  elemental subroutine pacify_LT (LT, tolerance)
    type(lorentz_transformation_t), intent(inout) :: LT
    real(default), intent(in) :: tolerance
    where (abs (LT%L) < tolerance) LT%L = zero
  end subroutine pacify_LT

<Lorentz: public>+≡
  public :: vector_set_reshuffle

<Lorentz: procedures>+≡
  subroutine vector_set_reshuffle (p1, list, p2)
    type(vector4_t), intent(in), dimension(:), allocatable :: p1
    integer, intent(in), dimension(:), allocatable :: list
    type(vector4_t), intent(out), dimension(:), allocatable :: p2
    integer :: n, n_p
    n_p = size (p1)
    if (size (list) /= n_p) return
    allocate (p2 (n_p))
    do n = 1, n_p
      p2(n) = p1(list(n))
    end do
  end subroutine vector_set_reshuffle

<Lorentz: public>+≡
  public :: vector_set_is_cms

<Lorentz: procedures>+≡
  function vector_set_is_cms (p, n_in) result (is_cms)
    logical :: is_cms
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: n_in
    integer :: i
    type(vector4_t) :: p_sum
    p_sum%p = 0._default

```

```

do i = 1, n_in
  p_sum = p_sum + p(i)
end do
is_cms = all (abs (p_sum%p(1:3)) < tiny_07)
end function vector_set_is_cms

```

<Lorentz: public>+≡

```
public :: vector_set_is_lab
```

<Lorentz: procedures>+≡

```

function vector_set_is_lab (p, n_in) result (is_lab)
  logical :: is_lab
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in) :: n_in
  is_lab = .not. vector_set_is_cms (p, n_in)
end function vector_set_is_lab

```

<Lorentz: public>+≡

```
public :: vector4_write_set
```

<Lorentz: procedures>+≡

```

subroutine vector4_write_set (p, unit, show_mass, testflag, &
  check_conservation, ultra, n_in)
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: show_mass
  logical, intent(in), optional :: testflag, ultra
  logical, intent(in), optional :: check_conservation
  integer, intent(in), optional :: n_in
  logical :: extreme
  integer :: i, j
  real(default), dimension(0:3) :: p_tot
  character(len=7) :: fmt
  integer :: u
  logical :: yorn, is_test
  integer :: n
  extreme = .false.; if (present (ultra)) extreme = ultra
  is_test = .false.; if (present (testflag)) is_test = testflag
  u = given_output_unit (unit); if (u < 0) return
  n = 2; if (present (n_in)) n = n_in
  p_tot = 0
  yorn = .false.; if (present (check_conservation)) yorn = check_conservation
  do i = 1, size (p)
    if (yorn .and. i > n) then
      forall (j=0:3) p_tot(j) = p_tot(j) - p(i)%p(j)
    else
      forall (j=0:3) p_tot(j) = p_tot(j) + p(i)%p(j)
    end if
    call vector4_write (p(i), u, show_mass=show_mass, &
      testflag=testflag, ultra=ultra)
  end do
  if (extreme) then
    call pac_fmt (fmt, FMT_19, FMT_11, testflag)
  else

```

```

        call pac_fmt (fmt, FMT_19, FMT_15, testflag)
    end if
    if (is_test) call pacify (p_tot, 1.E-9_default)
    if (.not. is_test) then
        write (u, "(A5)") 'Total: '
        write (u, "(1x,A,1x," // fmt // ")") "E = ", p_tot(0)
        write (u, "(1x,A,3(1x," // fmt // ")") "P = ", p_tot(1:)
    end if
end subroutine vector4_write_set

```

(Lorentz: public)+≡

```
public :: vector4_check_momentum_conservation
```

(Lorentz: procedures)+≡

```

subroutine vector4_check_momentum_conservation (p, n_in, unit, &
    abs_smallness, rel_smallness, verbose)
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: n_in
    integer, intent(in), optional :: unit
    real(default), intent(in), optional :: abs_smallness, rel_smallness
    logical, intent(in), optional :: verbose
    integer :: u, i
    type(vector4_t) :: psum_in, psum_out
    logical, dimension(0:3) :: p_diff
    logical :: verb
    u = given_output_unit (unit); if (u < 0) return
    verb = .false.; if (present (verbose)) verb = verbose
    psum_in = vector4_null
    do i = 1, n_in
        psum_in = psum_in + p(i)
    end do
    psum_out = vector4_null
    do i = n_in + 1, size (p)
        psum_out = psum_out + p(i)
    end do
    p_diff = vanishes (psum_in%p - psum_out%p, &
        abs_smallness = abs_smallness, rel_smallness = rel_smallness)
    if (.not. all (p_diff)) then
        call msg_warning ("Momentum conservation: FAIL", unit = u)
        if (verb) then
            write (u, "(A)") "Incoming:"
            call vector4_write (psum_in, u)
            write (u, "(A)") "Outgoing:"
            call vector4_write (psum_out, u)
        end if
    else
        if (verb) then
            write (u, "(A)") "Momentum conservation: CHECK"
        end if
    end if
end subroutine vector4_check_momentum_conservation

```

This computes the quantities

$$\langle ij \rangle = \sqrt{|S_{ij}|} e^{i\phi_{ij}}, [ij] = \sqrt{|S_{ij}|} e^{i\tilde{\phi}_{ij}},$$

with $S_{ij} = (p_i + p_j)^2$. The phase space factor ϕ_{ij} is determined by

$$\cos \phi_{ij} = \frac{p_i^1 p_j^+ - p_j^1 p_i^+}{\sqrt{p_i^+ p_j^+ S_{ij}}}, \sin \phi_{ij} = \frac{p_i^2 p_j^+ - p_j^2 p_i^+}{\sqrt{p_i^+ p_j^+ S_{ij}}}.$$

After $\langle ij \rangle$ has been computed according to these formulae, $[ij]$ can be obtained by using the relation $S_{ij} = \langle ij \rangle [ji]$ and taking into account that $[ij] = -[ji]$. Thus, a minus-sign has to be applied.

<Lorentz: public>+≡

`public :: spinor_product`

<Lorentz: procedures>+≡

```
subroutine spinor_product (p1, p2, prod1, prod2)
  type(vector4_t), intent(in) :: p1, p2
  complex(default), intent(out) :: prod1, prod2
  real(default) :: sij
  complex(default) :: phase
  real(default) :: pp_1, pp_2
  pp_1 = p1%p(0) + p1%p(3)
  pp_2 = p2%p(0) + p2%p(3)
  sij = (p1+p2)**2
  phase = cmplx ((p1%p(1)*pp_2 - p2%p(1)*pp_1)/sqrt (sij*pp_1*pp_2), &
    (p1%p(2)*pp_2 - p2%p(2)*pp_1)/sqrt (sij*pp_1*pp_2), &
    default)

  !!! <ij>
  prod1 = sqrt (sij) * phase
  !!! [ij]
  if (abs(prod1) > 0) then
    prod2 = - sij / prod1
  else
    prod2 = 0
  end if
end subroutine spinor_product
```

9.4 Collections of Lorentz Vectors

The `phs_point` type is a container for an array of Lorentz vectors. This allows us to transfer Lorentz-vector arrays more freely, and to collect vector arrays of non-uniform size.

<phs_points.f90>≡

<File header>

`module phs_points`

<Use kinds>

`use lorentz, only: vector4_t`

```

    use lorentz, only: vector4_null
    use lorentz, only: vector4_write_set
    use lorentz, only: lorentz_transformation_t
    use lorentz, only: operator(==)
    use lorentz, only: operator(*)
    use lorentz, only: operator(**)
    use lorentz, only: sum

    <Standard module head>

    <PHS points: public>

    <PHS points: types>

    <PHS points: interfaces>

contains

    <PHS points: procedures>

end module phs_points

```

9.4.1 PHS point definition

This is a trivial container for an array of momenta. The main application is to store a non-uniform array of phase-space points.

```

    <PHS points: public>≡
        public :: phs_point_t

    <PHS points: types>≡
        type :: phs_point_t
        private
            type(vector4_t), dimension(:), allocatable :: p
        contains
            <PHS points: phs point: TBP>
        end type phs_point_t

```

9.4.2 PHS point: basic tools

Output. This is instrumented with options, which have to be provided by the caller.

```

    <PHS points: phs point: TBP>≡
        procedure :: write => phs_point_write

    <PHS points: procedures>≡
        subroutine phs_point_write (phs_point, unit, show_mass, testflag, &
            check_conservation, ultra, n_in)
            class(phs_point_t), intent(in) :: phs_point
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: show_mass
            logical, intent(in), optional :: testflag, ultra
            logical, intent(in), optional :: check_conservation

```

```

integer, intent(in), optional :: n_in
if (allocated (phs_point%p)) then
  call vector4_write_set (phs_point%p, &
    unit = unit, &
    show_mass = show_mass, &
    testflag = testflag, &
    check_conservation = check_conservation, &
    ultra = ultra, &
    n_in = n_in)
end if
end subroutine phs_point_write

```

Non-intrinsic assignment

```

<PHS points: public>+≡
  public :: assignment(=)

<PHS points: interfaces>≡
  interface assignment(=)
    module procedure phs_point_from_n
    module procedure phs_point_from_vector4
    module procedure vector4_from_phs_point
  end interface

```

Initialize with zero momenta but fixed size

```

<PHS points: procedures>+≡
  pure subroutine phs_point_from_n (phs_point, n_particles)
    type(phs_point_t), intent(out) :: phs_point
    integer, intent(in) :: n_particles
    allocate (phs_point%p (n_particles), source = vector4_null)
  end subroutine phs_point_from_n

```

Transform from/to plain vector array

```

<PHS points: procedures>+≡
  pure subroutine phs_point_from_vector4 (phs_point, p)
    type(phs_point_t), intent(out) :: phs_point
    type(vector4_t), dimension(:), intent(in) :: p
    phs_point%p = p
  end subroutine phs_point_from_vector4

  pure subroutine vector4_from_phs_point (p, phs_point)
    class(phs_point_t), intent(in) :: phs_point
    type(vector4_t), dimension(:), allocatable, intent(out) :: p
    if (allocated (phs_point%p)) p = phs_point%p
  end subroutine vector4_from_phs_point

```

Query the size of the momentum array (assuming it is allocated).

```

<PHS points: public>+≡
  public :: size

<PHS points: interfaces>+≡
  interface size
    module procedure phs_point_size
  end interface size

```



```

<PHS points: procedures>+≡
pure function phs_point_size (phs_point) result (s)
  class(phs_point_t), intent(in) :: phs_point
  integer :: s
  if (allocated (phs_point%p)) then
    s = size (phs_point%p)
  else
    s = 0
  end if
end function phs_point_size

```

Equality, implemented only for valid points.

```

<PHS points: public>+≡
public :: operator(==)

<PHS points: interfaces>+≡
interface operator(==)
  module procedure phs_point_eq
end interface operator(==)

<PHS points: procedures>+≡
elemental function phs_point_eq (phs_point_1, phs_point_2) result (flag)
  class(phs_point_t), intent(in) :: phs_point_1, phs_point_2
  logical :: flag
  if (allocated (phs_point_1%p) .and. (allocated (phs_point_2%p))) then
    flag = all (phs_point_1%p == phs_point_2%p)
  else
    flag = .false.
  end if
end function phs_point_eq

```

Extract all momenta, as a method

```

<PHS points: phs point: TBP>+≡
procedure :: get => phs_point_get

<PHS points: procedures>+≡
pure function phs_point_get (phs_point) result (p)
  class(phs_point_t), intent(in) :: phs_point
  type(vector4_t), dimension(:), allocatable :: p
  if (allocated (phs_point%p)) then
    p = phs_point%p
  else
    allocate (p (0))
  end if
end function phs_point_get

```

Extract a subset of all momenta.

```

<PHS points: phs point: TBP>+≡
procedure :: select => phs_point_select

<PHS points: procedures>+≡
elemental function phs_point_select (phs_point, i) result (p)
  class(phs_point_t), intent(in) :: phs_point
  integer, intent(in) :: i

```

```

    type(vector4_t) :: p
    if (allocated (phs_point%p)) then
        p = phs_point%p(i)
    else
        p = vector4_null
    end if
end function phs_point_select

```

Return the invariant mass squared for a subset of momenta

```

<PHS points: phs_point: TBP>+≡
    procedure :: get_msq => phs_point_get_msq

<PHS points: procedures>+≡
    pure function phs_point_get_msq (phs_point, iarray) result (msq)
        class(phs_point_t), intent(in) :: phs_point
        integer, dimension(:), intent(in) :: iarray
        real(default) :: msq
        if (allocated (phs_point%p)) then
            msq = (sum (phs_point%p(iarray)))*2
        else
            msq = 0
        end if
    end function phs_point_get_msq

```

9.4.3 Lorentz algebra pieces

Lorentz transformation.

```

<PHS points: public>+≡
    public :: operator(*)

<PHS points: interfaces>+≡
    interface operator(*)
        module procedure prod_LT_phs_point
    end interface operator(*)

<PHS points: procedures>+≡
    elemental function prod_LT_phs_point (L, phs_point) result (phs_point_LT)
        type(lorentz_transformation_t), intent(in) :: L
        type(phs_point_t), intent(in) :: phs_point
        type(phs_point_t) :: phs_point_LT
        if (allocated (phs_point%p)) phs_point_LT%p = L * phs_point%p
    end function prod_LT_phs_point

```

Compute momentum sum, analogous to the standard `sum` function (mask), and additionally using an index array.

```

<PHS points: public>+≡
    public :: sum

<PHS points: interfaces>+≡
    interface sum
        module procedure phs_point_sum
        module procedure phs_point_sum_iarray
    end interface sum

```

```

<PHS points: procedures>+≡
  pure function phs_point_sum (phs_point, mask) result (p)
    class(phs_point_t), intent(in) :: phs_point
    logical, dimension(:), intent(in), optional :: mask
    type(vector4_t) :: p
    if (allocated (phs_point%p)) then
      p = sum (phs_point%p, mask)
    else
      p = vector4_null
    end if
  end function phs_point_sum

  pure function phs_point_sum_iarray (phs_point, iarray) result (p)
    class(phs_point_t), intent(in) :: phs_point
    integer, dimension(:), intent(in) :: iarray
    type(vector4_t) :: p
    logical, dimension(:), allocatable :: mask
    integer :: i
    allocate (mask (size (phs_point)), source = .false.)
    mask(iarray) = .true.
    p = sum (phs_point, mask)
  end function phs_point_sum_iarray

```

9.4.4 Methods for specific applications

Convenience method: compute the pair of energy fractions w.r.t. the specified beam energy. We assume that the momenta represent a scattering process (two incoming particles) in the c.m. frame.

```

<PHS points: phs point: TBP>+≡
  procedure :: get_x => phs_point_get_x

<PHS points: procedures>+≡
  pure function phs_point_get_x (phs_point, E_beam) result (x)
    class(phs_point_t), intent(in) :: phs_point
    real(default), dimension(2) :: x
    real(default), intent(in) :: E_beam
    x = phs_point%p(1:2)%p(0) / E_beam
  end function phs_point_get_x

```

9.4.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<phs_points_ut.f90>≡
  <File header>

  module phs_points_ut
    use unit_tests
    use phs_points_ut_i

    <Standard module head>

```

```

    <PHS points: public test>

contains

    <PHS points: test driver>

    end module phs_points_ut
<phs_points_util.f90>≡
    <File header>

    module phs_points_util

    <Use kinds>
        use phs_points

    <Standard module head>

    <PHS points: test declarations>

contains

    <PHS points: tests>

    end module phs_points_util
API: driver for the unit tests below.
<PHS points: public test>≡
    public :: phs_points_test
<PHS points: test driver>≡
    subroutine phs_points_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS points: execute tests>
    end subroutine phs_points_test

```

Splitting functions

```

<PHS points: execute tests>≡
    call test (phs_points_1, "phs_points_1", &
        "Dummy test", &
        u, results)
<PHS points: test declarations>≡
    public :: phs_points_1
<PHS points: tests>≡
    subroutine phs_points_1 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: phs_points_1"
        write (u, "(A)")  "* Purpose: none yet"
        write (u, "(A)")
    end subroutine phs_points_1

```

```
write (u, "(A)")  
write (u, "(A)")  "* Test output end: phs_points_1"  
  
end subroutine phs_points_1
```

9.5 Special Physics functions

Here, we declare functions that are specific for the Standard Model, including QCD: fixed and running α_s , Catani-Seymour dipole terms, loop functions, etc.

To make maximum use of this, all functions, if possible, are declared elemental (or pure, if this is not possible).

```

⟨sm_physics.f90⟩≡
  ⟨File header⟩

  module sm_physics

    ⟨Use kinds⟩
    use io_units
    use constants
    use numeric_utils
    use diagnostics
    use physics_defs
    use lorentz

    ⟨Standard module head⟩

    ⟨SM physics: public⟩

    ⟨SM physics: parameters⟩

    contains

    ⟨SM physics: procedures⟩

  end module sm_physics

```

9.5.1 Running α_s

Then we define the coefficients of the beta function of QCD (as a reference cf. the Particle Data Group), where n_f is the number of active flavors in two different schemes:

$$\beta_0 = 11 - \frac{2}{3}n_f \quad (9.5)$$

$$\beta_1 = 51 - \frac{19}{3}n_f \quad (9.6)$$

$$\beta_2 = 2857 - \frac{5033}{9}n_f + \frac{325}{27}n_f^2 \quad (9.7)$$

$$b_0 = \frac{1}{12\pi} (11C_A - 2n_f) \quad (9.8)$$

$$b_1 = \frac{1}{24\pi^2} (17C_A^2 - 5C_A n_f - 3C_F n_f) \quad (9.9)$$

$$b_2 = \frac{1}{(4\pi)^3} \left(\frac{2857}{54} C_A^3 - \frac{1415}{54} C_A^2 n_f - \frac{205}{18} C_A C_F n_f + C_F^2 n_f + \frac{79}{54} C_A n_f^2 + \frac{11}{9} C_F n_f^2 \right) \quad (9.10)$$

```

<SM physics: public>≡
  public :: beta0, beta1, beta2, coeff_b0, coeff_b1, coeff_b2

<SM physics: procedures>≡
  pure function beta0 (nf)
    real(default), intent(in) :: nf
    real(default) :: beta0
    beta0 = 11.0_default - two/three * nf
  end function beta0

  pure function beta1 (nf)
    real(default), intent(in) :: nf
    real(default) :: beta1
    beta1 = 51.0_default - 19.0_default/three * nf
  end function beta1

  pure function beta2 (nf)
    real(default), intent(in) :: nf
    real(default) :: beta2
    beta2 = 2857.0_default - 5033.0_default / 9.0_default * &
      nf + 325.0_default/27.0_default * nf**2
  end function beta2

  pure function coeff_b0 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b0
    coeff_b0 = (11.0_default * CA - two * nf) / (12.0_default * pi)
  end function coeff_b0

  pure function coeff_b1 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b1
    coeff_b1 = (17.0_default * CA**2 - five * CA * nf - three * CF * nf) / &
      (24.0_default * pi**2)
  end function coeff_b1

  pure function coeff_b2 (nf)
    real(default), intent(in) :: nf
    real(default) :: coeff_b2
    coeff_b2 = (2857.0_default/54.0_default * CA**3 - &
      1415.0_default/54.0_default * &
      CA**2 * nf - 205.0_default/18.0_default * CA*CF*nf &
      + 79.0_default/54.0_default * CA*nf**2 + &
      11.0_default/9.0_default * CF * nf**2) / (four*pi)**3
  end function coeff_b2

```

There should be two versions of running α_s , one which takes the scale and Λ_{QCD} as input, and one which takes the scale and e.g. $\alpha_s(m_Z)$ as input. Here, we take the one which takes the QCD scale and scale as inputs from the PDG book.

```

<SM physics: public>+≡
  public :: running_as, running_as_lam

<SM physics: procedures>+≡
  pure function running_as (scale, al_mz, mz, order, nf) result (ascale)

```

```

real(default), intent(in) :: scale
real(default), intent(in), optional :: al_mz, nf, mz
integer, intent(in), optional :: order
integer :: ord
real(default) :: az, m_z, as_log, n_f, b0, b1, b2, ascale
real(default) :: as0, as1
if (present (mz)) then
    m_z = mz
else
    m_z = MZ_REF
end if
if (present (order)) then
    ord = order
else
    ord = 0
end if
if (present (al_mz)) then
    az = al_mz
else
    az = ALPHA_QCD_MZ_REF
end if
if (present (nf)) then
    n_f = nf
else
    n_f = 5
end if
b0 = coeff_b0 (n_f)
b1 = coeff_b1 (n_f)
b2 = coeff_b2 (n_f)
as_log = one + b0 * az * log(scale**2/m_z**2)
as0 = az / as_log
as1 = as0 - as0**2 * b1/b0 * log(as_log)
select case (ord)
case (0)
    ascale = as0
case (1)
    ascale = as1
case (2)
    ascale = as1 + as0**3 * (b1**2/b0**2 * ((log(as_log))**2 - &
        log(as_log) + as_log - one) - b2/b0 * (as_log - one))
case default
    ascale = as0
end select
end function running_as

pure function running_as_lam (nf, scale, lambda, order) result (ascale)
real(default), intent(in) :: nf, scale
real(default), intent(in), optional :: lambda
integer, intent(in), optional :: order
real(default) :: lambda_qcd
real(default) :: as0, as1, logmul, b0, b1, b2, ascale
integer :: ord
if (present (lambda)) then
    lambda_qcd = lambda

```



```

else
  lambda_qcd = LAMBDA_QCD_REF
end if
if (present (order)) then
  ord = order
else
  ord = 0
end if
b0 = beta0(nf)
logmul = log(scale**2/lambda_qcd**2)
as0 = four*pi / b0 / logmul
if (ord > 0) then
  b1 = beta1(nf)
  as1 = as0 * (one - two* b1 / b0**2 * log(logmul) / logmul)
end if
select case (ord)
case (0)
  ascale = as0
case (1)
  ascale = as1
case (2)
  b2 = beta2(nf)
  ascale = as1 + as0 * four * b1**2/b0**4/logmul**2 * &
    ((log(logmul) - 0.5_default)**2 + &
    b2*b0/8.0_default/b1**2 - five/four)
case default
  ascale = as0
end select
end function running_as_lam

```

9.5.2 Catani-Seymour Parameters

These are fundamental constants of the Catani-Seymour dipole formalism. Since the corresponding parameters for the gluon case depend on the number of flavors which is treated as an argument, there we do have functions and not parameters.

$$\gamma_q = \gamma_{\bar{q}} = \frac{3}{2}C_F \quad \gamma_g = \frac{11}{6}C_A - \frac{2}{3}T_R N_f \quad (9.11)$$

$$K_q = K_{\bar{q}} = \left(\frac{7}{2} - \frac{\pi^2}{6}\right) C_F \quad K_g = \left(\frac{67}{18} - \frac{\pi^2}{6}\right) C_A - \frac{10}{9}T_R N_f \quad (9.12)$$

```

⟨SM physics: parameters⟩≡
real(kind=default), parameter, public :: gamma_q = three/two * CF, &
  k_q = (7.0_default/two - pi**2/6.0_default) * CF

```

```

⟨SM physics: public⟩+≡
public :: gamma_g, k_g

```

```

⟨SM physics: procedures⟩+≡
elemental function gamma_g (nf) result (gg)
  real(kind=default), intent(in) :: nf
  real(kind=default) :: gg

```

```

      gg = 11.0_default/6.0_default * CA - two/three * TR * nf
end function gamma_g

elemental function k_g (nf) result (kg)
  real(kind=default), intent(in) :: nf
  real(kind=default) :: kg
  kg = (67.0_default/18.0_default - pi**2/6.0_default) * CA - &
      10.0_default/9.0_default * TR * nf
end function k_g

```

9.5.3 Mathematical Functions

The dilogarithm. This simplified version is bound to double precision, and restricted to argument values less or equal to unity, so we do not need complex algebra. The wrapper converts it to default precision (which is, of course, a no-op if double=default).

The routine calculates the dilogarithm through mapping on the area where there is a quickly convergent series (adapted from an F77 routine by Hans Kuijf, 1988): Map x such that x is not in the neighbourhood of 1. Note that $|z| = -\ln(1-x)$ is always smaller than 1.10, but $\frac{1 \cdot 10^{19}}{19!} \text{Bernoulli}_{19} = 2.7 \times 10^{-15}$.

<SM physics: public>+≡
 public :: Li2

<SM physics: procedures>+≡
 elemental function Li2 (x)
 use kinds, only: double
 real(default), intent(in) :: x
 real(default) :: Li2
 Li2 = real(Li2_double (real(x, kind=double)), kind=default)
end function Li2

<SM physics: procedures>+≡
 elemental function Li2_double (x) result (Li2)
 use kinds, only: double
 real(kind=double), intent(in) :: x
 real(kind=double) :: Li2
 real(kind=double), parameter :: pi2_6 = pi**2/6
 if (abs(1-x) < tiny_07) then
 Li2 = pi2_6
 else if (abs(1-x) < 0.5_double) then
 Li2 = pi2_6 - log(1-x) * log(x) - Li2_restricted (1-x)
 else if (abs(x) > 1.d0) then
 ! Li2 = 0
 ! call msg_bug (" Dilogarithm called outside of defined range.")
 !!! Reactivate Dilogarithm identity
 Li2 = -pi2_6 - 0.5_default * log(-x) * log(-x) - Li2_restricted (1/x)
 else
 Li2 = Li2_restricted (x)
 end if
contains
 elemental function Li2_restricted (x) result (Li2)

```

      real(kind=double), intent(in) :: x
      real(kind=double) :: Li2
      real(kind=double) :: tmp, z, z2
      z = - log (1-x)
      z2 = z**2
! Horner's rule for the powers z^3 through z^19
      tmp = 43867._double/798._double
      tmp = tmp * z2 /342._double - 3617._double/510._double
      tmp = tmp * z2 /272._double + 7._double/6._double
      tmp = tmp * z2 /210._double - 691._double/2730._double
      tmp = tmp * z2 /156._double + 5._double/66._double
      tmp = tmp * z2 /110._double - 1._double/30._double
      tmp = tmp * z2 / 72._double + 1._double/42._double
      tmp = tmp * z2 / 42._double - 1._double/30._double
      tmp = tmp * z2 / 20._double + 1._double/6._double
! The first three terms of the power series
      Li2 = z2 * z * tmp / 6._double - 0.25_double * z2 + z
    end function Li2_restricted
end function Li2_double

```

9.5.4 Loop Integrals

These functions appear in the calculation of the effective one-loop coupling of a (pseudo)scalar to a vector boson pair.

```

<SM physics: public>+≡
  public :: faux

<SM physics: procedures>+≡
  elemental function faux (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
    if (1 <= x) then
      y = asin(sqrt(1/x))**2
    else
      y = - 1/4.0_default * (log((1 + sqrt(1 - x))/ &
        (1 - sqrt(1 - x)))) - cmplx (0.0_default, pi, kind=default))**2
    end if
  end function faux

<SM physics: public>+≡
  public :: fonehalf

<SM physics: procedures>+≡
  elemental function fonehalf (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
    if (abs(x) < eps0) then
      y = 0
    else
      y = - 2.0_default * x * (1 + (1 - x) * faux(x))
    end if
  end function fonehalf

```

```

<SM physics: public>+≡
  public :: fonehalf_pseudo

<SM physics: procedures>+≡
  function fonehalf_pseudo (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
    if (abs(x) < eps0) then
      y = 0
    else
      y = - 2.0_default * x * faux(x)
    end if
  end function fonehalf_pseudo

<SM physics: public>+≡
  public :: fone

<SM physics: procedures>+≡
  elemental function fone (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
    if (abs(x) < eps0) then
      y = 2.0_default
    else
      y = 2.0_default + 3.0_default * x + &
        3.0_default * x * (2.0_default - x) * &
        faux(x)
    end if
  end function fone

<SM physics: public>+≡
  public :: gaux

<SM physics: procedures>+≡
  elemental function gaux (x) result (y)
    real(default), intent(in) :: x
    complex(default) :: y
    if (1 <= x) then
      y = sqrt(x - 1) * asin(sqrt(1/x))
    else
      y = sqrt(1 - x) * (log((1 + sqrt(1 - x)) / &
        (1 - sqrt(1 - x)))) - &
        cmplx (0.0_default, pi, kind=default)) / 2.0_default
    end if
  end function gaux

<SM physics: public>+≡
  public :: tri_i1

<SM physics: procedures>+≡
  elemental function tri_i1 (a,b) result (y)
    real(default), intent(in) :: a,b
    complex(default) :: y
    if (a < eps0 .or. b < eps0) then

```

```

        y = 0
    else
        y = a*b/2.0_default/(a-b) + a**2 * b**2/2.0_default/(a-b)**2 * &
            (faux(a) - faux(b)) + &
            a**2 * b/(a-b)**2 * (gaux(a) - gaux(b))
    end if
end function tri_i1

```

```

⟨SM physics: public⟩+≡
public :: tri_i2

```

```

⟨SM physics: procedures⟩+≡
elemental function tri_i2 (a,b) result (y)
    real(default), intent(in) :: a,b
    complex(default) :: y
    if (a < eps0 .or. b < eps0) then
        y = 0
    else
        y = - a * b / 2.0_default / (a-b) * (faux(a) - faux(b))
    end if
end function tri_i2

```

9.5.5 More on α_s

These functions are for the running of the strong coupling constants, α_s .

```

⟨SM physics: public⟩+≡
public :: run_b0

```

```

⟨SM physics: procedures⟩+≡
elemental function run_b0 (nf) result (bnull)
    integer, intent(in) :: nf
    real(default) :: bnull
    bnull = 33.0_default - 2.0_default * nf
end function run_b0

```

```

⟨SM physics: public⟩+≡
public :: run_b1

```

```

⟨SM physics: procedures⟩+≡
elemental function run_b1 (nf) result (bone)
    integer, intent(in) :: nf
    real(default) :: bone
    bone = 6.0_default * (153.0_default - 19.0_default * nf)/run_b0(nf)**2
end function run_b1

```

```

⟨SM physics: public⟩+≡
public :: run_aa

```

```

<SM physics: procedures>+≡
  elemental function run_aa (nf) result (aaa)
    integer, intent(in) :: nf
    real(default) :: aaa
    aaa = 12.0_default * PI / run_b0(nf)
  end function run_aa

```

```

<SM physics: pubic functions>≡
  public :: run_bb

```

```

<SM physics: procedures>+≡
  elemental function run_bb (nf) result (bbb)
    integer, intent(in) :: nf
    real(default) :: bbb
    bbb = run_b1(nf) / run_aa(nf)
  end function run_bb

```

9.5.6 Functions for Catani-Seymour dipoles

For the automated Catani-Seymour dipole subtraction, we need the following functions.

```

<SM physics: public>+≡
  public :: ff_dipole

```

```

<SM physics: procedures>+≡
  pure subroutine ff_dipole (v_ijk,y_ijk,p_ij,pp_k,p_i,p_j,p_k)
    type(vector4_t), intent(in) :: p_i, p_j, p_k
    type(vector4_t), intent(out) :: p_ij, pp_k
    real(kind=default), intent(out) :: y_ijk
    real(kind=default) :: z_i
    real(kind=default), intent(out) :: v_ijk
    z_i = (p_i*p_k) / ((p_k*p_j) + (p_k*p_i))
    y_ijk = (p_i*p_j) / ((p_i*p_j) + (p_i*p_k) + (p_j*p_k))
    p_ij = p_i + p_j - y_ijk/(1.0_default - y_ijk) * p_k
    pp_k = (1.0/(1.0_default - y_ijk)) * p_k
    !!! We don't multiply by alpha_s right here:
    v_ijk = 8.0_default * PI * CF * &
      (2.0 / (1.0 - z_i*(1.0 - y_ijk)) - (1.0 + z_i))
  end subroutine ff_dipole

```

```

<SM physics: public>+≡
  public :: fi_dipole

```

```

<SM physics: procedures>+≡
  pure subroutine fi_dipole (v_ija,x_ija,p_ij,pp_a,p_i,p_j,p_a)
    type(vector4_t), intent(in) :: p_i, p_j, p_a
    type(vector4_t), intent(out) :: p_ij, pp_a
    real(kind=default), intent(out) :: x_ija
    real(kind=default) :: z_i
    real(kind=default), intent(out) :: v_ija
    z_i = (p_i*p_a) / ((p_a*p_j) + (p_a*p_i))
    x_ija = ((p_i*p_a) + (p_j*p_a) - (p_i*p_j)) &

```

```

      / ((p_i*p_a) + (p_j*p_a))
p_ij = p_i + p_j - (1.0_default - x_ija) * p_a
pp_a = x_ija * p_a
!!! We don't not multiply by alpha_s right here:
v_ija = 8.0_default * PI * CF * &
      (2.0 / (1.0 - z_i + (1.0 - x_ija)) - (1.0 + z_i)) / x_ija
end subroutine fi_dipole

```

```

<SM physics: public>+≡
public :: if_dipole

<SM physics: procedures>+≡
pure subroutine if_dipole (v_kja,u_j,p_aj,pp_k,p_k,p_j,p_a)
  type(vector4_t), intent(in) :: p_k, p_j, p_a
  type(vector4_t), intent(out) :: p_aj, pp_k
  real(kind=default), intent(out) :: u_j
  real(kind=default) :: x_kja
  real(kind=default), intent(out) :: v_kja
  u_j = (p_a*p_j) / ((p_a*p_j) + (p_a*p_k))
  x_kja = ((p_a*p_k) + (p_a*p_j) - (p_j*p_k)) &
    / ((p_a*p_j) + (p_a*p_k))
  p_aj = x_kja * p_a
  pp_k = p_k + p_j - (1.0_default - x_kja) * p_a
  v_kja = 8.0_default * PI * CF * &
    (2.0 / (1.0 - x_kja + u_j) - (1.0 + x_kja)) / x_kja
end subroutine if_dipole

```

This function depends on a variable number of final state particles whose kinematics all get changed by the initial-initial dipole insertion.

```

<SM physics: public>+≡
public :: ii_dipole

<SM physics: procedures>+≡
pure subroutine ii_dipole (v_jab,v_j,p_in,p_out,flag_1or2)
  type(vector4_t), dimension(:), intent(in) :: p_in
  type(vector4_t), dimension(size(p_in)-1), intent(out) :: p_out
  logical, intent(in) :: flag_1or2
  real(kind=default), intent(out) :: v_j
  real(kind=default), intent(out) :: v_jab
  type(vector4_t) :: p_a, p_b, p_j
  type(vector4_t) :: k, kk
  type(vector4_t) :: p_aj
  real(kind=default) :: x_jab
  integer :: i
  !!! flag_1or2 decides whether this a 12 or 21 dipole
  if (flag_1or2) then
    p_a = p_in(1)
    p_b = p_in(2)
  else
    p_b = p_in(1)
    p_a = p_in(2)
  end if
  !!! We assume that the unresolved particle has always the last
  !!! momentum

```

```

p_j = p_in(size(p_in))
x_jab = ((p_a*p_b) - (p_a*p_j) - (p_b*p_j)) / (p_a*p_b)
v_j = (p_a*p_j) / (p_a * p_b)
p_aj = x_jab * p_a
k = p_a + p_b - p_j
kk = p_aj + p_b
do i = 3, size(p_in)-1
  p_out(i) = p_in(i) - 2.0*((k+kk)*p_in(i))/((k+kk)*(k+kk)) * (k+kk) + &
    (2.0 * (k*p_in(i)) / (k*k)) * kk
end do
if (flag_1or2) then
  p_out(1) = p_aj
  p_out(2) = p_b
else
  p_out(1) = p_b
  p_out(2) = p_aj
end if
v_jab = 8.0_default * PI * CF * &
  (2.0 / (1.0 - x_jab) - (1.0 + x_jab)) / x_jab
end subroutine ii_dipole

```

9.5.7 Distributions for integrated dipoles and such

Note that the following formulae are only meaningful for $0 \leq x \leq 1$.

The Dirac delta distribution, modified for Monte-Carlo sampling, centered at $x = 1 - \frac{\epsilon}{2}$:

```

<SM physics: public>+≡
  public :: delta

<SM physics: procedures>+≡
  elemental function delta (x,eps) result (z)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: z
    if (x > one - eps) then
      z = one / eps
    else
      z = 0
    end if
  end function delta

```

The $+$ -distribution, $P_+(x) = \left(\frac{1}{1-x}\right)_+$, for the regularization of soft-collinear singularities. The constant part for the Monte-Carlo sampling is the integral over the splitting function divided by the weight for the WHIZARD numerical integration over the interval.

```

<SM physics: public>+≡
  public :: plus_distr

<SM physics: procedures>+≡
  elemental function plus_distr (x,eps) result (plused)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: plused
    if (x > one - eps) then
      plused = log(eps) / eps
    end if
  end function plus_distr

```



```

else
  plusd = one / (one - x)
end if
end function plus_distr

```

The splitting function in $D = 4$ dimensions, regularized as $+$ -distributions if necessary:

$$P^{qq}(x) = P^{\bar{q}q}(x) = C_F \cdot \left(\frac{1+x^2}{1-x} \right)_+ \quad (9.13)$$

$$P^{qg}(x) = P^{\bar{q}g}(x) = C_F \cdot \frac{1+(1-x)^2}{x} \quad (9.14)$$

$$P^{gq}(x) = P^{g\bar{q}}(x) = T_R \cdot [x^2 + (1-x)^2] \quad (9.15)$$

$$P^{gg}(x) = 2C_A \left[\left(\frac{1}{1-x} \right)_+ + \frac{1-x}{x} - 1 + x(1-x) \right] + \delta(1-x) \left(\frac{11}{6}C_A - \frac{2}{3}N_f T_R \right) \quad (9.16)$$

Since the number of flavors summed over in the gluon splitting function might depend on the physics case under consideration, it is implemented as an input variable.

```

⟨SM physics: public⟩+≡
  public :: pqq

⟨SM physics: procedures⟩+≡
  elemental function pqq (x,eps) result (pqqx)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: pqqx
    if (x > (1.0_default - eps)) then
      pqqx = (eps - one) / two + two * log(eps) / eps - &
        three * (eps - one) / eps / two
    else
      pqqx = (one + x**2) / (one - x)
    end if
    pqqx = CF * pqqx
  end function pqq

⟨SM physics: public⟩+≡
  public :: pgq

⟨SM physics: procedures⟩+≡
  elemental function pgq (x) result (pgqx)
    real(kind=default), intent(in) :: x
    real(kind=default) :: pgqx
    pgqx = TR * (x**2 + (one - x)**2)
  end function pgq

⟨SM physics: public⟩+≡
  public :: pqg

```

```

⟨SM physics: procedures⟩+≡
  elemental function pqg (x) result (pqgx)
    real(kind=default), intent(in) :: x
    real(kind=default) :: pqgx
    pqgx = CF * (one + (one - x)**2) / x
  end function pqg

⟨SM physics: public⟩+≡
  public :: pgg

⟨SM physics: procedures⟩+≡
  elemental function pgg (x, nf, eps) result (pggx)
    real(kind=default), intent(in) :: x, nf, eps
    real(kind=default) :: pggx
    pggx = two * CA * ( plus_distr (x, eps) + (one-x)/x - one + &
                        x*(one-x)) + delta (x, eps) * gamma_g(nf)
  end function pgg

```

For the qq and gg cases, there exist “regularized” versions of the splitting functions:

$$P_{\text{reg}}^{qq}(x) = -C_F \cdot (1 + x) \quad (9.17)$$

$$P_{\text{reg}}^{gg}(x) = 2C_A \left[\frac{1-x}{x} - 1 + x(1-x) \right] \quad (9.18)$$

```

⟨SM physics: public⟩+≡
  public :: pqq_reg

⟨SM physics: procedures⟩+≡
  elemental function pqq_reg (x) result (pqqregx)
    real(kind=default), intent(in) :: x
    real(kind=default) :: pqqregx
    pqqregx = - CF * (one + x)
  end function pqq_reg

⟨SM physics: public⟩+≡
  public :: pgg_reg

⟨SM physics: procedures⟩+≡
  elemental function pgg_reg (x) result (pggregx)
    real(kind=default), intent(in) :: x
    real(kind=default) :: pggregx
    pggregx = two * CA * ((one - x)/x - one + x*(one - x))
  end function pgg_reg

```

Here, we collect the expressions needed for integrated Catani-Seymour dipoles, and the so-called flavor kernels. We always distinguish between the “ordinary” Catani-Seymour version, and the one including a phase-space slicing parameter, α .

The standard flavor kernels \overline{K}^{ab} are:

$$\overline{K}^{qg}(x) = \overline{K}^{\bar{q}g}(x) = P^{qg}(x) \log((1-x)/x) + CF \times x \quad (9.19)$$

$$\overline{K}^{gg}(x) = \overline{K}^{\bar{q}\bar{q}}(x) = P^{gq}(x) \log((1-x)/x) + TR \times 2x(1-x) \quad (9.20)$$

$$\begin{aligned} \overline{K}^{qq} = & C_F \left[\left(\frac{2}{1-x} \log \frac{1-x}{x} \right)_+ - (1+x) \log((1-x)/x) + (1-x) \right] \\ & - (5 - \pi^2) \cdot C_F \cdot \delta(1-x) \end{aligned} \quad (9.21)$$

$$\begin{aligned} \overline{K}^{gq} = & 2C_A \left[\left(\frac{1}{1-x} \log \frac{1-x}{x} \right)_+ + \left(\frac{1-x}{x} - 1 + x(1-x) \right) \log((1-x)/x) \right] \\ & - \delta(1-x) \left[\left(\frac{50}{9} - \pi^2 \right) C_A - \frac{16}{9} T_R N_f \right] \end{aligned} \quad (9.22)$$

<SM physics: public>+≡
public :: kbarqg

<SM physics: procedures>+≡
function kbarqg (x) result (kbarqgx)
 real(kind=default), intent(in) :: x
 real(kind=default) :: kbarqgx
 kbarqgx = pqg(x) * log((one-x)/x) + CF * x
end function kbarqg

<SM physics: public>+≡
public :: kbargq

<SM physics: procedures>+≡
function kbargq (x) result (kbargqx)
 real(kind=default), intent(in) :: x
 real(kind=default) :: kbargqx
 kbargqx = pgq(x) * log((one-x)/x) + two * TR * x * (one - x)
end function kbargq

<SM physics: public>+≡
public :: kbarqq

<SM physics: procedures>+≡
function kbarqq (x,eps) result (kbarqqx)
 real(kind=default), intent(in) :: x, eps
 real(kind=default) :: kbarqqx
 kbarqqx = CF*(log_plus_distr(x,eps) - (one+x) * log((one-x)/x) + (one - &
 x) - (five - pi**2) * delta(x,eps))
end function kbarqq

<SM physics: public>+≡
public :: kbargg

<SM physics: procedures>+≡
function kbargg (x,eps,nf) result (kbarggx)
 real(kind=default), intent(in) :: x, eps, nf
 real(kind=default) :: kbarggx
 kbarggx = CA * (log_plus_distr(x,eps) + two * ((one-x)/x - one + &

```

x*(one-x) * log((1-x)/x))) - delta(x,eps) * &
((50.0_default/9.0_default - pi**2) * CA - &
16.0_default/9.0_default * TR * nf)
end function kbargg

```

The \tilde{K} are used when two identified hadrons participate:

$$\tilde{K}^{ab}(x) = P_{\text{reg}}^{ab}(x) \cdot \log(1-x) + \delta^{ab} \mathbf{T}_a^2 \left[\left(\frac{2}{1-x} \log(1-x) \right)_+ - \frac{\pi^2}{3} \delta(1-x) \right] \quad (9.23)$$

```

<SM physics: public>+≡
  public :: ktildeqq

<SM physics: procedures>+≡
  function ktildeqq (x,eps) result (ktildeqqx)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: ktildeqqx
    ktildeqqx = pqq_reg (x) * log(one-x) + CF * ( - log2_plus_distr (x,eps) &
      - pi**2/three * delta(x,eps))
  end function ktildeqq

<SM physics: public>+≡
  public :: ktildeqq

<SM physics: procedures>+≡
  function ktildeqq (x,eps) result (ktildeqqx)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: ktildeqqx
    ktildeqqx = pqq (x) * log(one-x)
  end function ktildeqq

<SM physics: public>+≡
  public :: ktildegg

<SM physics: procedures>+≡
  function ktildegg (x,eps) result (ktildeggx)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: ktildeggx
    ktildeggx = pgq (x) * log(one-x)
  end function ktildegg

<SM physics: public>+≡
  public :: ktildegg

<SM physics: procedures>+≡
  function ktildegg (x,eps) result (ktildeggx)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: ktildeggx
    ktildeggx = pgg_reg (x) * log(one-x) + CA * ( - &
      log2_plus_distr (x,eps) - pi**2/three * delta(x,eps))
  end function ktildegg

```

The insertion operator might not be necessary for a GOLEM interface but is demanded by the Les Houches NLO accord. It is a three-dimensional array, where the index always gives the inverse power of the DREG expansion parameter, ϵ .

```

⟨SM physics: public⟩+≡
  public :: insert_q

⟨SM physics: procedures⟩+≡
  pure function insert_q ()
    real(kind=default), dimension(0:2) :: insert_q
    insert_q(0) = gamma_q + k_q - pi**2/three * CF
    insert_q(1) = gamma_q
    insert_q(2) = CF
  end function insert_q

⟨SM physics: public⟩+≡
  public :: insert_g

⟨SM physics: procedures⟩+≡
  pure function insert_g (nf)
    real(kind=default), intent(in) :: nf
    real(kind=default), dimension(0:2) :: insert_g
    insert_g(0) = gamma_g (nf) + k_g (nf) - pi**2/three * CA
    insert_g(1) = gamma_g (nf)
    insert_g(2) = CA
  end function insert_g

```

For better convergence, one can exclude regions of phase space with a slicing parameter from the dipole subtraction procedure. First of all, the K functions get modified:

$$K_i(\alpha) = K_i - \mathbf{T}_i^2 \log^2 \alpha + \gamma_i(\alpha - 1 - \log \alpha) \quad (9.24)$$

```

⟨SM physics: public⟩+≡
  public :: k_q_al, k_g_al

⟨SM physics: procedures⟩+≡
  pure function k_q_al (alpha)
    real(kind=default), intent(in) :: alpha
    real(kind=default) :: k_q_al
    k_q_al = k_q - CF * (log(alpha))**2 + gamma_q * &
      (alpha - one - log(alpha))
  end function k_q_al

  pure function k_g_al (alpha, nf)
    real(kind=default), intent(in) :: alpha, nf
    real(kind=default) :: k_g_al
    k_g_al = k_g (nf) - CA * (log(alpha))**2 + gamma_g (nf) * &
      (alpha - one - log(alpha))
  end function k_g_al

```

The $+$ -distribution, but with a phase-space slicing parameter, α , $P_{1-\alpha}(x) = \left(\frac{1}{1-x}\right)_{1-x}$. Since we need the fatal error message here, this function cannot be elemental.

```

⟨SM physics: public⟩+≡
  public :: plus_distr_al

```

```

⟨SM physics: procedures⟩+≡
function plus_distr_al (x,alpha,eps) result (plusd_al)
  real(kind=default), intent(in) :: x,  eps, alpha
  real(kind=default) :: plusd_al
  if ((one - alpha) >= (one - eps)) then
    plusd_al = zero
    call msg_fatal ('sm_physics, plus_distr_al: alpha and epsilon chosen wrongly')
  elseif (x < (1.0_default - alpha)) then
    plusd_al = 0
  else if (x > (1.0_default - eps)) then
    plusd_al = log(eps/alpha)/eps
  else
    plusd_al = one/(one-x)
  end if
end function plus_distr_al

```

Introducing phase-space slicing parameters, these standard flavor kernels \overline{K}^{ab} become:

$$\overline{K}_\alpha^{qg}(x) = \overline{K}_\alpha^{\bar{q}g}(x) = P^{qg}(x) \log(\alpha(1-x)/x) + C_F \times x \quad (9.25)$$

$$\overline{K}_\alpha^{gq}(x) = \overline{K}_\alpha^{g\bar{q}}(x) = P^{gq}(x) \log(\alpha(1-x)/x) + T_R \times 2x(1-x) \quad (9.26)$$

$$\begin{aligned} \overline{K}_\alpha^{qq} = & C_F(1-x) + P_{\text{reg}}^{qq}(x) \log \frac{\alpha(1-x)}{x} \\ & + C_F \delta(1-x) \log^2 \alpha + C_F \left(\frac{2}{1-x} \log \frac{1-x}{x} \right)_+ \\ & - \left(\gamma_q + K_q(\alpha) - \frac{5}{6} \pi^2 C_F \right) \cdot \delta(1-x) C_F \left[+ \frac{2}{1-x} \log \left(\frac{\alpha(2-x)}{1+\alpha-x} \right) - \theta(1-\alpha-x) \cdot \left(\frac{2}{1-x} \right) \right] \end{aligned} \quad (9.27)$$

$$\begin{aligned} \overline{K}_\alpha^{gg} = & P_{\text{reg}}^{gg}(x) \log \frac{\alpha(1-x)}{x} + C_A \delta(1-x) \log^2 \alpha \\ & + C_A \left(\frac{2}{1-x} \log \frac{1-x}{x} \right)_+ - \left(\gamma_g + K_g(\alpha) - \frac{5}{6} \pi^2 C_A \right) \cdot \delta(1-x) C_A \left[+ \frac{2}{1-x} \log \left(\frac{\alpha(2-x)}{1+\alpha-x} \right) - \theta(1-\alpha-x) \cdot \left(\frac{2}{1-x} \right) \right] \end{aligned} \quad (9.28)$$

```

⟨SM physics: public⟩+≡
public :: kbarqg_al

```

```

⟨SM physics: procedures⟩+≡
function kbarqg_al (x,alpha,eps) result (kbarqgx)
  real(kind=default), intent(in) :: x, alpha, eps
  real(kind=default) :: kbarqgx
  kbarqgx = pqg (x) * log(alpha*(one-x)/x) + CF * x
end function kbarqg_al

```

```

⟨SM physics: public⟩+≡
public :: kbargq_al

```

```

⟨SM physics: procedures⟩+≡
function kbargq_al (x,alpha,eps) result (kbargqx)
  real(kind=default), intent(in) :: x, alpha, eps
  real(kind=default) :: kbargqx
  kbargqx = pgq (x) * log(alpha*(one-x)/x) + two * TR * x * (one-x)
end function kbargq_al

```

```

⟨SM physics: public⟩+≡
  public :: kbarqq_al
⟨SM physics: procedures⟩+≡
  function kbarqq_al (x,alpha,eps) result (kbarqqx)
    real(kind=default), intent(in) :: x, alpha, eps
    real(kind=default) :: kbarqqx
    kbarqqx = CF * (one - x) + pqq_reg(x) * log(alpha*(one-x)/x) &
      + CF * log_plus_distr(x,eps) &
      - (gamma_q + k_q_al(alpha) - CF * &
        five/6.0_default * pi**2 - CF * (log(alpha))**2) * &
        delta(x,eps) + &
        CF * two/(one -x)*log(alpha*(two-x)/(one+alpha-x))
    if (x < (one-alpha)) then
      kbarqqx = kbarqqx - CF * two/(one-x) * log((two-x)/(one-x))
    end if
  end function kbarqq_al

```

```

⟨SM physics: public⟩+≡
  public :: kbargg_al
⟨SM physics: procedures⟩+≡
  function kbargg_al (x,alpha,eps,nf) result (kbarggx)
    real(kind=default), intent(in) :: x, alpha, eps, nf
    real(kind=default) :: kbarggx
    kbarggx = pgg_reg(x) * log(alpha*(one-x)/x) &
      + CA * log_plus_distr(x,eps) &
      - (gamma_g(nf) + k_g_al(alpha,nf) - CA * &
        five/6.0_default * pi**2 - CA * (log(alpha))**2) * &
        delta(x,eps) + &
        CA * two/(one -x)*log(alpha*(two-x)/(one+alpha-x))
    if (x < (one-alpha)) then
      kbarggx = kbarggx - CA * two/(one-x) * log((two-x)/(one-x))
    end if
  end function kbargg_al

```

The \tilde{K} flavor kernels in the presence of a phase-space slicing parameter, are:

$$\tilde{K}^{ab}(x, \alpha) = P^{qq, \text{reg}}(x) \log \frac{1-x}{\alpha} + \dots \quad (9.29)$$

```

⟨SM physics: public⟩+≡
  public :: ktildeqq_al
⟨SM physics: procedures⟩+≡
  function ktildeqq_al (x,alpha,eps) result (ktildeqqx)
    real(kind=default), intent(in) :: x, eps, alpha
    real(kind=default) :: ktildeqqx
    ktildeqqx = pqq_reg(x) * log((one-x)/alpha) + CF*( &
      - log2_plus_distr_al(x,alpha,eps) - Pi**2/three * delta(x,eps) &
      + (one+x**2)/(one-x) * log(min(one,(alpha/(one-x)))) &
      + two/(one-x) * log((one+alpha-x)/alpha))
    if (x > (one-alpha)) then
      ktildeqqx = ktildeqqx - CF*two/(one-x)*log(two-x)
    end if
  end function ktildeqq_al

```

This is a logarithmic +-distribution, $\left(\frac{\log((1-x)/x)}{1-x}\right)_+$. For the sampling, we need the integral over this function over the incomplete sampling interval $[0, 1 - \epsilon]$, which is $\log^2(x) + 2Li_2(x) - \frac{\pi^2}{3}$. As this function is negative definite for $\epsilon > 0.1816$, we take a hard upper limit for that sampling parameter, irrespective of the fact what the user chooses.

```

⟨SM physics: public⟩+≡
  public :: log_plus_distr

⟨SM physics: procedures⟩+≡
  function log_plus_distr (x,eps) result (lpd)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: lpd, eps2
    eps2 = min (eps, 0.1816_default)
    if (x > (1.0_default - eps2)) then
      lpd = ((log(eps2))**2 + two*Li2(eps2) - pi**2/three)/eps2
    else
      lpd = two*log((one-x)/x)/(one-x)
    end if
  end function log_plus_distr

```

Logarithmic +-distribution, $2\left(\frac{\log(1/(1-x))}{1-x}\right)_+$.

```

⟨SM physics: public⟩+≡
  public :: log2_plus_distr

⟨SM physics: procedures⟩+≡
  function log2_plus_distr (x,eps) result (lpd)
    real(kind=default), intent(in) :: x, eps
    real(kind=default) :: lpd
    if (x > (1.0_default - eps)) then
      lpd = - (log(eps))**2/eps
    else
      lpd = two*log(one/(one-x))/(one-x)
    end if
  end function log2_plus_distr

```

Logarithmic +-distribution with phase-space slicing parameter, $2\left(\frac{\log(1/(1-x))}{1-x}\right)_{1-\alpha}$.

```

⟨SM physics: public⟩+≡
  public :: log2_plus_distr_al

⟨SM physics: procedures⟩+≡
  function log2_plus_distr_al (x,alpha,eps) result (lpd_al)
    real(kind=default), intent(in) :: x, eps, alpha
    real(kind=default) :: lpd_al
    if ((one - alpha) >= (one - eps)) then
      lpd_al = zero
      call msg_fatal ('alpha and epsilon chosen wrongly')
    elseif (x < (one - alpha)) then
      lpd_al = 0
    elseif (x > (1.0_default - eps)) then
      lpd_al = - ((log(eps))**2 - (log(alpha))**2)/eps
    else
      lpd_al = two*log(one/(one-x))/(one-x)
    end if
  end function log2_plus_distr_al

```



```

end if
end function log2_plus_distr_al

```

9.5.8 Splitting Functions

Analogue to the regularized distributions of the last subsection, we give here the unregularized splitting functions, relevant for the parton shower algorithm. We can use this unregularized version since there will be a cut-off ϵ that ensures that $\{z, 1 - z\} > \epsilon(t)$. This cut-off separates resolvable from unresolvable emissions. p_{xxx} are the kernels that are summed over helicity:

```

⟨SM physics: public⟩+≡
  public :: p_qqg
  public :: p_gqq
  public :: p_ggg

q → qq
⟨SM physics: procedures⟩+≡
  elemental function p_qqg (z) result (P)
    real(default), intent(in) :: z
    real(default) :: P
    P = CF * (one + z**2) / (one - z)
  end function p_qqg

g → q $\bar{q}$ 
⟨SM physics: procedures⟩+≡
  elemental function p_gqq (z) result (P)
    real(default), intent(in) :: z
    real(default) :: P
    P = TR * (z**2 + (one - z)**2)
  end function p_gqq

g → gg
⟨SM physics: procedures⟩+≡
  elemental function p_ggg (z) result (P)
    real(default), intent(in) :: z
    real(default) :: P
    P = NC * ((one - z) / z + z / (one - z) + z * (one - z))
  end function p_ggg

```

Analytically integrated splitting kernels:

```

⟨SM physics: public⟩+≡
  public :: integral_over_p_qqg
  public :: integral_over_p_gqq
  public :: integral_over_p_ggg

⟨SM physics: procedures⟩+≡
  pure function integral_over_p_qqg (zmin, zmax) result (integral)
    real(default), intent(in) :: zmin, zmax
    real(default) :: integral
    integral = (two / three) * (- zmax**2 + zmin**2 - &
      two * (zmax - zmin) + four * log((one - zmin) / (one - zmax)))
  end function integral_over_p_qqg

```

```

pure function integral_over_p_gqq (zmin, zmax) result (integral)
  real(default), intent(in) :: zmin, zmax
  real(default) :: integral
  integral = 0.5_default * ((two / three) * &
    (zmax**3 - zmin**3) - (zmax**2 - zmin**2) + (zmax - zmin))
end function integral_over_p_gqq

pure function integral_over_p_ggg (zmin, zmax) result (integral)
  real(default), intent(in) :: zmin, zmax
  real(default) :: integral
  integral = three * ((log(zmax) - two * zmax - &
    log(one - zmax) + zmax**2 / two - zmax**3 / three) - &
    (log(zmin) - zmin - zmin - log(one - zmin) + zmin**2 &
    / two - zmin**3 / three) )
end function integral_over_p_ggg

```

We can also use (massless) helicity dependent splitting functions:

<SM physics: public>+≡

```
public :: p_qqg_pol
```

$q_a \rightarrow q_b g_c$, the helicity of the quark is not changed by gluon emission and the gluon is preferably polarized in the branching plane ($l_c = 1$):

<SM physics: procedures>+≡

```

elemental function p_qqg_pol (z, l_a, l_b, l_c) result (P)
  real(default), intent(in) :: z
  integer, intent(in) :: l_a, l_b, l_c
  real(default) :: P
  if (l_a /= l_b) then
    P = zero
    return
  end if
  if (l_c == -1) then
    P = one - z
  else
    P = (one + z)**2 / (one - z)
  end if
  P = P * CF
end function p_qqg_pol

```

9.5.9 Top width

In order to produce sensible results, the widths have to be recomputed for each parameter and order. We start with the LO-expression for the top width given by the decay $t \rightarrow W^+, b$, cf. doi:10.1016/0550-3213(91)90530-B:

The analytic formula given there is

$$\Gamma = \frac{G_F m_t^2}{16\sqrt{2}\pi} \left[\mathcal{F}_0(\varepsilon, \xi^{-1/2}) - \frac{2\alpha_s}{3\pi} \mathcal{F}_1(\varepsilon, \xi^{-1/2}) \right],$$

with

$$\begin{aligned}\mathcal{F}_0 &= \frac{\sqrt{\lambda}}{2} f_0, \\ f_0 &= 4 \left[(1 - \varepsilon^2)^2 + w^2(1 + \varepsilon^2) - 2w^4 \right], \\ \lambda &= 1 + w^4 + \varepsilon^4 - 2(w^2 + \varepsilon^2 + w^2\varepsilon^2).\end{aligned}$$

Defining

$$u_q = \frac{1 + \varepsilon^2 - w^2 - \lambda^{1/2}}{1 + \varepsilon^2 - w^2 + \lambda^{1/2}}$$

and

$$u_w = \frac{1 - \varepsilon^2 + w^2 - \lambda^{1/2}}{1 - \varepsilon^2 + w^2 + \lambda^{1/2}}$$

the factor \mathcal{F}_1 can be expressed as

$$\begin{aligned}\mathcal{F}_1 &= \frac{1}{2} f_0 (1 + \varepsilon^2 - w^2) \left[\pi^2 + 2Li_2(u_w) - 2Li_2(1 - u_w) - 4Li_2(u_q) \right. \\ &\quad - 4Li_2(u_q u_w) + \log\left(\frac{1 - u_q}{w^2}\right) \log(1 - u_q) - \log^2(1 - u_q u_w) \\ &\quad + \frac{1}{4} \log^2\left(\frac{w^2}{u_w}\right) - \log(u_w) \log\left[\frac{(1 - u_q u_w)^2}{1 - u_q}\right] - 2 \log(u_q) \log[(1 - u_q)(1 - u_q u_w)] \\ &\quad - \sqrt{\lambda} f_0 (2 \log(w) + 3 \log(\varepsilon) - 2 \log \lambda) \\ &\quad + 4(1 - \varepsilon^2) [(1 - \varepsilon^2)^2 + w^2(1 + \varepsilon^2) - 4w^4] \log(u_w) \\ &\quad \left. + [(3 - \varepsilon^2 + 11\varepsilon^4 - \varepsilon^6) + w^2(6 - 12\varepsilon^2 + 2\varepsilon^4) - w^4(21 + 5\varepsilon^2) + 12w^6] \log(u_q) \right. \\ &\quad \left. + 6\sqrt{\lambda}(1 - \varepsilon^2)(1 + \varepsilon^2 - w^2) \log(\varepsilon) + \sqrt{\lambda} [-5 + 22\varepsilon^2 - 5\varepsilon^4 - 9w^2(1 + \varepsilon^2) + 6w^4] \right].\end{aligned}$$

<SM physics: public>+≡

`public :: top_width_sm_lo`

<SM physics: procedures>+≡

```
elemental function top_width_sm_lo (alpha, sinthw, vtb, mtop, mw, mb) &
  result (gamma)
  real(default) :: gamma
  real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb
  real(default) :: kappa
  kappa = sqrt ((mtop**2 - (mw + mb)**2) * (mtop**2 - (mw - mb)**2))
  gamma = alpha / four * mtop / (two * sinthw**2) * &
    vtb**2 * kappa / mtop**2 * &
    ((mtop**2 + mb**2) / (two * mtop**2) + &
    (mtop**2 - mb**2)**2 / (two * mtop**2 * mw**2) - &
    mw**2 / mtop**2)
end function top_width_sm_lo
```

<SM physics: public>+≡

`public :: g_mu_from_alpha`

<SM physics: procedures>+≡

```
elemental function g_mu_from_alpha (alpha, mw, sinthw) result (g_mu)
  real(default) :: g_mu
  real(default), intent(in) :: alpha, mw, sinthw
  g_mu = pi * alpha / sqrt(two) / mw**2 / sinthw**2
end function g_mu_from_alpha
```

```

⟨SM physics: public⟩+≡
  public :: alpha_from_g_mu

⟨SM physics: procedures⟩+≡
  elemental function alpha_from_g_mu (g_mu, mw, sinthw) result (alpha)
    real(default) :: alpha
    real(default), intent(in) :: g_mu, mw, sinthw
    alpha = g_mu * sqrt(two) / pi * mw**2 * sinthw**2
  end function alpha_from_g_mu

```

Cf. (3.3)-(3.7) in 1207.5018.

```

⟨SM physics: public⟩+≡
  public :: top_width_sm_qcd_nlo_massless_b

⟨SM physics: procedures⟩+≡
  elemental function top_width_sm_qcd_nlo_massless_b &
    (alpha, sinthw, vtb, mtop, mw, alphas) result (gamma)
    real(default) :: gamma
    real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, alphas
    real(default) :: prefac, g_mu, w2
    g_mu = g_mu_from_alpha (alpha, mw, sinthw)
    prefac = g_mu * mtop**3 * vtb**2 / (16 * sqrt(two) * pi)
    w2 = mw**2 / mtop**2
    gamma = prefac * (f0 (w2) - (two * alphas) / (3 * Pi) * f1 (w2))
  end function top_width_sm_qcd_nlo_massless_b

```

```

⟨SM physics: public⟩+≡
  public :: f0

⟨SM physics: procedures⟩+≡
  elemental function f0 (w2) result (f)
    real(default) :: f
    real(default), intent(in) :: w2
    f = two * (one - w2)**2 * (1 + 2 * w2)
  end function f0

```

```

⟨SM physics: public⟩+≡
  public :: f1

⟨SM physics: procedures⟩+≡
  elemental function f1 (w2) result (f)
    real(default) :: f
    real(default), intent(in) :: w2
    f = f0 (w2) * (pi**2 + two * Li2 (w2) - two * Li2 (one - w2)) &
      + four * w2 * (one - w2 - two * w2**2) * log (w2) &
      + two * (one - w2)**2 * (five + four * w2) * log (one - w2) &
      - (one - w2) * (five + 9 * w2 - 6 * w2**2)
  end function f1

```

Basically, the same as above but with m_b dependence, cf. Jezabek / Kuehn 1989.

```

⟨SM physics: public⟩+≡
  public :: top_width_sm_qcd_nlo_jk

```

```

<SM physics: procedures>+≡
elemental function top_width_sm_qcd_nlo_jk &
  (alpha, sinthw, vtb, mtop, mw, mb, alphas) result (gamma)
  real(default) :: gamma
  real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb, alphas
  real(default) :: prefac, g_mu, eps2, i_xi
  g_mu = g_mu_from_alpha (alpha, mw, sinthw)
  prefac = g_mu * mtop**3 * vtb**2 / (16 * sqrt(two) * pi)
  eps2 = (mb / mtop)**2
  i_xi = (mw / mtop)**2
  gamma = prefac * (ff0 (eps2, i_xi) - &
    (two * alphas) / (3 * Pi) * ff1 (eps2, i_xi))
end function top_width_sm_qcd_nlo_jk

```

Same as above, $m_b > 0$, with the slightly different implementation (2.6) of arXiv:1204.1513v1 by Campbell and Ellis.

```

<SM physics: public>+≡
public :: top_width_sm_qcd_nlo_ce

<SM physics: procedures>+≡
elemental function top_width_sm_qcd_nlo_ce &
  (alpha, sinthw, vtb, mtop, mw, mb, alpha_s) result (gamma)
  real(default) :: gamma
  real(default), intent(in) :: alpha, sinthw, vtb, mtop, mw, mb, alpha_s
  real(default) :: pm, pp, p0, p3
  real(default) :: yw, yp
  real(default) :: W0, Wp, Wm, w2
  real(default) :: beta2
  real(default) :: f
  real(default) :: g_mu, gamma0
  beta2 = (mb / mtop)**2
  w2 = (mw / mtop)**2
  p0 = (one - w2 + beta2) / two
  p3 = sqrt (lambda (one, w2, beta2)) / two
  pp = p0 + p3
  pm = p0 - p3
  W0 = (one + w2 - beta2) / two
  Wp = W0 + p3
  Wm = W0 - p3
  yp = log (pp / pm) / two
  yw = log (Wp / Wm) / two
  f = (one - beta2)**2 + w2 * (one + beta2) - two * w2**2
  g_mu = g_mu_from_alpha (alpha, mw, sinthw)
  gamma0 = g_mu * mtop**3 * vtb**2 / (8 * pi * sqrt(two))
  gamma = gamma0 * alpha_s / twopi * CF * &
    (8 * f * p0 * (Li2(one - pm) - Li2(one - pp) - two * Li2(one - pm / pp)) &
    + yp * log((four * p3**2) / (pp**2 * Wp)) + yw * log (pp)) &
    + four * (one - beta2) * ((one - beta2)**2 + w2 * (one + beta2) - four * w2**2) * yw &
    + (3 - beta2 + 11 * beta2**2 - beta2**3 + w2 * (6 - 12 * beta2 + two * beta2**2)) &
    - w2**2 * (21 + 5 * beta2) + 12 * w2**3) * yp &
    + 8 * f * p3 * log (sqrt(w2) / (four * p3**2)) &
    + 6 * (one - four * beta2 + 3 * beta2**2 + w2 * (3 + beta2) - four * w2**2) * p3 * log(sq
    + (5 - 22 * beta2 + 5 * beta2**2 + 9 * w2 * (one + beta2) - 6 * w2**2) * p3)
end function top_width_sm_qcd_nlo_ce

```

```

⟨SM physics: public⟩+≡
  public :: ff0

⟨SM physics: procedures⟩+≡
  elemental function ff0 (eps2, w2) result (f)
    real(default) :: f
    real(default), intent(in) :: eps2, w2
    f = one / two * sqrt(ff_lambda (eps2, w2)) * ff_f0 (eps2, w2)
  end function ff0

⟨SM physics: public⟩+≡
  public :: ff_f0

⟨SM physics: procedures⟩+≡
  elemental function ff_f0 (eps2, w2) result (f)
    real(default) :: f
    real(default), intent(in) :: eps2, w2
    f = four * ((1 - eps2)**2 + w2 * (1 + eps2) - 2 * w2**2)
  end function ff_f0

⟨SM physics: public⟩+≡
  public :: ff_lambda

⟨SM physics: procedures⟩+≡
  elemental function ff_lambda (eps2, w2) result (l)
    real(default) :: l
    real(default), intent(in) :: eps2, w2
    l = one + w2**2 + eps2**2 - two * (w2 + eps2 + w2 * eps2)
  end function ff_lambda

⟨SM physics: public⟩+≡
  public :: ff1

⟨SM physics: procedures⟩+≡
  elemental function ff1 (eps2, w2) result (f)
    real(default) :: f
    real(default), intent(in) :: eps2, w2
    real(default) :: uq, uw, sq_lam, fff
    sq_lam = sqrt (ff_lambda (eps2, w2))
    fff = ff_f0 (eps2, w2)
    uw = (one - eps2 + w2 - sq_lam) / &
      (one - eps2 + w2 + sq_lam)
    uq = (one + eps2 - w2 - sq_lam) / &
      (one + eps2 - w2 + sq_lam)
    f = one / two * fff * (one + eps2 - w2) * &
      (pi**2 + two * Li2 (uw) - two * Li2 (one - uw) - four * Li2 (uq) &
        - four * Li2 (uq * uw) + log ((one - uq) / w2) * log (one - uq) &
        - log (one - uq * uw)**2 + one / four * log (w2 / uw)**2 &
        - log (uw) * log ((one - uq * uw)**2 / (one - uq)) &
        - two * log (uq) * log ((one - uq) * (one - uq * uw))) &
        - sq_lam * fff * (two * log (sqrt (w2)) &
          + three * log (sqrt (eps2)) - two * log (sq_lam**2)) &
        + four * (one - eps2) * ((one - eps2)**2 + w2 * (one + eps2) &

```

```

      - four * w2**2) * log (uw) &
      + (three - eps2 + 11 * eps2**2 - eps2**3 + w2 * &
        (6 - 12 * eps2 + 2 * eps2**2) - w2**2 * (21 + five * eps2) &
      + 12 * w2**3) * log (uq) &
      + 6 * sq_lam * (one - eps2) * &
        (one + eps2 - w2) * log (sqrt (eps2)) &
      + sq_lam * (- five + 22 * eps2 - five * eps2**2 - 9 * w2 * &
        (one + eps2) + 6 * w2**2)
end function ff1

```

9.5.10 Unit tests

Test module, followed by the corresponding implementation module.

`<sm_physics_ut.f90>`≡
<File header>

```

module sm_physics_ut
  use unit_tests
  use sm_physics_ut

```

<Standard module head>

<SM physics: public test>

contains

<SM physics: test driver>

```

end module sm_physics_ut

```

`<sm_physics_uti.f90>`≡
<File header>

```

module sm_physics_uti

<Use kinds>
  use numeric_utils
  use format_defs, only: FMT_15
  use constants

  use sm_physics

```

<Standard module head>

<SM physics: test declarations>

contains

<SM physics: tests>

```

end module sm_physics_uti

```

API: driver for the unit tests below.

```

<SM physics: public test>≡
  public :: sm_physics_test

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

```

Splitting functions

```

<SM physics: execute tests>≡
  call test (sm_physics_1, "sm_physics_1", &
    "Splitting functions", &
    u, results)

<SM physics: test declarations>≡
  public :: sm_physics_1

<SM physics: tests>≡
  subroutine sm_physics_1 (u)
    integer, intent(in) :: u
    real(default) :: z = 0.75_default

    write (u, "(A)")  "* Test output: sm_physics_1"
    write (u, "(A)")  "* Purpose: check analytic properties"
    write (u, "(A)")

    write (u, "(A)")  "* Splitting functions:"
    write (u, "(A)")

    call assert (u, vanishes (p_qqg_pol (z, +1, -1, +1)), "+--")
    call assert (u, vanishes (p_qqg_pol (z, +1, -1, -1)), "+--")
    call assert (u, vanishes (p_qqg_pol (z, -1, +1, +1)), "-+-")
    call assert (u, vanishes (p_qqg_pol (z, -1, +1, -1)), "-+-")

    !call assert (u, nearly_equal ( &
      !p_qqg_pol (z, +1, +1, -1) + p_qqg_pol (z, +1, +1, +1), &
      !p_qqg (z)), "pol sum")

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: sm_physics_1"

  end subroutine sm_physics_1

```

Top width

```

<SM physics: execute tests>+≡
  call test(sm_physics_2, "sm_physics_2", &
    "Top width", u, results)

```



```

<SM physics: test declarations>+≡
public :: sm_physics_2

<SM physics: tests>+≡
subroutine sm_physics_2 (u)
  integer, intent(in) :: u
  real(default) :: mtop, mw, mz, mb, g_mu, sinthw, alpha, vtb, gamma0
  real(default) :: w2, alphas, alphas_mz, gamma1
  write (u, "(A)")  "* Test output: sm_physics_2"
  write (u, "(A)")  "* Purpose: Check different top width computations"
  write (u, "(A)")

  write (u, "(A)")  "* Values from [[1207.5018]] (massless b)"
  mtop = 172.0
  mw = 80.399
  mz = 91.1876
  mb = zero
  mb = 0.00001
  g_mu = 1.16637E-5
  sinthw = sqrt(one - mw**2 / mz**2)
  alpha = alpha_from_g_mu (g_mu, mw, sinthw)
  vtb = one
  w2 = mw**2 / mtop**2

  write (u, "(A)")  "* Check Li2 implementation"
  call assert_equal (u, Li2(w2), 0.2317566263959552_default, &
    "Li2(w2)", rel_smallness=1.0E-6_default)
  call assert_equal (u, Li2(one - w2), 1.038200378935867_default, &
    "Li2(one - w2)", rel_smallness=1.0E-6_default)

  write (u, "(A)")  "* Check LO Width"
  gamma0 = top_width_sm_lo (alpha, sinthw, vtb, mtop, mw, mb)
  call assert_equal (u, gamma0, 1.4655_default, &
    "top_width_sm_lo", rel_smallness=1.0E-5_default)
  alphas = zero
  gamma0 = top_width_sm_qcd_nlo_massless_b &
    (alpha, sinthw, vtb, mtop, mw, alphas)
  call assert_equal (u, gamma0, 1.4655_default, &
    "top_width_sm_qcd_nlo_massless_b", rel_smallness=1.0E-5_default)
  gamma0 = top_width_sm_qcd_nlo_jk &
    (alpha, sinthw, vtb, mtop, mw, mb, alphas)
  call assert_equal (u, gamma0, 1.4655_default, &
    "top_width_sm_qcd_nlo", rel_smallness=1.0E-5_default)

  write (u, "(A)")  "* Check NLO Width"
  alphas_mz = 0.1202      ! MSTW2008 NLO fit
  alphas = running_as (mtop, alphas_mz, mz, 1, 5.0_default)
  gamma1 = top_width_sm_qcd_nlo_massless_b &
    (alpha, sinthw, vtb, mtop, mw, alphas)
  call assert_equal (u, gamma1, 1.3376_default, rel_smallness=1.0E-4_default)
  gamma1 = top_width_sm_qcd_nlo_jk &
    (alpha, sinthw, vtb, mtop, mw, mb, alphas)
  ! It would be nice to get one more significant digit but the
  ! expression is numerically rather unstable for mb -> 0
  call assert_equal (u, gamma1, 1.3376_default, rel_smallness=1.0E-3_default)

```

```

write (u, "(A)")  "*"  Values from threshold validation (massive b)"
alpha = one / 125.924
! ee = 0.315901
! cw = 0.881903
! v = 240.024
mtop = 172.0 ! This is the value for M1S !!!
mb = 4.2
sinthw = 0.47143
mz = 91.188
mw = 80.419
call assert_equal (u, sqrt(one - mw**2 / mz**2), sinthw, &
    "sinthw", rel_smallness=1.0E-6_default)

write (u, "(A)")  "*"  Check LO Width"
gamma0 = top_width_sm_lo (alpha, sinthw, vtb, mtop, mw, mb)
call assert_equal (u, gamma0, 1.5386446_default, &
    "gamma0", rel_smallness=1.0E-7_default)
alphas = zero
gamma0 = top_width_sm_qcd_nlo_jk &
    (alpha, sinthw, vtb, mtop, mw, mb, alphas)
call assert_equal (u, gamma0, 1.5386446_default, &
    "gamma0", rel_smallness=1.0E-7_default)

write (u, "(A)")  "*"  Check NLO Width"
alphas_mz = 0.118 !(Z pole, NLL running to mu_h)
alphas = running_as (mtop, alphas_mz, mz, 1, 5.0_default)
write (u, "(A," // FMT_15 // ")")  "*"  alphas = ", alphas
gamma1 = top_width_sm_qcd_nlo_jk &
    (alpha, sinthw, vtb, mtop, mw, mb, alphas)
write (u, "(A," // FMT_15 // ")")  "*"  Gamma1 = ", gamma1

mb = zero
gamma1 = top_width_sm_qcd_nlo_massless_b &
    (alpha, sinthw, vtb, mtop, mw, alphas)
alphas = running_as (mtop, alphas_mz, mz, 1, 5.0_default)
write (u, "(A," // FMT_15 // ")")  "*"  Gamma1(mb=0) = ", gamma1

write (u, "(A)")
write (u, "(A)")  "*" Test output end: sm_physics_2"
end subroutine sm_physics_2

```

9.6 QCD Coupling

We provide various distinct implementations of the QCD coupling. In this module, we define an abstract data type and three implementations: fixed, running with $\alpha_s(M_Z)$ as input, and running with Λ_{QCD} as input. We use the functions defined above in the module `sm_physics` but provide a common interface. Later modules may define additional implementations.

```
<sm_qcd.f90>≡  
<File header>  
  
module sm_qcd  
  
  <Use kinds>  
  use io_units  
  use format_defs, only: FMT_12  
  use numeric_utils  
  use diagnostics  
  use md5  
  use physics_defs  
  use sm_physics  
  
  <Standard module head>  
  
  <SM qcd: public>  
  
  <SM qcd: types>  
  
  <SM qcd: interfaces>  
  
  contains  
  
  <SM qcd: procedures>  
  
end module sm_qcd
```

9.6.1 Coupling: Abstract Data Type

This is the abstract version of the QCD coupling implementation.

```
<SM qcd: public>≡  
  public :: alpha_qcd_t  
  
<SM qcd: types>≡  
  type, abstract :: alpha_qcd_t  
  contains  
    <SM qcd: alpha qcd: TBP>  
  end type alpha_qcd_t
```

There must be an output routine.

```
<SM qcd: alpha qcd: TBP>≡  
  procedure (alpha_qcd_write), deferred :: write
```

```

⟨SM qcd: interfaces⟩≡
  abstract interface
    subroutine alpha_qcd_write (object, unit)
      import
      class(alpha_qcd_t), intent(in) :: object
      integer, intent(in), optional :: unit
    end subroutine alpha_qcd_write
  end interface

```

This method computes the running coupling, given a certain scale. All parameters (reference value, order of the approximation, etc.) must be set before calling this.

```

⟨SM qcd: alpha qcd: TBP⟩+≡
  procedure (alpha_qcd_get), deferred :: get

⟨SM qcd: interfaces⟩+≡
  abstract interface
    function alpha_qcd_get (alpha_qcd, scale) result (alpha)
      import
      class(alpha_qcd_t), intent(in) :: alpha_qcd
      real(default), intent(in) :: scale
      real(default) :: alpha
    end function alpha_qcd_get
  end interface

```

9.6.2 Fixed Coupling

In this version, the α_s value is fixed, the `scale` argument of the `get` method is ignored. There is only one parameter, the value. By default, this is the value at M_Z .

```

⟨SM qcd: public⟩+≡
  public :: alpha_qcd_fixed_t

⟨SM qcd: types⟩+≡
  type, extends (alpha_qcd_t) :: alpha_qcd_fixed_t
    real(default) :: val = ALPHA_QCD_MZ_REF
  contains
    ⟨SM qcd: alpha qcd fixed: TBP⟩
  end type alpha_qcd_fixed_t

```

Output.

```

⟨SM qcd: alpha qcd fixed: TBP⟩≡
  procedure :: write => alpha_qcd_fixed_write

⟨SM qcd: procedures⟩≡
  subroutine alpha_qcd_fixed_write (object, unit)
    class(alpha_qcd_fixed_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3x,A)") "QCD parameters (fixed coupling):"
    write (u, "(5x,A," // FMT_12 // ")") "alpha = ", object%val
  end subroutine alpha_qcd_fixed_write

```

```
end subroutine alpha_qcd_fixed_write
```

Calculation: the scale is ignored in this case.

```
<SM qcd: alpha qcd fixed: TBP>+≡
  procedure :: get => alpha_qcd_fixed_get

<SM qcd: procedures>+≡
  function alpha_qcd_fixed_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_fixed_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
    alpha = alpha_qcd%val
  end function alpha_qcd_fixed_get
```

9.6.3 Running Coupling

In this version, the α_s value runs relative to the value at a given reference scale. There are two parameters: the value of this scale (default: M_Z), the value of α_s at this scale, and the number of effective flavors. Furthermore, we have the order of the approximation.

```
<SM qcd: public>+≡
  public :: alpha_qcd_from_scale_t

<SM qcd: types>+≡
  type, extends (alpha_qcd_t) :: alpha_qcd_from_scale_t
    real(default) :: mu_ref = MZ_REF
    real(default) :: ref = ALPHA_QCD_MZ_REF
    integer :: order = 0
    integer :: nf = 5
  contains
    <SM qcd: alpha qcd from scale: TBP>
  end type alpha_qcd_from_scale_t
```

Output.

```
<SM qcd: alpha qcd from scale: TBP>≡
  procedure :: write => alpha_qcd_from_scale_write

<SM qcd: procedures>+≡
  subroutine alpha_qcd_from_scale_write (object, unit)
    class(alpha_qcd_from_scale_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3x,A)") "QCD parameters (running coupling):"
    write (u, "(5x,A," // FMT_12 // ")") "Scale mu = ", object%mu_ref
    write (u, "(5x,A," // FMT_12 // ")") "alpha(mu) = ", object%ref
    write (u, "(5x,A,I0)") "LL order = ", object%order
    write (u, "(5x,A,I0)") "N(flav) = ", object%nf
  end subroutine alpha_qcd_from_scale_write
```

Calculation: here, we call the function for running α_s that was defined in `sm.physics` above. The function does not take into account thresholds, so the number of flavors should be the correct one for the chosen scale. Normally, this should be the Z boson mass.

```

<SM qcd: alpha qcd from scale: TBP>+≡
  procedure :: get => alpha_qcd_from_scale_get

<SM qcd: procedures>+≡
  function alpha_qcd_from_scale_get (alpha_qcd, scale) result (alpha)
    class(alpha_qcd_from_scale_t), intent(in) :: alpha_qcd
    real(default), intent(in) :: scale
    real(default) :: alpha
    alpha = running_as (scale, alpha_qcd%ref, alpha_qcd%mu_ref, &
      alpha_qcd%order, real (alpha_qcd%nf, kind=default))
  end function alpha_qcd_from_scale_get

```

9.6.4 Running Coupling, determined by Λ_{QCD}

In this version, the inputs are the value Λ_{QCD} and the order of the approximation.

```

<SM qcd: public>+≡
  public :: alpha_qcd_from_lambda_t

<SM qcd: types>+≡
  type, extends (alpha_qcd_t) :: alpha_qcd_from_lambda_t
    real(default) :: lambda = LAMBDA_QCD_REF
    integer :: order = 0
    integer :: nf = 5
  contains
    <SM qcd: alpha qcd from lambda: TBP>
  end type alpha_qcd_from_lambda_t

```

Output.

```

<SM qcd: alpha qcd from lambda: TBP>≡
  procedure :: write => alpha_qcd_from_lambda_write

<SM qcd: procedures>+≡
  subroutine alpha_qcd_from_lambda_write (object, unit)
    class(alpha_qcd_from_lambda_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3x,A)") "QCD parameters (Lambda_QCD as input):"
    write (u, "(5x,A," // FMT_12 // ")") "Lambda_QCD = ", object%lambda
    write (u, "(5x,A,I0)") "LL order = ", object%order
    write (u, "(5x,A,I0)") "N(flν) = ", object%nf
  end subroutine alpha_qcd_from_lambda_write

```

Calculation: here, we call the second function for running α_s that was defined in `sm.physics` above. The Λ value should be the one that is appropriate for the chosen number of effective flavors. Again, thresholds are not incorporated.

```

<SM qcd: alpha qcd from lambda: TBP>+≡
  procedure :: get => alpha_qcd_from_lambda_get

```

```

⟨SM qcd: procedures⟩+≡
function alpha_qcd_from_lambda_get (alpha_qcd, scale) result (alpha)
  class(alpha_qcd_from_lambda_t), intent(in) :: alpha_qcd
  real(default), intent(in) :: scale
  real(default) :: alpha
  alpha = running_as_lam (real (alpha_qcd%nf, kind=default), scale, &
    alpha_qcd%lambda, alpha_qcd%order)
end function alpha_qcd_from_lambda_get

```

9.6.5 QCD Wrapper type

We could get along with a polymorphic QCD type, but a monomorphic wrapper type with a polymorphic component is easier to handle and probably safer (w.r.t. compiler bugs). However, we keep the object transparent, so we can set the type-specific parameters directly (by a `dispatch` routine).

```

⟨SM qcd: public⟩+≡
  public :: qcd_t

⟨SM qcd: types⟩+≡
  type :: qcd_t
    class(alpha_qcd_t), allocatable :: alpha
    character(32) :: md5sum = ""
    integer :: n_f = -1
  contains
    ⟨SM qcd: qcd: TBP⟩
  end type qcd_t

```

Output. We first print the polymorphic `alpha` which contains a headline, then any extra components.

```

⟨SM qcd: qcd: TBP⟩≡
  procedure :: write => qcd_write

⟨SM qcd: procedures⟩+≡
  subroutine qcd_write (qcd, unit, show_md5sum)
    class(qcd_t), intent(in) :: qcd
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_md5sum
    logical :: show_md5
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    show_md5 = .true.; if (present (show_md5sum)) show_md5 = show_md5sum
    if (allocated (qcd%alpha)) then
      call qcd%alpha%write (u)
    else
      write (u, "(3x,A)") "QCD parameters (coupling undefined)"
    end if
    if (show_md5 .and. qcd%md5sum /= "") &
      write (u, "(5x,A,A,A)") "md5sum = '", qcd%md5sum, "'"
  end subroutine qcd_write

```

Compute an MD5 sum for the `alpha_s` setup. This is done by writing them to a temporary file, using a standard format.

```

⟨SM qcd: qcd: TBP⟩+≡
  procedure :: compute_alphas_md5sum => qcd_compute_alphas_md5sum

⟨SM qcd: procedures⟩+≡
  subroutine qcd_compute_alphas_md5sum (qcd)
    class(qcd_t), intent(inout) :: qcd
    integer :: unit
    if (allocated (qcd%alpha)) then
      unit = free_unit ()
      open (unit, status="scratch", action="readwrite")
      call qcd%alpha%write (unit)
      rewind (unit)
      qcd%md5sum = md5sum (unit)
      close (unit)
    end if
  end subroutine qcd_compute_alphas_md5sum

```

Retrieve the MD5 sum of the `qcd` setup.

```

⟨SM qcd: qcd: TBP⟩+≡
  procedure :: get_md5sum => qcd_get_md5sum

⟨SM qcd: procedures⟩+≡
  function qcd_get_md5sum (qcd) result (md5sum)
    character(32) :: md5sum
    class(qcd_t), intent(inout) :: qcd
    md5sum = qcd%md5sum
  end function qcd_get_md5sum

```

9.6.6 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sm_qcd.ut.f90⟩≡
  ⟨File header⟩

  module sm_qcd_ut
    use unit_tests
    use sm_qcd_util

    ⟨Standard module head⟩

    ⟨SM qcd: public test⟩

    contains

    ⟨SM qcd: test driver⟩

  end module sm_qcd_ut

```



```

⟨sm_qcd_util.f90⟩≡
  ⟨File header⟩

  module sm_qcd_util

    ⟨Use kinds⟩
    use physics_defs, only: MZ_REF

    use sm_qcd

    ⟨Standard module head⟩

    ⟨SM qcd: test declarations⟩

    contains

    ⟨SM qcd: tests⟩

  end module sm_qcd_util
API: driver for the unit tests below.
⟨SM qcd: public test⟩≡
  public :: sm_qcd_test
⟨SM qcd: test driver⟩≡
  subroutine sm_qcd_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    ⟨SM qcd: execute tests⟩
  end subroutine sm_qcd_test

```

QCD Coupling

We check two different implementations of the abstract QCD coupling.

```

⟨SM qcd: execute tests⟩≡
  call test (sm_qcd_1, "sm_qcd_1", &
    "running alpha_s", &
    u, results)
⟨SM qcd: test declarations⟩≡
  public :: sm_qcd_1
⟨SM qcd: tests⟩≡
  subroutine sm_qcd_1 (u)
    integer, intent(in) :: u
    type(qcd_t) :: qcd

    write (u, "(A)")  "* Test output: sm_qcd_1"
    write (u, "(A)")  "* Purpose: compute running alpha_s"
    write (u, "(A)")

    write (u, "(A)")  "* Fixed:"
    write (u, "(A)")

    allocate (alpha_qcd_fixed_t :: qcd%alpha)

```

```

call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz)   =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)
deallocate (qcd%alpha)

write (u, "(A)")  "* Running from MZ (LO):"
write (u, "(A)")

allocate (alpha_qcd_from_scale_t :: qcd%alpha)
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz)   =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from MZ (NLO):"
write (u, "(A)")

select type (alpha => qcd%alpha)
type is (alpha_qcd_from_scale_t)
    alpha%order = 1
end select
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz)   =", &
    qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
    qcd%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from MZ (NNLO):"
write (u, "(A)")

select type (alpha => qcd%alpha)
type is (alpha_qcd_from_scale_t)
    alpha%order = 2
end select
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz)   =", &

```

```

      qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
      qcd%alpha%get (1000._default)
write (u, *)

deallocate (qcd%alpha)
write (u, "(A)")  "* Running from Lambda_QCD (LO):"
write (u, "(A)")

allocate (alpha_qcd_from_lambda_t :: qcd%alpha)
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz)      =", &
      qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
      qcd%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from Lambda_QCD (NLO):"
write (u, "(A)")

select type (alpha => qcd%alpha)
type is (alpha_qcd_from_lambda_t)
      alpha%order = 1
end select
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz)      =", &
      qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
      qcd%alpha%get (1000._default)
write (u, *)

write (u, "(A)")  "* Running from Lambda_QCD (NNLO):"
write (u, "(A)")

select type (alpha => qcd%alpha)
type is (alpha_qcd_from_lambda_t)
      alpha%order = 2
end select
call qcd%compute_alphas_md5sum ()

call qcd%write (u)
write (u, *)
write (u, "(1x,A,F10.7)") "alpha_s (mz)      =", &
      qcd%alpha%get (MZ_REF)
write (u, "(1x,A,F10.7)") "alpha_s (1 TeV) =", &
      qcd%alpha%get (1000._default)

write (u, "(A)")

```

```
write (u, "(A)")  "* Test output end: sm_qcd_1"  
end subroutine sm_qcd_1
```

9.7 QED Coupling

On the surface similar to the QCD coupling module but much simpler. Only a fixed QED coupling α_{em} is allowed. Can be extended later if we want to enable a running of α_{em} as well.

```

⟨sm_qed.f90⟩≡
  ⟨File header⟩

  module sm_qed

    ⟨Use kinds⟩
    use io_units
    use format_defs, only: FMT_12

    ⟨Standard module head⟩

    ⟨SM qed: public⟩

    ⟨SM qed: types⟩

    contains

    ⟨SM qed: procedures⟩

  end module sm_qed

```

9.7.1 QED type

Slightly similar to qcd_t but way simpler. It just needs to store `alpha_em`.

```

⟨SM qed: public⟩≡
  public :: qed_t

⟨SM qed: types⟩≡
  type :: qed_t
    private
    real(default) :: alpha_qed = -1
    contains
    ⟨SM qed: TBP⟩
  end type qed_t

```

Output routine

```

⟨SM qed: TBP⟩≡
  procedure :: write => qed_write

⟨SM qed: procedures⟩≡
  subroutine qed_write (qed, unit)
    class(qed_t), intent(in) :: qed
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3x,A)") "QED parameters (fixed coupling):"
    write (u, "(5x,A," // FMT_12 // ")") "alpha_qed = ", qed%alpha_qed
  end subroutine qed_write

```

Setter for `alpha_qed`

$\langle SM \text{ qed: TBP} \rangle + \equiv$

```
procedure :: set_alpha_qed => qed_set_alpha_qed
```

$\langle SM \text{ qed: procedures} \rangle + \equiv$

```
subroutine qed_set_alpha_qed (qed, alpha_qed_in)
  class(qed_t), intent(inout) :: qed
  real(default), intent(in) :: alpha_qed_in
  qed%alpha_qed = alpha_qed_in
end subroutine qed_set_alpha_qed
```

Getter for `alpha_qed`

$\langle SM \text{ qed: TBP} \rangle + \equiv$

```
procedure :: get_alpha_qed => qed_get_alpha_qed
```

$\langle SM \text{ qed: procedures} \rangle + \equiv$

```
function qed_get_alpha_qed (qed) result (alpha_qed_out)
  class(qed_t), intent(in) :: qed
  real(default) :: alpha_qed_out
  alpha_qed_out = qed%alpha_qed
end function qed_get_alpha_qed
```

9.8 Shower algorithms

```

<shower_algorithms.f90>≡
  <File header>

  module shower_algorithms

    <Use kinds>
    use diagnostics
    use constants

    <Standard module head>

    <shower_algorithms: public>

    <shower_algorithms: interfaces>

    contains

    <shower_algorithms: procedures>

    <shower_algorithms: tests>

  end module shower_algorithms

```

We want to generate emission variables $\mathbf{x} \in \mathbb{R}^d$ proportional to

$$f(\mathbf{x}) \propto \Delta(f, h(\mathbf{x})) \quad \text{with} \quad (9.30)$$

$$\Delta(f, H) = \exp \left\{ - \int d^d x' f(\mathbf{x}') \Theta(h(\mathbf{x}') - H) \right\} \quad (9.31)$$

The `true_function` f is however too complicated and we are only able to generate \mathbf{x} according to the `overestimator` F . This algorithm is described in Appendix B of 0709.2092 and is proven e.g. in 1211.7204 and hep-ph/0606275. Intuitively speaking, we overestimate the emission probability and can therefore set `scale_max = scale` if the emission is rejected.

```

<shower_algorithms: procedures>≡
  subroutine generate_vetoed (x, overestimator, true_function, &
    sudakov, inverse_sudakov, scale_min)
    real(default), dimension(:), intent(out) :: x
    !class(rng_t), intent(inout) :: rng
    procedure(XXX_function), pointer, intent(in) :: overestimator, true_function
    procedure(sudakov_p), pointer, intent(in) :: sudakov, inverse_sudakov
    real(default), intent(in) :: scale_min
    real(default) :: random, scale_max, scale
    scale_max = inverse_sudakov (one)
    do while (scale_max > scale_min)
      !call rng%generate (random)
      scale = inverse_sudakov (random * sudakov (scale_max))
      call generate_on_hypersphere (x, overestimator, scale)
      !call rng%generate (random)
      if (random < true_function (x) / overestimator (x)) then
        return !!! accept x
      end if
    end while
  end subroutine

```

```

        scale_max = scale
    end do
end subroutine generate_vetoed

<shower algorithms: procedures>+=
subroutine generate_on_hypersphere (x, overestimator, scale)
    real(default), dimension(:), intent(out) :: x
    procedure(XXX_function), pointer, intent(in) :: overestimator
    real(default), intent(in) :: scale
    call msg_bug ("generate_on_hypersphere: not implemented")
end subroutine generate_on_hypersphere

<shower algorithms: interfaces>=
interface
    pure function XXX_function (x)
        import
        real(default) :: XXX_function
        real(default), dimension(:), intent(in) :: x
    end function XXX_function
end interface
interface
    pure function sudakov_p (x)
        import
        real(default) :: sudakov_p
        real(default), intent(in) :: x
    end function sudakov_p
end interface

```

9.8.1 Unit tests

(Currently unused.)

```

<XXX shower algorithms: public>=
public :: shower_algorithms_test

<XXX shower algorithms: tests>=
subroutine shower_algorithms_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
<shower algorithms: execute tests>
end subroutine shower_algorithms_test

```

Splitting functions

```

<XXX shower algorithms: execute tests>=
call test (shower_algorithms_1, "shower_algorithms_1", &
    "veto technique", &
    u, results)

<XXX shower algorithms: tests>+=
subroutine shower_algorithms_1 (u)
    integer, intent(in) :: u

```



```

write (u, "(A)")  "* Test output: shower_algorithms_1"
write (u, "(A)")  "* Purpose: check veto technique"
write (u, "(A)")

write (u, "(A)")  "* Splitting functions:"
write (u, "(A)")

!call assert (u, vanishes (p_qqg_pol (z, +1, -1, +1)))
!call assert (u, nearly_equal ( &
    !p_qqg_pol (z, +1, +1, -1) + p_qqg_pol (z, +1, +1, +1),
    !p_qqg (z))

write (u, "(A)")
write (u, "(A)")  "* Test output end: shower_algorithms_1"

end subroutine shower_algorithms_1

```

Chapter 10

QED Parton Distribution Functions

We start with a module that gives access to the ISR structure function:

`electron.pdfs`

10.1 Electron PDFs

This module contains the formulae for the numerical evaluation of different incarnations of the QED initial-state radiation (ISR) structure functions (a.k.a. electron PDFs).

```
(electron.pdfs.f90)≡  
  <File header>  
  
  module electron_pdfs  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use constants, only: pi  
    use format_defs, only: FMT_19  
    use numeric_utils  
    use sm_physics, only: Li2  
  
    <Standard module head>  
  
    <Electron PDFs: public>  
  
    <Electron PDFs: types>  
  
    contains  
  
    <Electron PDFs: procedures>  
  
  end module electron_pdfs
```

No internal dependencies

Figure 10.1: Module dependencies in `src/qed_pdf`.

10.1.1 The physics for electron beam structure functions

The ISR structure function is in the most crude approximation (LLA without α corrections, i.e. ϵ^0)

$$f_0(x) = \epsilon(1-x)^{-1+\epsilon} \quad \text{with} \quad \epsilon = \frac{\alpha}{\pi} q_e^2 \ln \frac{s}{m^2}, \quad (10.1)$$

where m is the mass of the incoming (and outgoing) particle, which is initially assumed on-shell.

Here, the form of ϵ results from the kinematical bounds for the momentum squared of the outgoing particle, which in the limit $m^2 \ll s$ are given by

$$t_0 = -2\bar{x}E(E+p) + m^2 \approx -\bar{x}s, \quad (10.2)$$

$$t_1 = -2\bar{x}E(E-p) + m^2 \approx xm^2, \quad (10.3)$$

so the integration over the propagator $1/(t-m^2)$ yields

$$\ln \frac{t_0 - m^2}{t_1 - m^2} = \ln \frac{s}{m^2}. \quad (10.4)$$

The structure function has three parameters: α , m_{in} of the incoming particle and s , the hard scale. Internally, we store the exponent ϵ which is the relevant parameter. (In conventional notation, $\epsilon = \beta/2$.) As defaults, we take the actual values of α (which is probably $\alpha(s)$), the actual mass m_{in} and the squared total c.m. energy s .

Including ϵ , ϵ^2 , and ϵ^3 corrections, the successive approximation of the ISR

structure function read

$$f_0(x) = \epsilon(1-x)^{-1+\epsilon} \quad (10.5)$$

$$f_1(x) = g_1(\epsilon) f_0(x) - \frac{\epsilon}{2}(1+x) \quad (10.6)$$

$$f_2(x) = g_2(\epsilon) f_0(x) - \frac{\epsilon}{2}(1+x) - \frac{\epsilon^2}{8} \left(\frac{1+3x^2}{1-x} \ln x + 4(1+x) \ln(1-x) + 5+x \right) \quad (10.7)$$

$$\begin{aligned} f_3(x) = g_3(\epsilon) f_0(x) - \frac{\epsilon}{2}(1+x) & - \frac{\epsilon^2}{8} \left(\frac{1+3x^2}{1-x} \ln x + 4(1+x) \ln(1-x) + 5+x \right) \\ & - \frac{\epsilon^3}{48} \left((1+x) [6 \text{Li}_2(x) + 12 \ln^2(1-x) - 3\pi^2] + 6(x+5) \ln(1-x) \right. \\ & \quad \left. + \frac{1}{1-x} \left[\frac{3}{2}(1+8x+3x^2) \ln x + 12(1+x^2) \ln x \ln(1-x) \right. \right. \\ & \quad \left. \left. - \frac{1}{2}(1+7x^2) \ln^2 x + \frac{1}{4}(39-24x-15x^2) \right] \right) \end{aligned} \quad (10.8)$$

where the successive approximations to the prefactor of the leading singularity

$$g(\epsilon) = \frac{\exp\left(\epsilon(-\gamma_E + \frac{3}{4})\right)}{\Gamma(1+\epsilon)}, \quad (10.9)$$

are given by

$$g_0(\epsilon) = 1 \quad (10.10)$$

$$g_1(\epsilon) = 1 + \frac{3}{4}\epsilon \quad (10.11)$$

$$g_2(\epsilon) = 1 + \frac{3}{4}\epsilon + \frac{27-8\pi^2}{96}\epsilon^2 \quad (10.12)$$

$$g_3(\epsilon) = 1 + \frac{3}{4}\epsilon + \frac{27-8\pi^2}{96}\epsilon^2 + \frac{27-24\pi^2+128\zeta(3)}{384}\epsilon^3, \quad (10.13)$$

where, numerically

$$\zeta(3) = 1.20205690315959428539973816151\dots \quad (10.14)$$

Although one could calculate the function $g(\epsilon)$ exactly, truncating its Taylor expansion ensures the exact normalization of the truncated structure function at each given order:

$$\int_0^1 dx f_i(x) = 1 \quad \text{for all } i. \quad (10.15)$$

Effectively, the $O(\epsilon)$ correction reduces the low- x tail of the structure function by 50% while increasing the coefficient of the singularity by $O(\epsilon)$. Relative to this, the $O(\epsilon^2)$ correction slightly enhances $x > \frac{1}{2}$ compared to $x < \frac{1}{2}$. At $x = 0$, $f_2(x)$ introduces a logarithmic singularity which should be cut off at

$x_0 = O(e^{-1/\epsilon})$: for lower x the perturbative series breaks down. The f_3 correction is slightly positive for low x values and negative near $x = 1$, where the Li_2 piece slightly softens the singularity at $x = 1$.

Instead of the definition for ϵ given above, it is customary to include a universal nonlogarithmic piece:

$$\epsilon = \frac{\alpha}{\pi} q_e^2 \left(\ln \frac{s}{m^2} - 1 \right) \quad (10.16)$$

10.1.2 Implementation

The basic type for lepton beam (QED) structure functions:

```

<Electron PDFs: public>≡
  public :: qed_pdf_t

<Electron PDFs: types>≡
  type :: qed_pdf_t
    private
    integer :: flv = 0
    real(default) :: mass = 0
    real(default) :: q_max = 0
    real(default) :: alpha = 0
    real(default) :: eps = 0
    integer :: order
  contains
    <Electron PDFs: QED PDF: TBP>
  end type qed_pdf_t

<Electron PDFs: QED PDF: TBP>≡
  procedure :: init => qed_pdf_init

<Electron PDFs: procedures>≡
  subroutine qed_pdf_init &
    (qed_pdf, mass, alpha, charge, q_max, order)
    class(qed_pdf_t), intent(out) :: qed_pdf
    real(default), intent(in) :: mass, alpha, q_max, charge
    integer, intent(in) :: order
    qed_pdf%mass = mass
    qed_pdf%q_max = q_max
    qed_pdf%alpha = alpha
    qed_pdf%order = order
    qed_pdf%eps = alpha/pi * charge**2 &
      * (2 * log (q_max / mass) - 1)
  end subroutine qed_pdf_init

Write routine.

<Electron PDFs: QED PDF: TBP>+≡
  procedure :: write => qed_pdf_write

<Electron PDFs: procedures>+≡
  subroutine qed_pdf_write (qed_pdf, unit)
    class(qed_pdf_t), intent(in) :: qed_pdf
    integer, intent(in), optional :: unit
    integer :: u

```

```

u = given_output_unit (unit)
write (u, "(3x,A)") "QED structure function (PDF):"
write (u, "(5x,A,I0)") "Flavor      = ", qed_pdf%flv
write (u, "(5x,A," // FMT_19 // ")") "Mass      = ", qed_pdf%mass
write (u, "(5x,A," // FMT_19 // ")") "q_max     = ", qed_pdf%q_max
write (u, "(5x,A," // FMT_19 // ")") "alpha     = ", qed_pdf%alpha
write (u, "(5x,A,I0)") "Order      = ", qed_pdf%order
write (u, "(5x,A," // FMT_19 // ")") "epsilon   = ", qed_pdf%eps
end subroutine qed_pdf_write

```

For some unit tests, the order has to be set explicitly.

```

<Electron PDFs: QED PDF: TBP>+≡
  procedure :: set_order => qed_pdf_set_order

<Electron PDFs: procedures>+≡
  subroutine qed_pdf_set_order (qed_pdf, order)
    class(qed_pdf_t), intent(inout) :: qed_pdf
    integer, intent(in) :: order
    qed_pdf%order = order
  end subroutine qed_pdf_set_order

```

Calculate the actual value depending on the order and a possible mapping parameter.

```

<Electron PDFs: QED PDF: TBP>+≡
  procedure :: evolve_qed_pdf => qed_pdf_evolve_qed_pdf

<Electron PDFs: procedures>+≡
  subroutine qed_pdf_evolve_qed_pdf (qed_pdf, x, xb, rb, ff)
    class(qed_pdf_t), intent(inout) :: qed_pdf
    real(default), intent(in) :: x, xb, rb
    real(default), intent(inout) :: ff
    real(default), parameter :: &
      & xmin = 0.00714053329734592839549879772019_default
    real(default), parameter :: &
      & zeta3 = 1.20205690315959428539973816151_default
    real(default), parameter :: &
      g1 = 3._default / 4._default, &
      g2 = (27 - 8 * pi**2) / 96._default, &
      g3 = (27 - 24 * pi**2 + 128 * zeta3) / 384._default
    real(default) :: x_2, log_x, log_xb
    if (ff > 0 .and. qed_pdf%order > 0) then
      ff = ff * (1 + g1 * qed_pdf%eps)
      x_2 = x * x
      if (rb > 0) ff = ff * (1 - (1-x_2) / (2 * rb))
      if (qed_pdf%order > 1) then
        ff = ff * (1 + g2 * qed_pdf%eps**2)
        if (rb > 0 .and. xb > 0 .and. x > xmin) then
          log_x = log_prec (x, xb)
          log_xb = log_prec (xb, x)
          ff = ff * (1 - ((1 + 3 * x_2) * log_x + xb * (4 * (1 + x) * &
            log_xb + 5 + x)) / (8 * rb) * qed_pdf%eps)
        end if
      if (qed_pdf%order > 2) then
        ff = ff * (1 + g3 * qed_pdf%eps**3)

```

```

      if (rb > 0 .and. xb > 0 .and. x > xmin) then
        ff = ff * (1 - ((1 + x) * xb &
          * (6 * Li2(x) + 12 * log_xb**2 - 3 * pi**2) &
          + 1.5_default * (1 + 8 * x + 3 * x_2) * log_x &
          + 6 * (x + 5) * xb * log_xb &
          + 12 * (1 + x_2) * log_x * log_xb &
          - (1 + 7 * x_2) * log_x**2 / 2 &
          + (39 - 24 * x - 15 * x_2) / 4) &
          / (48 * rb) * qed_pdf%eps**2)
      end if
    end if
  end if
end subroutine qed_pdf_evolve_qed_pdf

```

Chapter 11

Quantum Field Theory Concepts

The objects and methods defined here implement concepts and data for the underlying quantum field theory that we use for computing matrix elements and processes.

model_data Fields and coupling parameters, operators as vertex structures, for a specific model.

model_testbed Provide hooks to deal with a **model_data** extension without referencing it explicitly.

helicities Types and methods for spin density matrices.

colors Dealing with colored particles, using the color-flow representation.

flavors PDG codes and particle properties, depends on the model.

quantum_numbers Quantum numbers and density matrices for entangled particle systems.

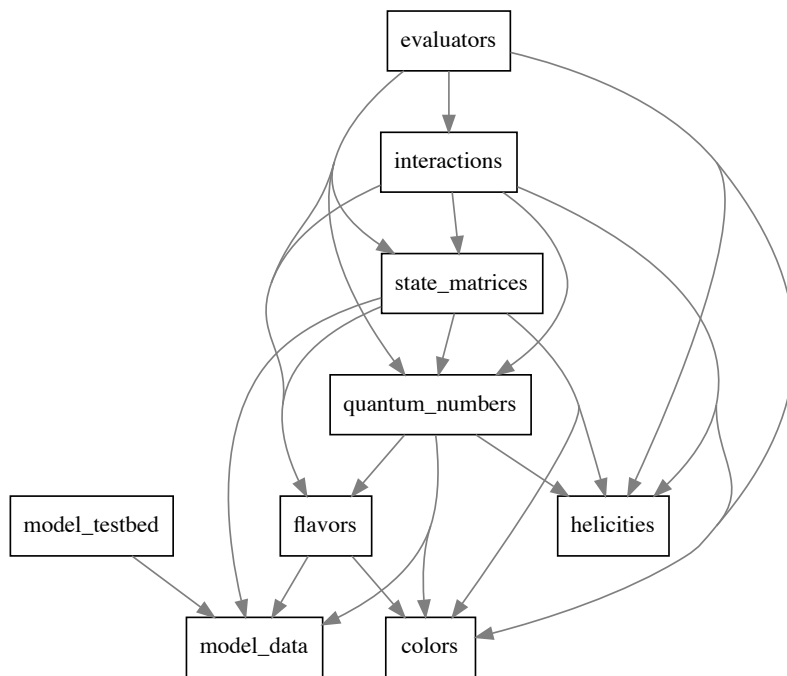


Figure 11.1: Module dependencies in `src/qft`.

11.1 Model Data

These data represent a specific Lagrangian in numeric terms. That is, we have the fields with their quantum numbers, the masses, widths and couplings as numerical values, and the vertices as arrays of fields.

We do not store the relations between coupling parameters. They should be represented by expressions for evaluation, implemented as Sindarin objects in a distinct data structure. Neither do we need the algebraic structure of vertices. The field content of vertices is required for the sole purpose of setting up phase space.

```
<model_data.f90>≡  
  <File header>  
  
  module model_data  
  
    use, intrinsic :: iso_c_binding !NODEP!  
  
    <Use kinds>  
    use kinds, only: i8, i32  
    use kinds, only: c_default_float  
    <Use strings>  
    use format_defs, only: FMT_19  
    use io_units  
    use diagnostics  
    use md5  
    use hashes, only: hash  
    use physics_defs, only: UNDEFINED, SCALAR  
  
    <Standard module head>  
  
    <Model data: public>  
  
    <Model data: parameters>  
  
    <Model data: types>  
  
    contains  
  
    <Model data: procedures>  
  
  end module model_data
```

11.1.1 Physics Parameters

Couplings, masses, and widths are physics parameters. Each parameter has a unique name (used, essentially, for diagnostics output and debugging) and a value. The value may be a real or a complex number, so we provide to implementations of an abstract type.

```
<Model data: public>≡  
  public :: modelpar_data_t  
  
<Model data: types>≡  
  type, abstract :: modelpar_data_t
```

```

    private
    type(string_t) :: name
contains
  <Model data: par data: TBP>
end type modelpar_data_t

type, extends (modelpar_data_t) :: modelpar_real_t
  private
  real(default) :: value
end type modelpar_real_t

type, extends (modelpar_data_t) :: modelpar_complex_t
  private
  complex(default) :: value
end type modelpar_complex_t

```

Output for diagnostics. Non-advancing.

```

<Model data: par data: TBP>≡
  procedure :: write => par_write

<Model data: procedures>≡
  subroutine par_write (par, unit)
    class(modelpar_data_t), intent(in) :: par
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,1x,A)", advance="no") char (par%name), "= "
    select type (par)
    type is (modelpar_real_t)
      write (u, "(" // FMT_19 // ")", advance="no") par%value
    type is (modelpar_complex_t)
      write (u, "(" // FMT_19 // ",1x,'+',1x," // FMT_19 // ",1x,'I')", &
        advance="no") par%value
    end select
  end subroutine par_write

```

Pretty-printed on separate line, with fixed line length

```

<Model data: par data: TBP>+≡
  procedure :: show => par_show

<Model data: procedures>+≡
  subroutine par_show (par, l, u)
    class(modelpar_data_t), intent(in) :: par
    integer, intent(in) :: l, u
    character(len=l) :: buffer
    buffer = par%name
    select type (par)
    type is (modelpar_real_t)
      write (u, "(4x,A,1x,'=',1x," // FMT_19 // ")", buffer, par%value
    type is (modelpar_complex_t)
      write (u, "(4x,A,1x,'=',1x," // FMT_19 // ",1x,'+',1x," &
        // FMT_19 // ",1x,'I')", buffer, par%value
    end select
  end subroutine par_show

```

Initialize with name and value. The type depends on the argument type. If the type does not match, the value is converted following Fortran rules.

```

<Model data: par data: TBP>+≡
  generic :: init => modelpar_data_init_real, modelpar_data_init_complex
  procedure, private :: modelpar_data_init_real
  procedure, private :: modelpar_data_init_complex

<Model data: procedures>+≡
  subroutine modelpar_data_init_real (par, name, value)
    class(modelpar_data_t), intent(out) :: par
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
    par%name = name
    par = value
  end subroutine modelpar_data_init_real

  subroutine modelpar_data_init_complex (par, name, value)
    class(modelpar_data_t), intent(out) :: par
    type(string_t), intent(in) :: name
    complex(default), intent(in) :: value
    par%name = name
    par = value
  end subroutine modelpar_data_init_complex

```

Modify the value. We assume that the parameter has been initialized. The type (real or complex) must not be changed, and the name is also fixed.

```

<Model data: par data: TBP>+≡
  generic :: assignment(=) => modelpar_data_set_real, modelpar_data_set_complex
  procedure, private :: modelpar_data_set_real
  procedure, private :: modelpar_data_set_complex

<Model data: procedures>+≡
  elemental subroutine modelpar_data_set_real (par, value)
    class(modelpar_data_t), intent(inout) :: par
    real(default), intent(in) :: value
    select type (par)
      type is (modelpar_real_t)
        par%value = value
      type is (modelpar_complex_t)
        par%value = value
    end select
  end subroutine modelpar_data_set_real

  elemental subroutine modelpar_data_set_complex (par, value)
    class(modelpar_data_t), intent(inout) :: par
    complex(default), intent(in) :: value
    select type (par)
      type is (modelpar_real_t)
        par%value = value
      type is (modelpar_complex_t)
        par%value = value
    end select
  end subroutine modelpar_data_set_complex

```

Return the parameter name.

```
<Model data: par data: TBP>+≡  
  procedure :: get_name => modelpar_data_get_name  
  
<Model data: procedures>+≡  
  function modelpar_data_get_name (par) result (name)  
    class(modelpar_data_t), intent(in) :: par  
    type(string_t) :: name  
    name = par%name  
  end function modelpar_data_get_name
```

Return the value. In case of a type mismatch, follow Fortran conventions.

```
<Model data: par data: TBP>+≡  
  procedure, pass :: get_real => modelpar_data_get_real  
  procedure, pass :: get_complex => modelpar_data_get_complex  
  
<Model data: procedures>+≡  
  elemental function modelpar_data_get_real (par) result (value)  
    class(modelpar_data_t), intent(in), target :: par  
    real(default) :: value  
    select type (par)  
      type is (modelpar_real_t)  
        value = par%value  
      type is (modelpar_complex_t)  
        value = par%value  
    end select  
  end function modelpar_data_get_real  
  
  elemental function modelpar_data_get_complex (par) result (value)  
    class(modelpar_data_t), intent(in), target :: par  
    complex(default) :: value  
    select type (par)  
      type is (modelpar_real_t)  
        value = par%value  
      type is (modelpar_complex_t)  
        value = par%value  
    end select  
  end function modelpar_data_get_complex
```

Return a pointer to the value. This makes sense only for matching types.

```
<Model data: par data: TBP>+≡  
  procedure :: get_real_ptr => modelpar_data_get_real_ptr  
  procedure :: get_complex_ptr => modelpar_data_get_complex_ptr  
  
<Model data: procedures>+≡  
  function modelpar_data_get_real_ptr (par) result (ptr)  
    class(modelpar_data_t), intent(in), target :: par  
    real(default), pointer :: ptr  
    select type (par)  
      type is (modelpar_real_t)  
        ptr => par%value  
    class default  
      ptr => null ()
```

```

        end select
    end function modelpar_data_get_real_ptr

function modelpar_data_get_complex_ptr (par) result (ptr)
    class(modelpar_data_t), intent(in), target :: par
    complex(default), pointer :: ptr
    select type (par)
    type is (modelpar_complex_t)
        ptr => par%value
    class default
        ptr => null ()
    end select
end function modelpar_data_get_complex_ptr

```

11.1.2 Field Data

The field-data type holds all information that pertains to a particular field (or particle) within a particular model. Information such as spin type, particle code etc. is stored within the object itself, while mass and width are associated to parameters, otherwise assumed zero.

```

<Model data: public>+≡
    public :: field_data_t

<Model data: types>+≡
    type :: field_data_t
        private
        type(string_t) :: longname
        integer :: pdg = UNDEFINED
        logical :: visible = .true.
        logical :: parton = .false.
        logical :: gauge = .false.
        logical :: left_handed = .false.
        logical :: right_handed = .false.
        logical :: has_anti = .false.
        logical :: p_is_stable = .true.
        logical :: p_decays_isotropically = .false.
        logical :: p_decays_diagonal = .false.
        logical :: p_has_decay_helicity = .false.
        integer :: p_decay_helicity = 0
        logical :: a_is_stable = .true.
        logical :: a_decays_isotropically = .false.
        logical :: a_decays_diagonal = .false.
        logical :: a_has_decay_helicity = .false.
        integer :: a_decay_helicity = 0
        logical :: p_polarized = .false.
        logical :: a_polarized = .false.
        type(string_t), dimension(:), allocatable :: name, anti
        type(string_t) :: tex_name, tex_anti
        integer :: spin_type = UNDEFINED
        integer :: isospin_type = 1
        integer :: charge_type = 1
        integer :: color_type = 1
        real(default), pointer :: mass_val => null ()
    end type

```

```

class(modelpar_data_t), pointer :: mass_data => null ()
real(default), pointer :: width_val => null ()
class(modelpar_data_t), pointer :: width_data => null ()
integer :: multiplicity = 1
type(string_t), dimension(:), allocatable :: p_decay
type(string_t), dimension(:), allocatable :: a_decay
contains
  <Model data: field data: TBP>
end type field_data_t

```

Initialize field data with PDG long name and PDG code. T_EX names should be initialized to avoid issues with accessing unallocated string contents.

```

<Model data: field data: TBP>≡
  procedure :: init => field_data_init

<Model data: procedures>+≡
  subroutine field_data_init (prt, longname, pdg)
    class(field_data_t), intent(out) :: prt
    type(string_t), intent(in) :: longname
    integer, intent(in) :: pdg
    prt%longname = longname
    prt%pdg = pdg
    prt%tex_name = ""
    prt%tex_anti = ""
  end subroutine field_data_init

```

Copy quantum numbers from another particle. Do not compute the multiplicity yet, because this depends on the association of the `mass_data` pointer.

```

<Model data: field data: TBP>+≡
  procedure :: copy_from => field_data_copy_from

<Model data: procedures>+≡
  subroutine field_data_copy_from (prt, prt_src)
    class(field_data_t), intent(inout) :: prt
    class(field_data_t), intent(in) :: prt_src
    prt%visible = prt_src%visible
    prt%parton = prt_src%parton
    prt%gauge = prt_src%gauge
    prt%left_handed = prt_src%left_handed
    prt%right_handed = prt_src%right_handed
    prt%p_is_stable = prt_src%p_is_stable
    prt%p_decays_isotropically = prt_src%p_decays_isotropically
    prt%p_decays_diagonal = prt_src%p_decays_diagonal
    prt%p_has_decay_helicity = prt_src%p_has_decay_helicity
    prt%p_decay_helicity = prt_src%p_decay_helicity
    prt%p_decays_diagonal = prt_src%p_decays_diagonal
    prt%a_is_stable = prt_src%a_is_stable
    prt%a_decays_isotropically = prt_src%a_decays_isotropically
    prt%a_decays_diagonal = prt_src%a_decays_diagonal
    prt%a_has_decay_helicity = prt_src%a_has_decay_helicity
    prt%a_decay_helicity = prt_src%a_decay_helicity
    prt%p_polarized = prt_src%p_polarized
    prt%a_polarized = prt_src%a_polarized
    prt%spin_type = prt_src%spin_type
  end subroutine field_data_copy_from

```

```

prt%isospin_type = prt_src%isospin_type
prt%charge_type = prt_src%charge_type
prt%color_type = prt_src%color_type
prt%has_anti = prt_src%has_anti
if (allocated (prt_src%name)) then
    if (allocated (prt%name)) deallocate (prt%name)
    allocate (prt%name (size (prt_src%name)), source = prt_src%name)
end if
if (allocated (prt_src%anti)) then
    if (allocated (prt%anti)) deallocate (prt%anti)
    allocate (prt%anti (size (prt_src%anti)), source = prt_src%anti)
end if
prt%tex_name = prt_src%tex_name
prt%tex_anti = prt_src%tex_anti
if (allocated (prt_src%p_decay)) then
    if (allocated (prt%p_decay)) deallocate (prt%p_decay)
    allocate (prt%p_decay (size (prt_src%p_decay)), source = prt_src%p_decay)
end if
if (allocated (prt_src%a_decay)) then
    if (allocated (prt%a_decay)) deallocate (prt%a_decay)
    allocate (prt%a_decay (size (prt_src%a_decay)), source = prt_src%a_decay)
end if
end subroutine field_data_copy_from

```

Set particle quantum numbers.

(Model data: field data: TBP)+≡

```

procedure :: set => field_data_set

```

(Model data: procedures)+≡

```

subroutine field_data_set (prt, &
    is_visible, is_parton, is_gauge, is_left_handed, is_right_handed, &
    p_is_stable, p_decays_isotropically, p_decays_diagonal, &
    p_decay_helicity, &
    a_is_stable, a_decays_isotropically, a_decays_diagonal, &
    a_decay_helicity, &
    p_polarized, a_polarized, &
    name, anti, tex_name, tex_anti, &
    spin_type, isospin_type, charge_type, color_type, &
    mass_data, width_data, &
    p_decay, a_decay)
class(field_data_t), intent(inout) :: prt
logical, intent(in), optional :: is_visible, is_parton, is_gauge
logical, intent(in), optional :: is_left_handed, is_right_handed
logical, intent(in), optional :: p_is_stable
logical, intent(in), optional :: p_decays_isotropically, p_decays_diagonal
integer, intent(in), optional :: p_decay_helicity
logical, intent(in), optional :: a_is_stable
logical, intent(in), optional :: a_decays_isotropically, a_decays_diagonal
integer, intent(in), optional :: a_decay_helicity
logical, intent(in), optional :: p_polarized, a_polarized
type(string_t), dimension(:), intent(in), optional :: name, anti
type(string_t), intent(in), optional :: tex_name, tex_anti
integer, intent(in), optional :: spin_type, isospin_type
integer, intent(in), optional :: charge_type, color_type

```



```

class(modelpar_data_t), intent(in), pointer, optional :: mass_data, width_data
type(string_t), dimension(:), intent(in), optional :: p_decay, a_decay
if (present (is_visible)) prt%visible = is_visible
if (present (is_parton)) prt%parton = is_parton
if (present (is_gauge)) prt%gauge = is_gauge
if (present (is_left_handed)) prt%left_handed = is_left_handed
if (present (is_right_handed)) prt%right_handed = is_right_handed
if (present (p_is_stable)) prt%p_is_stable = p_is_stable
if (present (p_decays_isotropically)) &
    prt%p_decays_isotropically = p_decays_isotropically
if (present (p_decays_diagonal)) &
    prt%p_decays_diagonal = p_decays_diagonal
if (present (p_decay_helicity)) then
    prt%p_has_decay_helicity = .true.
    prt%p_decay_helicity = p_decay_helicity
end if
if (present (a_is_stable)) prt%a_is_stable = a_is_stable
if (present (a_decays_isotropically)) &
    prt%a_decays_isotropically = a_decays_isotropically
if (present (a_decays_diagonal)) &
    prt%a_decays_diagonal = a_decays_diagonal
if (present (a_decay_helicity)) then
    prt%a_has_decay_helicity = .true.
    prt%a_decay_helicity = a_decay_helicity
end if
if (present (p_polarized)) prt%p_polarized = p_polarized
if (present (a_polarized)) prt%a_polarized = a_polarized
if (present (name)) then
    if (allocated (prt%name)) deallocate (prt%name)
    allocate (prt%name (size (name)), source = name)
end if
if (present (anti)) then
    if (allocated (prt%anti)) deallocate (prt%anti)
    allocate (prt%anti (size (anti)), source = anti)
    prt%has_anti = .true.
end if
if (present (tex_name)) prt%tex_name = tex_name
if (present (tex_anti)) prt%tex_anti = tex_anti
if (present (spin_type)) prt%spin_type = spin_type
if (present (isospin_type)) prt%isospin_type = isospin_type
if (present (charge_type)) prt%charge_type = charge_type
if (present (color_type)) prt%color_type = color_type
if (present (mass_data)) then
    prt%mass_data => mass_data
    if (associated (mass_data)) then
        prt%mass_val => mass_data%get_real_ptr ()
    else
        prt%mass_val => null ()
    end if
end if
if (present (width_data)) then
    prt%width_data => width_data
    if (associated (width_data)) then
        prt%width_val => width_data%get_real_ptr ()
    end if
end if

```

```

        else
            prt%width_val => null ()
        end if
    end if
end if
if (present (spin_type) .or. present (mass_data)) then
    call prt%set_multiplicity ()
end if
if (present (p_decay)) then
    if (allocated (prt%p_decay)) deallocate (prt%p_decay)
    if (size (p_decay) > 0) &
        allocate (prt%p_decay (size (p_decay)), source = p_decay)
end if
if (present (a_decay)) then
    if (allocated (prt%a_decay)) deallocate (prt%a_decay)
    if (size (a_decay) > 0) &
        allocate (prt%a_decay (size (a_decay)), source = a_decay)
end if
end subroutine field_data_set

```

Calculate the multiplicity given spin type and mass.

```

<Model data: field data: TBP>+≡
    procedure, private :: &
        set_multiplicity => field_data_set_multiplicity
<Model data: procedures>+≡
    subroutine field_data_set_multiplicity (prt)
        class(field_data_t), intent(inout) :: prt
        if (prt%spin_type /= SCALAR) then
            if (associated (prt%mass_data)) then
                prt%multiplicity = prt%spin_type
            else if (prt%left_handed .or. prt%right_handed) then
                prt%multiplicity = 1
            else
                prt%multiplicity = 2
            end if
        end if
    end if
end subroutine field_data_set_multiplicity

```

Set the mass/width value (not the pointer). The mass/width pointer must be allocated.

```

<Model data: field data: TBP>+≡
    procedure, private :: set_mass => field_data_set_mass
    procedure, private :: set_width => field_data_set_width
<Model data: procedures>+≡
    subroutine field_data_set_mass (prt, mass)
        class(field_data_t), intent(inout) :: prt
        real(default), intent(in) :: mass
        if (associated (prt%mass_val)) prt%mass_val = mass
    end subroutine field_data_set_mass

    subroutine field_data_set_width (prt, width)
        class(field_data_t), intent(inout) :: prt
        real(default), intent(in) :: width
    end subroutine field_data_set_width

```

```

        if (associated (prt%width_val)) prt%width_val = width
    end subroutine field_data_set_width

```

Loose ends: name arrays should be allocated.

<Model data: field data: TBP>+≡

```

    procedure :: freeze => field_data_freeze

```

<Model data: procedures>+≡

```

    elemental subroutine field_data_freeze (prt)
        class(field_data_t), intent(inout) :: prt
        if (.not. associated (prt%name)) allocate (prt%name (0))
        if (.not. associated (prt%anti)) allocate (prt%anti (0))
    end subroutine field_data_freeze

```

Output

<Model data: field data: TBP>+≡

```

    procedure :: write => field_data_write

```

<Model data: procedures>+≡

```

    subroutine field_data_write (prt, unit)
        class(field_data_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(3x,A,1x,A)", advance="no") "particle", char (prt%longname)
        write (u, "(1x,I0)", advance="no") prt%pdg
        if (.not. prt%visible) write (u, "(2x,A)", advance="no") "invisible"
        if (prt%parton) write (u, "(2x,A)", advance="no") "parton"
        if (prt%gauge) write (u, "(2x,A)", advance="no") "gauge"
        if (prt%left_handed) write (u, "(2x,A)", advance="no") "left"
        if (prt%right_handed) write (u, "(2x,A)", advance="no") "right"
        write (u, *)
        write (u, "(5x,A)", advance="no") "name"
        if (associated (prt%name)) then
            do i = 1, size (prt%name)
                write (u, "(1x,A)", advance="no") ' ' // char (prt%name(i)) // ' '
            end do
        end if
        write (u, *)
        if (prt%has_anti) then
            write (u, "(5x,A)", advance="no") "anti"
            do i = 1, size (prt%anti)
                write (u, "(1x,A)", advance="no") ' ' // char (prt%anti(i)) // ' '
            end do
        end if
        write (u, *)
        if (prt%tex_name /= "") then
            write (u, "(5x,A)") &
                "tex_name " // ' ' // char (prt%tex_name) // ' '
        end if
        if (prt%has_anti .and. prt%tex_anti /= "") then
            write (u, "(5x,A)") &
                "tex_anti " // ' ' // char (prt%tex_anti) // ' '
        end if
    else

```

```

        write (u, "(A)") "???"
    end if
    write (u, "(5x,A)", advance="no") "spin "
    select case (mod (prt%spin_type - 1, 2))
    case (0); write (u, "(I0)", advance="no") (prt%spin_type-1) / 2
    case default; write (u, "(I0,A)", advance="no") prt%spin_type-1, "/2"
    end select
    ! write (u, "(2x,A,I1,A)") "! [multiplicity = ", prt%multiplicity, "]"
    if (abs (prt%isospin_type) /= 1) then
        write (u, "(2x,A)", advance="no") "isospin "
        select case (mod (abs (prt%isospin_type) - 1, 2))
        case (0); write (u, "(I0)", advance="no") &
            sign (abs (prt%isospin_type) - 1, prt%isospin_type) / 2
        case default; write (u, "(I0,A)", advance="no") &
            sign (abs (prt%isospin_type) - 1, prt%isospin_type), "/2"
        end select
    end if
    if (abs (prt%charge_type) /= 1) then
        write (u, "(2x,A)", advance="no") "charge "
        select case (mod (abs (prt%charge_type) - 1, 3))
        case (0); write (u, "(I0)", advance="no") &
            sign (abs (prt%charge_type) - 1, prt%charge_type) / 3
        case default; write (u, "(I0,A)", advance="no") &
            sign (abs (prt%charge_type) - 1, prt%charge_type), "/3"
        end select
    end if
    if (prt%color_type /= 1) then
        write (u, "(2x,A,I0)", advance="no") "color ", prt%color_type
    end if
    write (u, *)
    if (associated (prt%mass_data)) then
        write (u, "(5x,A)", advance="no") &
            "mass " // char (prt%mass_data%get_name ())
        if (associated (prt%width_data)) then
            write (u, "(2x,A)") &
                "width " // char (prt%width_data%get_name ())
        else
            write (u, *)
        end if
    end if
    call prt%write_decays (u)
end subroutine field_data_write

```

Write decay and polarization data.

```

<Model data: field data: TBP>+≡
    procedure :: write_decays => field_data_write_decays

<Model data: procedures>+≡
    subroutine field_data_write_decays (prt, unit)
        class(field_data_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        if (.not. prt%p_is_stable) then

```

```

    if (allocated (prt%p_decay)) then
      write (u, "(5x,A)", advance="no") "p_decay"
      do i = 1, size (prt%p_decay)
        write (u, "(1x,A)", advance="no") char (prt%p_decay(i))
      end do
      if (prt%p_decays_isotropically) then
        write (u, "(1x,A)", advance="no") "isotropic"
      else if (prt%p_decays_diagonal) then
        write (u, "(1x,A)", advance="no") "diagonal"
      else if (prt%p_has_decay_helicity) then
        write (u, "(1x,A,I0)", advance="no") "helicity = ", &
          prt%p_decay_helicity
      end if
      write (u, *)
    end if
  else if (prt%p_polarized) then
    write (u, "(5x,A)") "p_polarized"
  end if
  if (.not. prt%a_is_stable) then
    if (allocated (prt%a_decay)) then
      write (u, "(5x,A)", advance="no") "a_decay"
      do i = 1, size (prt%a_decay)
        write (u, "(1x,A)", advance="no") char (prt%a_decay(i))
      end do
      if (prt%a_decays_isotropically) then
        write (u, "(1x,A)", advance="no") "isotropic"
      else if (prt%a_decays_diagonal) then
        write (u, "(1x,A)", advance="no") "diagonal"
      else if (prt%a_has_decay_helicity) then
        write (u, "(1x,A,I0)", advance="no") "helicity = ", &
          prt%a_decay_helicity
      end if
      write (u, *)
    end if
  else if (prt%a_polarized) then
    write (u, "(5x,A)") "a_polarized"
  end if
end subroutine field_data_write_decays

```

Screen version of output.

```

<Model data: field data: TBP>+≡
  procedure :: show => field_data_show

<Model data: procedures>+≡
  subroutine field_data_show (prt, l, u)
    class(field_data_t), intent(in) :: prt
    integer, intent(in) :: l, u
    character(len=1) :: buffer
    integer :: i
    type(string_t), dimension(:), allocatable :: decay
    buffer = prt%get_name (.false.)
    write (u, "(4x,A,1x,I8)", advance="no") buffer, &
      prt%get_pdg ()
    if (prt%is_polarized ()) then

```

```

        write (u, "(3x,A)" "polarized"
    else if (.not. prt%is_stable ()) then
        write (u, "(3x,A)", advance="no") "decays:"
        call prt%get_decays (decay)
        do i = 1, size (decay)
            write (u, "(1x,A)", advance="no") char (decay(i))
        end do
        write (u, *)
    else
        write (u, *)
    end if
    if (prt%has_antiparticle ()) then
        buffer = prt%get_name (.true.)
        write (u, "(4x,A,1x,I8)", advance="no") buffer, &
            prt%get_pdg_anti ()
        if (prt%is_polarized (.true.)) then
            write (u, "(3x,A)" "polarized"
        else if (.not. prt%is_stable (.true.)) then
            write (u, "(3x,A)", advance="no") "decays:"
            call prt%get_decays (decay, .true.)
            do i = 1, size (decay)
                write (u, "(1x,A)", advance="no") char (decay(i))
            end do
            write (u, *)
        else
            write (u, *)
        end if
    end if
end if
end subroutine field_data_show

```

Retrieve data:

```

<Model data: field data: TBP>+≡
    procedure :: get_pdg => field_data_get_pdg
    procedure :: get_pdg_anti => field_data_get_pdg_anti

<Model data: procedures>+≡
    elemental function field_data_get_pdg (prt) result (pdg)
        integer :: pdg
        class(field_data_t), intent(in) :: prt
        pdg = prt%pdg
    end function field_data_get_pdg

    elemental function field_data_get_pdg_anti (prt) result (pdg)
        integer :: pdg
        class(field_data_t), intent(in) :: prt
        if (prt%has_anti) then
            pdg = - prt%pdg
        else
            pdg = prt%pdg
        end if
    end function field_data_get_pdg_anti

```

Predicates:

```

<Model data: field data: TBP>+≡

```

```

procedure :: is_visible => field_data_is_visible
procedure :: is_parton => field_data_is_parton
procedure :: is_gauge => field_data_is_gauge
procedure :: is_left_handed => field_data_is_left_handed
procedure :: is_right_handed => field_data_is_right_handed
procedure :: has_antiparticle => field_data_has_antiparticle
procedure :: is_stable => field_data_is_stable
procedure :: get_decays => field_data_get_decays
procedure :: decays_isotropically => field_data_decays_isotropically
procedure :: decays_diagonal => field_data_decays_diagonal
procedure :: has_decay_helicity => field_data_has_decay_helicity
procedure :: decay_helicity => field_data_decay_helicity
procedure :: is_polarized => field_data_is_polarized

(Model data: procedures)+≡
  elemental function field_data_is_visible (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    flag = prt%visible
  end function field_data_is_visible

  elemental function field_data_is_parton (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    flag = prt%parton
  end function field_data_is_parton

  elemental function field_data_is_gauge (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    flag = prt%gauge
  end function field_data_is_gauge

  elemental function field_data_is_left_handed (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    flag = prt%left_handed
  end function field_data_is_left_handed

  elemental function field_data_is_right_handed (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    flag = prt%right_handed
  end function field_data_is_right_handed

  elemental function field_data_has_antiparticle (prt) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    flag = prt%has_anti
  end function field_data_has_antiparticle

  elemental function field_data_is_stable (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti

```

```

if (present (anti)) then
  if (anti) then
    flag = prt%a_is_stable
  else
    flag = prt%p_is_stable
  end if
else
  flag = prt%p_is_stable
end if
end function field_data_is_stable

subroutine field_data_get_decays (prt, decay, anti)
  class(field_data_t), intent(in) :: prt
  type(string_t), dimension(:), intent(out), allocatable :: decay
  logical, intent(in), optional :: anti
  if (present (anti)) then
    if (anti) then
      allocate (decay (size (prt%a_decay)), source = prt%a_decay)
    else
      allocate (decay (size (prt%p_decay)), source = prt%p_decay)
    end if
  else
    allocate (decay (size (prt%p_decay)), source = prt%p_decay)
  end if
end subroutine field_data_get_decays

elemental function field_data_decays_isotropically &
  (prt, anti) result (flag)
  logical :: flag
  class(field_data_t), intent(in) :: prt
  logical, intent(in), optional :: anti
  if (present (anti)) then
    if (anti) then
      flag = prt%a_decays_isotropically
    else
      flag = prt%p_decays_isotropically
    end if
  else
    flag = prt%p_decays_isotropically
  end if
end function field_data_decays_isotropically

elemental function field_data_decays_diagonal &
  (prt, anti) result (flag)
  logical :: flag
  class(field_data_t), intent(in) :: prt
  logical, intent(in), optional :: anti
  if (present (anti)) then
    if (anti) then
      flag = prt%a_decays_diagonal
    else
      flag = prt%p_decays_diagonal
    end if
  else

```



```

        flag = prt%p_decays_diagonal
    end if
end function field_data_decays_diagonal

elemental function field_data_has_decay_helicity &
    (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    if (present (anti)) then
        if (anti) then
            flag = prt%a_has_decay_helicity
        else
            flag = prt%p_has_decay_helicity
        end if
    else
        flag = prt%p_has_decay_helicity
    end if
end function field_data_has_decay_helicity

elemental function field_data_decay_helicity &
    (prt, anti) result (hel)
    integer :: hel
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    if (present (anti)) then
        if (anti) then
            hel = prt%a_decay_helicity
        else
            hel = prt%p_decay_helicity
        end if
    else
        hel = prt%p_decay_helicity
    end if
end function field_data_decay_helicity

elemental function field_data_is_polarized (prt, anti) result (flag)
    logical :: flag
    class(field_data_t), intent(in) :: prt
    logical, intent(in), optional :: anti
    logical :: a
    if (present (anti)) then
        a = anti
    else
        a = .false.
    end if
    if (a) then
        flag = prt%a_polarized
    else
        flag = prt%p_polarized
    end if
end function field_data_is_polarized

```

Names. Return the first name in the list (or the first antiparticle name)

```

<Model data: field data: TBP>+≡
  procedure :: get_longname => field_data_get_longname
  procedure :: get_name => field_data_get_name
  procedure :: get_name_array => field_data_get_name_array

<Model data: procedures>+≡
  pure function field_data_get_longname (prt) result (name)
    type(string_t) :: name
    class(field_data_t), intent(in) :: prt
    name = prt%longname
  end function field_data_get_longname

  pure function field_data_get_name (prt, is_antiparticle) result (name)
    type(string_t) :: name
    class(field_data_t), intent(in) :: prt
    logical, intent(in) :: is_antiparticle
    name = prt%longname
    if (is_antiparticle) then
      if (prt%has_anti) then
        if (allocated (prt%anti)) then
          if (size(prt%anti) > 0) name = prt%anti(1)
        end if
      else
        if (allocated (prt%name)) then
          if (size (prt%name) > 0) name = prt%name(1)
        end if
      end if
    else
      if (allocated (prt%name)) then
        if (size (prt%name) > 0) name = prt%name(1)
      end if
    end if
  end function field_data_get_name

  subroutine field_data_get_name_array (prt, is_antiparticle, name)
    class(field_data_t), intent(in) :: prt
    logical, intent(in) :: is_antiparticle
    type(string_t), dimension(:), allocatable, intent(inout) :: name
    if (allocated (name)) deallocate (name)
    if (is_antiparticle) then
      if (prt%has_anti) then
        allocate (name (size (prt%anti)))
        name = prt%anti
      else
        allocate (name (0))
      end if
    else
      allocate (name (size (prt%name)))
      name = prt%name
    end if
  end subroutine field_data_get_name_array

```

Same for the \TeX name.

```

<Model data: field data: TBP>+≡

```

```

procedure :: get_tex_name => field_data_get_tex_name
<Model data: procedures>+≡
  elemental function field_data_get_tex_name &
    (prt, is_antiparticle) result (name)
    type(string_t) :: name
    class(field_data_t), intent(in) :: prt
    logical, intent(in) :: is_antiparticle
    if (is_antiparticle) then
      if (prt%has_anti) then
        name = prt%tex_anti
      else
        name = prt%tex_name
      end if
    else
      name = prt%tex_name
    end if
    if (name == "") name = prt%get_name (is_antiparticle)
  end function field_data_get_tex_name

```

Check if any of the field names matches the given string.

```

<Model data: field data: TBP>+≡
  procedure, private :: matches_name => field_data_matches_name
<Model data: procedures>+≡
  function field_data_matches_name (field, name, is_antiparticle) result (flag)
    class(field_data_t), intent(in) :: field
    type(string_t), intent(in) :: name
    logical, intent(in) :: is_antiparticle
    logical :: flag
    if (is_antiparticle) then
      if (field%has_anti) then
        flag = any (name == field%anti)
      else
        flag = .false.
      end if
    else
      flag = name == field%longname .or. any (name == field%name)
    end if
  end function field_data_matches_name

```

Quantum numbers

```

<Model data: field data: TBP>+≡
  procedure :: get_spin_type => field_data_get_spin_type
  procedure :: get_multiplicity => field_data_get_multiplicity
  procedure :: get_isospin_type => field_data_get_isospin_type
  procedure :: get_charge_type => field_data_get_charge_type
  procedure :: get_color_type => field_data_get_color_type
<Model data: procedures>+≡
  elemental function field_data_get_spin_type (prt) result (type)
    integer :: type
    class(field_data_t), intent(in) :: prt
    type = prt%spin_type

```

```

end function field_data_get_spin_type

elemental function field_data_get_multiplicity (prt) result (type)
  integer :: type
  class(field_data_t), intent(in) :: prt
  type = prt%multiplicity
end function field_data_get_multiplicity

elemental function field_data_get_isospin_type (prt) result (type)
  integer :: type
  class(field_data_t), intent(in) :: prt
  type = prt%isospin_type
end function field_data_get_isospin_type

elemental function field_data_get_charge_type (prt) result (type)
  integer :: type
  class(field_data_t), intent(in) :: prt
  type = prt%charge_type
end function field_data_get_charge_type

elemental function field_data_get_color_type (prt) result (type)
  integer :: type
  class(field_data_t), intent(in) :: prt
  type = prt%color_type
end function field_data_get_color_type

```

In the MSSM, neutralinos can have a negative mass. This is relevant for computing matrix elements. However, within the WHIZARD main program we are interested only in kinematics, therefore we return the absolute value of the particle mass. If desired, we can extract the sign separately.

```

<Model data: field data: TBP>+=
  procedure :: get_charge => field_data_get_charge
  procedure :: get_isospin => field_data_get_isospin
  procedure :: get_mass => field_data_get_mass
  procedure :: get_mass_sign => field_data_get_mass_sign
  procedure :: get_width => field_data_get_width

<Model data: procedures>+=
  elemental function field_data_get_charge (prt) result (charge)
    real(default) :: charge
    class(field_data_t), intent(in) :: prt
    if (prt%charge_type /= 0) then
      charge = real (sign ((abs(prt%charge_type) - 1), &
        prt%charge_type), default) / 3
    else
      charge = 0
    end if
  end function field_data_get_charge

  elemental function field_data_get_isospin (prt) result (isospin)
    real(default) :: isospin
    class(field_data_t), intent(in) :: prt
    if (prt%isospin_type /= 0) then
      isospin = real (sign (abs(prt%isospin_type) - 1, &

```

```

        prt%isospin_type), default) / 2
    else
        isospin = 0
    end if
end function field_data_get_isospin

elemental function field_data_get_mass (prt) result (mass)
    real(default) :: mass
    class(field_data_t), intent(in) :: prt
    if (associated (prt%mass_val)) then
        mass = abs (prt%mass_val)
    else
        mass = 0
    end if
end function field_data_get_mass

elemental function field_data_get_mass_sign (prt) result (sgn)
    integer :: sgn
    class(field_data_t), intent(in) :: prt
    if (associated (prt%mass_val)) then
        sgn = sign (1._default, prt%mass_val)
    else
        sgn = 0
    end if
end function field_data_get_mass_sign

elemental function field_data_get_width (prt) result (width)
    real(default) :: width
    class(field_data_t), intent(in) :: prt
    if (associated (prt%width_val)) then
        width = prt%width_val
    else
        width = 0
    end if
end function field_data_get_width

```

Find the model containing the PDG given two model files.

```

<Model data: public>+≡
    public :: find_model

<Model data: procedures>+≡
    subroutine find_model (model, PDG, model_A, model_B)
        class(model_data_t), pointer, intent(out) :: model
        integer, intent(in) :: PDG
        class(model_data_t), intent(in), target :: model_A, model_B
        character(len=10) :: buffer
        if (model_A%test_field (PDG)) then
            model => model_A
        else if (model_B%test_field (PDG)) then
            model => model_B
        else
            call model_A%write ()
            call model_B%write ()
            write (buffer, "(I10)") PDG

```

```

        call msg_fatal ("Parton " // buffer // &
            " not found in the given model files")
    end if
end subroutine find_model

```

11.1.3 Vertex data

The vertex object contains an array of particle-data pointers, for which we need a separate type. (We could use the flavor type defined in another module.)

The program does not (yet?) make use of vertex definitions, so they are not stored here.

```

<Model data: types>+≡
    type :: field_data_p
        type(field_data_t), pointer :: p => null ()
    end type field_data_p

<Model data: types>+≡
    type :: vertex_t
        private
        logical :: trilinear
        integer, dimension(:), allocatable :: pdg
        type(field_data_p), dimension(:), allocatable :: prt
        contains
        <Model data: vertex: TBP>
    end type vertex_t

<Model data: vertex: TBP>≡
    procedure :: write => vertex_write

<Model data: procedures>+≡
    subroutine vertex_write (vtx, unit)
        class(vertex_t), intent(in) :: vtx
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(3x,A)", advance="no") "vertex"
        do i = 1, size (vtx%prt)
            if (associated (vtx%prt(i)%p)) then
                write (u, "(1x,A)", advance="no") &
                    ''' // char (vtx%prt(i)%p%get_name (vtx%pdg(i) < 0)) &
                    // '''
            else
                write (u, "(1x,I7)", advance="no") vtx%pdg(i)
            end if
        end do
        write (u, *)
    end subroutine vertex_write

```

Initialize using PDG codes. The model is used for finding particle data pointers associated with the pdg codes.

```

<Model data: vertex: TBP>+≡
    procedure :: init => vertex_init

```

```

<Model data: procedures>+≡
subroutine vertex_init (vtx, pdg, model)
  class(vertex_t), intent(out) :: vtx
  integer, dimension(:), intent(in) :: pdg
  type(model_data_t), intent(in), target, optional :: model
  integer :: i
  allocate (vtx%pdg (size (pdg)))
  allocate (vtx%prt (size (pdg)))
  vtx%trilinear = size (pdg) == 3
  vtx%pdg = pdg
  if (present (model)) then
    do i = 1, size (pdg)
      vtx%prt(i)%p => model%get_field_ptr (pdg(i))
    end do
  end if
end subroutine vertex_init

```

Copy vertex: we must reassign the field-data pointer to a new model.

```

<Model data: vertex: TBP>+≡
procedure :: copy_from => vertex_copy_from

<Model data: procedures>+≡
subroutine vertex_copy_from (vtx, old_vtx, new_model)
  class(vertex_t), intent(out) :: vtx
  class(vertex_t), intent(in) :: old_vtx
  type(model_data_t), intent(in), target, optional :: new_model
  call vtx%init (old_vtx%pdg, new_model)
end subroutine vertex_copy_from

```

Single-particle lookup: Given a particle code, we return matching codes if present, otherwise zero. Actually, we return the antiparticles of the matching codes, as appropriate for computing splittings.

```

<Model data: vertex: TBP>+≡
procedure :: get_match => vertex_get_match

<Model data: procedures>+≡
subroutine vertex_get_match (vtx, pdg1, pdg2)
  class(vertex_t), intent(in) :: vtx
  integer, intent(in) :: pdg1
  integer, dimension(:), allocatable, intent(out) :: pdg2
  integer :: i, j
  do i = 1, size (vtx%pdg)
    if (vtx%pdg(i) == pdg1) then
      allocate (pdg2 (size (vtx%pdg) - 1))
      do j = 1, i-1
        pdg2(j) = anti (j)
      end do
      do j = i, size (pdg2)
        pdg2(j) = anti (j+1)
      end do
      exit
    end if
  end do
contains

```

```

function anti (i) result (pdg)
  integer, intent(in) :: i
  integer :: pdg
  if (vtx%prt(i)%p%has_antiparticle ()) then
    pdg = - vtx%pdg(i)
  else
    pdg = vtx%pdg(i)
  end if
end function anti
end subroutine vertex_get_match

```

To access this from the outside, we create an iterator. The iterator has the sole purpose of returning the matching particles for a given array of PDG codes.

```

<Model data: public>+≡
  public :: vertex_iterator_t

<Model data: types>+≡
  type :: vertex_iterator_t
  private
  class(model_data_t), pointer :: model => null ()
  integer, dimension(:), allocatable :: pdg
  integer :: vertex_index = 0
  integer :: pdg_index = 0
  logical :: save_pdg_index
  contains
  procedure :: init => vertex_iterator_init
  procedure :: get_next_match => vertex_iterator_get_next_match
end type vertex_iterator_t

```

We initialize the iterator for a particular model with the pdg index of the particle we are looking at.

```

<Model data: procedures>+≡
  subroutine vertex_iterator_init (it, model, pdg, save_pdg_index)
    class(vertex_iterator_t), intent(out) :: it
    class(model_data_t), intent(in), target :: model
    integer, dimension(:), intent(in) :: pdg
    logical, intent(in) :: save_pdg_index
    it%model => model
    allocate (it%pdg (size (pdg)), source = pdg)
    it%save_pdg_index = save_pdg_index
  end subroutine vertex_iterator_init

  subroutine vertex_iterator_get_next_match (it, pdg_match)
    class(vertex_iterator_t), intent(inout) :: it
    integer, dimension(:), allocatable, intent(out) :: pdg_match
    integer :: i, j
    do i = it%vertex_index + 1, size (it%model%vtx)
      do j = it%pdg_index + 1, size (it%pdg)
        call it%model%vtx(i)%get_match (it%pdg(j), pdg_match)
        if (it%save_pdg_index) then
          if (allocated (pdg_match) .and. j < size (it%pdg)) then
            it%pdg_index = j
            return
          end if
        end if
      end do
    end do
  end subroutine vertex_iterator_get_next_match

```



```

        else if (allocated (pdg_match) .and. j == size (it%pdg)) then
            it%vertex_index = i
            it%pdg_index = 0
            return
        end if
    else if (allocated (pdg_match)) then
        it%vertex_index = i
        return
    end if
end do
end do
it%vertex_index = 0
it%pdg_index = 0
end subroutine vertex_iterator_get_next_match

```

11.1.4 Vertex lookup table

The vertex lookup table is a hash table: given two particle codes, we check which codes are allowed for the third one.

The size of the hash table should be large enough that collisions are rare. We first select a size based on the number of vertices (multiplied by six because all permutations count), with some margin, and then choose the smallest integer power of two larger than this.

```

<Model data: parameters>≡
    integer, parameter :: VERTEX_TABLE_SCALE_FACTOR = 60

<Model data: procedures>+≡
    function vertex_table_size (n_vtx) result (n)
        integer(i32) :: n
        integer, intent(in) :: n_vtx
        integer :: i, s
        s = VERTEX_TABLE_SCALE_FACTOR * n_vtx
        n = 1
        do i = 1, 31
            n = ishft (n, 1)
            s = ishft (s,-1)
            if (s == 0) exit
        end do
    end function vertex_table_size

```

The specific hash function takes two particle codes (arbitrary integers) and returns a 32-bit integer. It makes use of the universal function `hash` which operates on a byte array.

```

<Model data: procedures>+≡
    function hash2 (pdg1, pdg2)
        integer(i32) :: hash2
        integer, intent(in) :: pdg1, pdg2
        integer(i8), dimension(1) :: mold
        hash2 = hash (transfer ([pdg1, pdg2], mold))
    end function hash2

```

Each entry in the vertex table stores the two particle codes and an array of possibilities for the third code.

```

<Model data: types>+≡
  type :: vertex_table_entry_t
  private
    integer :: pdg1 = 0, pdg2 = 0
    integer :: n = 0
    integer, dimension(:), allocatable :: pdg3
  end type vertex_table_entry_t

```

The vertex table:

```

<Model data: types>+≡
  type :: vertex_table_t
    type(vertex_table_entry_t), dimension(:), allocatable :: entry
    integer :: n_collisions = 0
    integer(i32) :: mask
  contains
    <Model data: vertex table: TBP>
  end type vertex_table_t

```

Output.

```

<Model data: vertex table: TBP>≡
  procedure :: write => vertex_table_write

<Model data: procedures>+≡
  subroutine vertex_table_write (vt, unit)
    class(vertex_table_t), intent(in) :: vt
    integer, intent(in), optional :: unit
    integer :: u, i
    character(9) :: size_pdg3
    u = given_output_unit (unit)
    write (u, "(A)") "vertex hash table:"
    write (u, "(A,I7)") " size = ", size (vt%entry)
    write (u, "(A,I7)") " used = ", count (vt%entry%n /= 0)
    write (u, "(A,I7)") " coll = ", vt%n_collisions
    do i = lbound (vt%entry, 1), ubound (vt%entry, 1)
      if (vt%entry(i)%n /= 0) then
        write (size_pdg3, "(I7)") size (vt%entry(i)%pdg3)
        write (u, "(A,1x,I7,1x,A,2(1x,I7),A," // &
              size_pdg3 // "(1x,I7))") &
              " ", i, ":", vt%entry(i)%pdg1, &
              vt%entry(i)%pdg2, "->", vt%entry(i)%pdg3
      end if
    end do
  end subroutine vertex_table_write

```

Initializing the vertex table: This is done in two passes. First, we scan all permutations for all vertices and count the number of entries in each bucket of the hashtable. Then, the buckets are allocated accordingly and filled.

Collision resolution is done by just incrementing the hash value until an empty bucket is found. The vertex table size is fixed, since we know from the beginning the number of entries.

```

<Model data: vertex table: TBP>+≡

```

```

procedure :: init => vertex_table_init

<Model data: procedures>+≡
subroutine vertex_table_init (vt, prt, vtx)
  class(vertex_table_t), intent(out) :: vt
  type(field_data_t), dimension(:), intent(in) :: prt
  type(vertex_t), dimension(:), intent(in) :: vtx
  integer :: n_vtx, vt_size, i, p1, p2, p3
  integer, dimension(3) :: p
  n_vtx = size (vtx)
  vt_size = vertex_table_size (count (vtx%trilinear))
  vt%mask = vt_size - 1
  allocate (vt%entry (0:vt_size-1))
  do i = 1, n_vtx
    if (vtx(i)%trilinear) then
      p = vtx(i)%pdg
      p1 = p(1); p2 = p(2)
      call create (hash2 (p1, p2))
      if (p(2) /= p(3)) then
        p2 = p(3)
        call create (hash2 (p1, p2))
      end if
      if (p(1) /= p(2)) then
        p1 = p(2); p2 = p(1)
        call create (hash2 (p1, p2))
        if (p(1) /= p(3)) then
          p2 = p(3)
          call create (hash2 (p1, p2))
        end if
      end if
      if (p(1) /= p(3)) then
        p1 = p(3); p2 = p(1)
        call create (hash2 (p1, p2))
        if (p(1) /= p(2)) then
          p2 = p(2)
          call create (hash2 (p1, p2))
        end if
      end if
    end if
  end do
  do i = 0, vt_size - 1
    allocate (vt%entry(i)%pdg3 (vt%entry(i)%n))
  end do
  vt%entry%n = 0
  do i = 1, n_vtx
    if (vtx(i)%trilinear) then
      p = vtx(i)%pdg
      p1 = p(1); p2 = p(2); p3 = p(3)
      call register (hash2 (p1, p2))
      if (p(2) /= p(3)) then
        p2 = p(3); p3 = p(2)
        call register (hash2 (p1, p2))
      end if
      if (p(1) /= p(2)) then
        p1 = p(2); p2 = p(1); p3 = p(3)

```

```

        call register (hash2 (p1, p2))
        if (p(1) /= p(3)) then
            p2 = p(3); p3 = p(1)
            call register (hash2 (p1, p2))
        end if
    end if
    if (p(1) /= p(3)) then
        p1 = p(3); p2 = p(1); p3 = p(2)
        call register (hash2 (p1, p2))
        if (p(1) /= p(2)) then
            p2 = p(2); p3 = p(1)
            call register (hash2 (p1, p2))
        end if
    end if
end if
end do
contains
recursive subroutine create (hashval)
    integer(i32), intent(in) :: hashval
    integer :: h
    h = iand (hashval, vt%mask)
    if (vt%entry(h)%n == 0) then
        vt%entry(h)%pdg1 = p1
        vt%entry(h)%pdg2 = p2
        vt%entry(h)%n = 1
    else if (vt%entry(h)%pdg1 == p1 .and. vt%entry(h)%pdg2 == p2) then
        vt%entry(h)%n = vt%entry(h)%n + 1
    else
        vt%n_collisions = vt%n_collisions + 1
        call create (hashval + 1)
    end if
end subroutine create
recursive subroutine register (hashval)
    integer(i32), intent(in) :: hashval
    integer :: h
    h = iand (hashval, vt%mask)
    if (vt%entry(h)%pdg1 == p1 .and. vt%entry(h)%pdg2 == p2) then
        vt%entry(h)%n = vt%entry(h)%n + 1
        vt%entry(h)%pdg3(vt%entry(h)%n) = p3
    else
        call register(hashval + 1)
    end if
end subroutine register
end subroutine vertex_table_init

```

Return the array of particle codes that match the given pair.

<Model data: vertex table: TBP>+≡

```
procedure :: match => vertex_table_match
```

<Model data: procedures>+≡

```

subroutine vertex_table_match (vt, pdg1, pdg2, pdg3)
    class(vertex_table_t), intent(in) :: vt
    integer, intent(in) :: pdg1, pdg2
    integer, dimension(:), allocatable, intent(out) :: pdg3

```

```

    call match (hash2 (pdg1, pdg2))
contains
    recursive subroutine match (hashval)
        integer(i32), intent(in) :: hashval
        integer :: h
        h = iand (hashval, vt%mask)
        if (vt%entry(h)%n == 0) then
            allocate (pdg3 (0))
        else if (vt%entry(h)%pdg1 == pdg1 .and. vt%entry(h)%pdg2 == pdg2) then
            allocate (pdg3 (size (vt%entry(h)%pdg3)))
            pdg3 = vt%entry(h)%pdg3
        else
            call match (hashval + 1)
        end if
    end subroutine match
end subroutine vertex_table_match

```

Return true if the triplet is represented as a vertex.

```

<Model data: vertex table: TBP>+≡
    procedure :: check => vertex_table_check

<Model data: procedures>+≡
    function vertex_table_check (vt, pdg1, pdg2, pdg3) result (flag)
        class(vertex_table_t), intent(in) :: vt
        integer, intent(in) :: pdg1, pdg2, pdg3
        logical :: flag
        flag = check (hash2 (pdg1, pdg2))
contains
        recursive function check (hashval) result (flag)
            integer(i32), intent(in) :: hashval
            integer :: h
            logical :: flag
            h = iand (hashval, vt%mask)
            if (vt%entry(h)%n == 0) then
                flag = .false.
            else if (vt%entry(h)%pdg1 == pdg1 .and. vt%entry(h)%pdg2 == pdg2) then
                flag = any (vt%entry(h)%pdg3 == pdg3)
            else
                flag = check (hashval + 1)
            end if
        end function check
    end function vertex_table_check

```

11.1.5 Model Data Record

This type collects the model data as defined above.

We deliberately implement the parameter arrays as pointer arrays. We thus avoid keeping track of TARGET attributes.

The `scheme` identifier provides meta information. It doesn't give the client code an extra parameter, but it tells something about the interpretation of the parameters. If the scheme ID is left as default (zero), it is ignored.

```

<Model data: public>+≡

```

```

public :: model_data_t
<Model data: types>+=
  type :: model_data_t
    private
    type(string_t) :: name
    integer :: scheme = 0
    type(modelpar_real_t), dimension(:), pointer :: par_real => null ()
    type(modelpar_complex_t), dimension(:), pointer :: par_complex => null ()
    type(field_data_t), dimension(:), allocatable :: field
    type(vertex_t), dimension(:), allocatable :: vtx
    type(vertex_table_t) :: vt
  contains
    <Model data: model data: TBP>
  end type model_data_t

```

Finalizer, deallocate pointer arrays.

```

<Model data: model data: TBP>=
  procedure :: final => model_data_final

<Model data: procedures>+=
  subroutine model_data_final (model)
    class(model_data_t), intent(inout) :: model
    if (associated (model%par_real)) then
      deallocate (model%par_real)
    end if
    if (associated (model%par_complex)) then
      deallocate (model%par_complex)
    end if
  end subroutine model_data_final

```

Output. The signature matches the signature of the high-level `model_write` procedure, so some of the options don't actually apply.

```

<Model data: model data: TBP>+=
  procedure :: write => model_data_write

<Model data: procedures>+=
  subroutine model_data_write (model, unit, verbose, &
    show_md5sum, show_variables, show_parameters, &
    show_particles, show_vertices, show_scheme)
    class(model_data_t), intent(in) :: model
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    logical, intent(in), optional :: show_md5sum
    logical, intent(in), optional :: show_variables
    logical, intent(in), optional :: show_parameters
    logical, intent(in), optional :: show_particles
    logical, intent(in), optional :: show_vertices
    logical, intent(in), optional :: show_scheme
    logical :: show_sch, show_par, show_prt, show_vtx
    integer :: u, i
    u = given_output_unit (unit)
    show_sch = .false.; if (present (show_scheme)) &
      show_sch = show_scheme

```

```

show_par = .true.; if (present (show_parameters)) &
    show_par = show_parameters
show_prt = .true.; if (present (show_particles)) &
    show_prt = show_particles
show_vtx = .true.; if (present (show_vertices)) &
    show_vtx = show_vertices
if (show_sch) then
    write (u, "(3x,A,1X,I0)") "scheme =", model%scheme
end if
if (show_par) then
    do i = 1, size (model%par_real)
        call model%par_real(i)%write (u)
        write (u, "(A)")
    end do
    do i = 1, size (model%par_complex)
        call model%par_complex(i)%write (u)
        write (u, "(A)")
    end do
end if
if (show_prt) then
    write (u, "(A)")
    call model%write_fields (u)
end if
if (show_vtx) then
    write (u, "(A)")
    call model%write_vertices (u, verbose)
end if
end subroutine model_data_write

```

Initialize, allocating pointer arrays. The second version makes a deep copy.

```

<Model data: model data: TBP>+≡
generic :: init => model_data_init
procedure, private :: model_data_init

<Model data: procedures>+≡
subroutine model_data_init (model, name, &
    n_par_real, n_par_complex, n_field, n_vtx)
class(model_data_t), intent(out) :: model
type(string_t), intent(in) :: name
integer, intent(in) :: n_par_real, n_par_complex
integer, intent(in) :: n_field
integer, intent(in) :: n_vtx
model%name = name
allocate (model%par_real (n_par_real))
allocate (model%par_complex (n_par_complex))
allocate (model%field (n_field))
allocate (model%vtx (n_vtx))
end subroutine model_data_init

```

Set the scheme ID.

```

<Model data: model data: TBP>+≡
procedure :: set_scheme_num => model_data_set_scheme_num

```

```

<Model data: procedures>+≡
  subroutine model_data_set_scheme_num (model, scheme)
    class(model_data_t), intent(inout) :: model
    integer, intent(in) :: scheme
    model%scheme = scheme
  end subroutine model_data_set_scheme_num

```

Complete model data initialization.

```

<Model data: model data: TBP>+≡
  procedure :: freeze_fields => model_data_freeze_fields

<Model data: procedures>+≡
  subroutine model_data_freeze_fields (model)
    class(model_data_t), intent(inout) :: model
    call model%field%freeze ()
  end subroutine model_data_freeze_fields

```

Deep copy. The new model should already be initialized, so we do not allocate memory.

```

<Model data: model data: TBP>+≡
  procedure :: copy_from => model_data_copy

<Model data: procedures>+≡
  subroutine model_data_copy (model, src)
    class(model_data_t), intent(inout), target :: model
    class(model_data_t), intent(in), target :: src
    class(modelpar_data_t), pointer :: data, src_data
    integer :: i
    model%scheme = src%scheme
    model%par_real = src%par_real
    model%par_complex = src%par_complex
    do i = 1, size (src%field)
      associate (field => model%field(i), src_field => src%field(i))
        call field%init (src_field%get_longname (), src_field%get_pdg ())
        call field%copy_from (src_field)
        src_data => src_field%mass_data
        if (associated (src_data)) then
          data => model%get_par_data_ptr (src_data%get_name ())
          call field%set (mass_data = data)
        end if
        src_data => src_field%width_data
        if (associated (src_data)) then
          data => model%get_par_data_ptr (src_data%get_name ())
          call field%set (width_data = data)
        end if
        call field%set_multiplicity ()
      end associate
    end do
    do i = 1, size (src%vtx)
      call model%vtx(i)%copy_from (src%vtx(i), model)
    end do
    call model%freeze_vertices ()
  end subroutine model_data_copy

```


Return the model name and numeric scheme.

```

<Model data: model data: TBP>+=
  procedure :: get_name => model_data_get_name
  procedure :: get_scheme_num => model_data_get_scheme_num

<Model data: procedures>+=
  function model_data_get_name (model) result (name)
    class(model_data_t), intent(in) :: model
    type(string_t) :: name
    name = model%name
  end function model_data_get_name

  function model_data_get_scheme_num (model) result (scheme)
    class(model_data_t), intent(in) :: model
    integer :: scheme
    scheme = model%scheme
  end function model_data_get_scheme_num

```

Retrieve a MD5 sum for the current model parameter values and decay/polarization settings. This is done by writing them to a temporary file, using a standard format. If the model scheme is nonzero, it is also written.

```

<Model data: model data: TBP>+=
  procedure :: get_parameters_md5sum => model_data_get_parameters_md5sum

<Model data: procedures>+=
  function model_data_get_parameters_md5sum (model) result (par_md5sum)
    character(32) :: par_md5sum
    class(model_data_t), intent(in) :: model
    real(default), dimension(:), allocatable :: par
    type(field_data_t), pointer :: field
    integer :: unit, i
    allocate (par (model%get_n_real ()))
    call model%real_parameters_to_array (par)
    unit = free_unit ()
    open (unit, status="scratch", action="readwrite")
    if (model%scheme /= 0) write (unit, "(I0)") model%scheme
    write (unit, "(" // FMT_19 // ")") par
    do i = 1, model%get_n_field ()
      field => model%get_field_ptr_by_index (i)
      if (.not. field%is_stable (.false.) .or. .not. field%is_stable (.true.) &
        .or. field%is_polarized (.false.) .or. field%is_polarized (.true.))&
      then
        write (unit, "(3x,A)") char (field%get_longname ())
        call field%write_decays (unit)
      end if
    end do
    rewind (unit)
    par_md5sum = md5sum (unit)
    close (unit)
  end function model_data_get_parameters_md5sum

```

Return the MD5 sum. This is a placeholder, to be overwritten for the complete model definition.

```

<Model data: model data: TBP>+=

```

```

    procedure :: get_md5sum => model_data_get_md5sum
<Model data: procedures>+≡
    function model_data_get_md5sum (model) result (md5sum)
        class(model_data_t), intent(in) :: model
        character(32) :: md5sum
        md5sum = model%get_parameters_md5sum ()
    end function model_data_get_md5sum

```

Initialize a real or complex parameter.

```

<Model data: model data: TBP>+≡
    generic :: init_par => model_data_init_par_real, model_data_init_par_complex
    procedure, private :: model_data_init_par_real
    procedure, private :: model_data_init_par_complex
<Model data: procedures>+≡
    subroutine model_data_init_par_real (model, i, name, value)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: i
        type(string_t), intent(in) :: name
        real(default), intent(in) :: value
        call model%par_real(i)%init (name, value)
    end subroutine model_data_init_par_real

    subroutine model_data_init_par_complex (model, i, name, value)
        class(model_data_t), intent(inout) :: model
        integer, intent(in) :: i
        type(string_t), intent(in) :: name
        complex(default), intent(in) :: value
        call model%par_complex(i)%init (name, value)
    end subroutine model_data_init_par_complex

```

After initialization, return size of parameter array.

```

<Model data: model data: TBP>+≡
    procedure :: get_n_real => model_data_get_n_real
    procedure :: get_n_complex => model_data_get_n_complex
<Model data: procedures>+≡
    function model_data_get_n_real (model) result (n)
        class(model_data_t), intent(in) :: model
        integer :: n
        n = size (model%par_real)
    end function model_data_get_n_real

    function model_data_get_n_complex (model) result (n)
        class(model_data_t), intent(in) :: model
        integer :: n
        n = size (model%par_complex)
    end function model_data_get_n_complex

```

After initialization, extract the whole parameter array.

```

<Model data: model data: TBP>+≡
    procedure :: real_parameters_to_array &
        => model_data_real_par_to_array

```

```

        procedure :: complex_parameters_to_array &
            => model_data_complex_par_to_array

<Model data: procedures>+=
    subroutine model_data_real_par_to_array (model, array)
        class(model_data_t), intent(in) :: model
        real(default), dimension(:), intent(inout) :: array
        array = model%par_real%get_real ()
    end subroutine model_data_real_par_to_array

    subroutine model_data_complex_par_to_array (model, array)
        class(model_data_t), intent(in) :: model
        complex(default), dimension(:), intent(inout) :: array
        array = model%par_complex%get_complex ()
    end subroutine model_data_complex_par_to_array

```

After initialization, set the whole parameter array.

```

<Model data: model data: TBP>+=
    procedure :: real_parameters_from_array &
        => model_data_real_par_from_array
    procedure :: complex_parameters_from_array &
        => model_data_complex_par_from_array

<Model data: procedures>+=
    subroutine model_data_real_par_from_array (model, array)
        class(model_data_t), intent(inout) :: model
        real(default), dimension(:), intent(in) :: array
        model%par_real = array
    end subroutine model_data_real_par_from_array

    subroutine model_data_complex_par_from_array (model, array)
        class(model_data_t), intent(inout) :: model
        complex(default), dimension(:), intent(in) :: array
        model%par_complex = array
    end subroutine model_data_complex_par_from_array

```

Analogous, for a C parameter array.

```

<Model data: model data: TBP>+=
    procedure :: real_parameters_to_c_array &
        => model_data_real_par_to_c_array

<Model data: procedures>+=
    subroutine model_data_real_par_to_c_array (model, array)
        class(model_data_t), intent(in) :: model
        real(c_default_float), dimension(:), intent(inout) :: array
        array = model%par_real%get_real ()
    end subroutine model_data_real_par_to_c_array

```

After initialization, set the whole parameter array.

```

<Model data: model data: TBP>+=
    procedure :: real_parameters_from_c_array &
        => model_data_real_par_from_c_array

```

```

<Model data: procedures>+≡
  subroutine model_data_real_par_from_c_array (model, array)
    class(model_data_t), intent(inout) :: model
    real(c_default_float), dimension(:), intent(in) :: array
    model%par_real = real (array, default)
  end subroutine model_data_real_par_from_c_array

```

After initialization, get pointer to a real or complex parameter, directly by index.

```

<Model data: model data: TBP>+≡
  procedure :: get_par_real_ptr => model_data_get_par_real_ptr_index
  procedure :: get_par_complex_ptr => model_data_get_par_complex_ptr_index

<Model data: procedures>+≡
  function model_data_get_par_real_ptr_index (model, i) result (ptr)
    class(model_data_t), intent(inout) :: model
    integer, intent(in) :: i
    class(modelpar_data_t), pointer :: ptr
    ptr => model%par_real(i)
  end function model_data_get_par_real_ptr_index

  function model_data_get_par_complex_ptr_index (model, i) result (ptr)
    class(model_data_t), intent(inout) :: model
    integer, intent(in) :: i
    class(modelpar_data_t), pointer :: ptr
    ptr => model%par_complex(i)
  end function model_data_get_par_complex_ptr_index

```

After initialization, get pointer to a parameter by name.

```

<Model data: model data: TBP>+≡
  procedure :: get_par_data_ptr => model_data_get_par_data_ptr_name

<Model data: procedures>+≡
  function model_data_get_par_data_ptr_name (model, name) result (ptr)
    class(model_data_t), intent(in) :: model
    type(string_t), intent(in) :: name
    class(modelpar_data_t), pointer :: ptr
    integer :: i
    do i = 1, size (model%par_real)
      if (model%par_real(i)%name == name) then
        ptr => model%par_real(i)
        return
      end if
    end do
    do i = 1, size (model%par_complex)
      if (model%par_complex(i)%name == name) then
        ptr => model%par_complex(i)
        return
      end if
    end do
    ptr => null ()
  end function model_data_get_par_data_ptr_name

```

Return the value by name. Again, type conversion is allowed.

```

<Model data: model data: TBP>+=
  procedure :: get_real => model_data_get_par_real_value
  procedure :: get_complex => model_data_get_par_complex_value

<Model data: procedures>+=
  function model_data_get_par_real_value (model, name) result (value)
    class(model_data_t), intent(in) :: model
    type(string_t), intent(in) :: name
    class(modelpar_data_t), pointer :: par
    real(default) :: value
    par => model%get_par_data_ptr (name)
    value = par%get_real ()
  end function model_data_get_par_real_value

  function model_data_get_par_complex_value (model, name) result (value)
    class(model_data_t), intent(in) :: model
    type(string_t), intent(in) :: name
    class(modelpar_data_t), pointer :: par
    complex(default) :: value
    par => model%get_par_data_ptr (name)
    value = par%get_complex ()
  end function model_data_get_par_complex_value

```

Modify a real or complex parameter.

```

<Model data: model data: TBP>+=
  generic :: set_par => model_data_set_par_real, model_data_set_par_complex
  procedure, private :: model_data_set_par_real
  procedure, private :: model_data_set_par_complex

<Model data: procedures>+=
  subroutine model_data_set_par_real (model, name, value)
    class(model_data_t), intent(inout) :: model
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
    class(modelpar_data_t), pointer :: par
    par => model%get_par_data_ptr (name)
    par = value
  end subroutine model_data_set_par_real

  subroutine model_data_set_par_complex (model, name, value)
    class(model_data_t), intent(inout) :: model
    type(string_t), intent(in) :: name
    complex(default), intent(in) :: value
    class(modelpar_data_t), pointer :: par
    par => model%get_par_data_ptr (name)
    par = value
  end subroutine model_data_set_par_complex

```

List all fields in the model.

```

<Model data: model data: TBP>+=
  procedure :: write_fields => model_data_write_fields

```

```

<Model data: procedures>+≡
subroutine model_data_write_fields (model, unit)
  class(model_data_t), intent(in) :: model
  integer, intent(in), optional :: unit
  integer :: i
  do i = 1, size (model%field)
    call model%field(i)%write (unit)
  end do
end subroutine model_data_write_fields

```

After initialization, return number of fields (particles):

```

<Model data: model data: TBP>+≡
  procedure :: get_n_field => model_data_get_n_field

<Model data: procedures>+≡
function model_data_get_n_field (model) result (n)
  class(model_data_t), intent(in) :: model
  integer :: n
  n = size (model%field)
end function model_data_get_n_field

```

Return the PDG code of a field. The field is identified by name or by index. If the field is not found, return zero.

```

<Model data: model data: TBP>+≡
  generic :: get_pdg => &
    model_data_get_field_pdg_index, &
    model_data_get_field_pdg_name
  procedure, private :: model_data_get_field_pdg_index
  procedure, private :: model_data_get_field_pdg_name

<Model data: procedures>+≡
function model_data_get_field_pdg_index (model, i) result (pdg)
  class(model_data_t), intent(in) :: model
  integer, intent(in) :: i
  integer :: pdg
  pdg = model%field(i)%get_pdg ()
end function model_data_get_field_pdg_index

function model_data_get_field_pdg_name (model, name, check) result (pdg)
  class(model_data_t), intent(in) :: model
  type(string_t), intent(in) :: name
  logical, intent(in), optional :: check
  integer :: pdg
  integer :: i
  do i = 1, size (model%field)
    associate (field => model%field(i))
      if (field%matches_name (name, .false.)) then
        pdg = field%get_pdg ()
        return
      else if (field%matches_name (name, .true.)) then
        pdg = - field%get_pdg ()
        return
      end if
    end associate
  end do
end function model_data_get_field_pdg_name

```

```

end do
pdg = 0
call model%field_error (check, name)
end function model_data_get_field_pdg_name

```

Return an array of all PDG codes, including antiparticles. The antiparticle are sorted after all particles.

```

⟨Model data: model data: TBP⟩+≡
  procedure :: get_all_pdg => model_data_get_all_pdg

⟨Model data: procedures⟩+≡
  subroutine model_data_get_all_pdg (model, pdg)
    class(model_data_t), intent(in) :: model
    integer, dimension(:), allocatable, intent(inout) :: pdg
    integer :: n0, n1, i, k
    n0 = size (model%field)
    n1 = n0 + count (model%field%has_antiparticle ())
    allocate (pdg (n1))
    pdg(1:n0) = model%field%get_pdg ()
    k = n0
    do i = 1, size (model%field)
      associate (field => model%field(i))
        if (field%has_antiparticle ()) then
          k = k + 1
          pdg(k) = - field%get_pdg ()
        end if
      end associate
    end do
  end subroutine model_data_get_all_pdg

```

Return pointer to the field array.

```

⟨Model data: model data: TBP⟩+≡
  procedure :: get_field_array_ptr => model_data_get_field_array_ptr

⟨Model data: procedures⟩+≡
  function model_data_get_field_array_ptr (model) result (ptr)
    class(model_data_t), intent(in), target :: model
    type(field_data_t), dimension(:), pointer :: ptr
    ptr => model%field
  end function model_data_get_field_array_ptr

```

Return pointer to a field. The identifier should be the unique long name, the PDG code, or the index.

We can issue an error message, if the `check` flag is set. We never return an error if the PDG code is zero, this yields just a null pointer.

```

⟨Model data: model data: TBP⟩+≡
  generic :: get_field_ptr => &
    model_data_get_field_ptr_name, &
    model_data_get_field_ptr_pdg
  procedure, private :: model_data_get_field_ptr_name
  procedure, private :: model_data_get_field_ptr_pdg
  procedure :: get_field_ptr_by_index => model_data_get_field_ptr_index

```

```

<Model data: procedures>+≡
function model_data_get_field_ptr_name (model, name, check) result (ptr)
  class(model_data_t), intent(in), target :: model
  type(string_t), intent(in) :: name
  logical, intent(in), optional :: check
  type(field_data_t), pointer :: ptr
  integer :: i
  do i = 1, size (model%field)
    if (model%field(i)%matches_name (name, .false.)) then
      ptr => model%field(i)
      return
    else if (model%field(i)%matches_name (name, .true.)) then
      ptr => model%field(i)
      return
    end if
  end do
  ptr => null ()
  call model%field_error (check, name)
end function model_data_get_field_ptr_name

function model_data_get_field_ptr_pdg (model, pdg, check) result (ptr)
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: pdg
  logical, intent(in), optional :: check
  type(field_data_t), pointer :: ptr
  integer :: i, pdg_abs
  if (pdg == 0) then
    ptr => null ()
    return
  end if
  pdg_abs = abs (pdg)
  do i = 1, size (model%field)
    if (abs(model%field(i)%get_pdg ()) == pdg_abs) then
      ptr => model%field(i)
      return
    end if
  end do
  ptr => null ()
  call model%field_error (check, pdg=pdg)
end function model_data_get_field_ptr_pdg

function model_data_get_field_ptr_index (model, i) result (ptr)
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: i
  type(field_data_t), pointer :: ptr
  ptr => model%field(i)
end function model_data_get_field_ptr_index

```

Don't assign a pointer, just check.

```

<Model data: model data: TBP>+≡
  procedure :: test_field => model_data_test_field_pdg

<Model data: procedures>+≡
  function model_data_test_field_pdg (model, pdg, check) result (exist)

```



```

class(model_data_t), intent(in), target :: model
integer, intent(in) :: pdg
logical, intent(in), optional :: check
logical :: exist
exist = associated (model%get_field_ptr (pdg, check))
end function model_data_test_field_pdg

```

Error message, if check is set.

```

<Model data: model data: TBP>+≡
  procedure :: field_error => model_data_field_error

<Model data: procedures>+≡
  subroutine model_data_field_error (model, check, name, pdg)
    class(model_data_t), intent(in) :: model
    logical, intent(in), optional :: check
    type(string_t), intent(in), optional :: name
    integer, intent(in), optional :: pdg
    if (present (check)) then
      if (check) then
        if (present (name)) then
          write (msg_buffer, "(A,1x,A,1x,A,1x,A)" &
            "No particle with name", char (name), &
            "is contained in model", char (model%name)
          else if (present (pdg)) then
            write (msg_buffer, "(A,1x,I0,1x,A,1x,A)" &
              "No particle with PDG code", pdg, &
              "is contained in model", char (model%name)
            else
              write (msg_buffer, "(A,1x,A,1x,A)" &
                "Particle missing", &
                "in model", char (model%name)
            end if
            call msg_fatal ()
          end if
        end if
      end if
    end subroutine model_data_field_error

```

Assign mass and width value, which are associated via pointer. Identify the particle via pdg.

```

<Model data: model data: TBP>+≡
  procedure :: set_field_mass => model_data_set_field_mass_pdg
  procedure :: set_field_width => model_data_set_field_width_pdg

<Model data: procedures>+≡
  subroutine model_data_set_field_mass_pdg (model, pdg, value)
    class(model_data_t), intent(inout) :: model
    integer, intent(in) :: pdg
    real(default), intent(in) :: value
    type(field_data_t), pointer :: field
    field => model%get_field_ptr (pdg, check = .true.)
    call field%set_mass (value)
  end subroutine model_data_set_field_mass_pdg

  subroutine model_data_set_field_width_pdg (model, pdg, value)

```

```

class(model_data_t), intent(inout) :: model
integer, intent(in) :: pdg
real(default), intent(in) :: value
type(field_data_t), pointer :: field
field => model%get_field_ptr (pdg, check = .true.)
call field%set_width (value)
end subroutine model_data_set_field_width_pdg

```

Mark a particle as unstable and provide a list of names for its decay processes. In contrast with the previous subroutine which is for internal use, we address the particle by its PDG code. If the index is negative, we address the antiparticle.

```

<Model data: model data: TBP>+≡
  procedure :: set_unstable => model_data_set_unstable
  procedure :: set_stable => model_data_set_stable

<Model data: procedures>+≡
  subroutine model_data_set_unstable &
    (model, pdg, decay, isotropic, diagonal, decay_helicity)
    class(model_data_t), intent(inout), target :: model
    integer, intent(in) :: pdg
    type(string_t), dimension(:), intent(in) :: decay
    logical, intent(in), optional :: isotropic, diagonal
    integer, intent(in), optional :: decay_helicity
    type(field_data_t), pointer :: field
    field => model%get_field_ptr (pdg)
    if (pdg > 0) then
      call field%set ( &
        p_is_stable = .false., p_decay = decay, &
        p_decays_isotropically = isotropic, &
        p_decays_diagonal = diagonal, &
        p_decay_helicity = decay_helicity)
    else
      call field%set ( &
        a_is_stable = .false., a_decay = decay, &
        a_decays_isotropically = isotropic, &
        a_decays_diagonal = diagonal, &
        a_decay_helicity = decay_helicity)
    end if
  end subroutine model_data_set_unstable

  subroutine model_data_set_stable (model, pdg)
    class(model_data_t), intent(inout), target :: model
    integer, intent(in) :: pdg
    type(field_data_t), pointer :: field
    field => model%get_field_ptr (pdg)
    if (pdg > 0) then
      call field%set (p_is_stable = .true.)
    else
      call field%set (a_is_stable = .true.)
    end if
  end subroutine model_data_set_stable

```

Mark a particle as polarized.

```

<Model data: model data: TBP>+=
  procedure :: set_polarized => model_data_set_polarized
  procedure :: set_unpolarized => model_data_set_unpolarized

<Model data: procedures>+=
  subroutine model_data_set_polarized (model, pdg)
    class(model_data_t), intent(inout), target :: model
    integer, intent(in) :: pdg
    type(field_data_t), pointer :: field
    field => model%get_field_ptr (pdg)
    if (pdg > 0) then
      call field%set (p_polarized = .true.)
    else
      call field%set (a_polarized = .true.)
    end if
  end subroutine model_data_set_polarized

  subroutine model_data_set_unpolarized (model, pdg)
    class(model_data_t), intent(inout), target :: model
    integer, intent(in) :: pdg
    type(field_data_t), pointer :: field
    field => model%get_field_ptr (pdg)
    if (pdg > 0) then
      call field%set (p_polarized = .false.)
    else
      call field%set (a_polarized = .false.)
    end if
  end subroutine model_data_set_unpolarized

```

Revert all polarized (unstable) particles to unpolarized (stable) status, respectively.

```

<Model data: model data: TBP>+=
  procedure :: clear_unstable => model_clear_unstable
  procedure :: clear_polarized => model_clear_polarized

<Model data: procedures>+=
  subroutine model_clear_unstable (model)
    class(model_data_t), intent(inout), target :: model
    integer :: i
    type(field_data_t), pointer :: field
    do i = 1, model%get_n_field ()
      field => model%get_field_ptr_by_index (i)
      call field%set (p_is_stable = .true.)
      if (field%has_antiparticle ()) then
        call field%set (a_is_stable = .true.)
      end if
    end do
  end subroutine model_clear_unstable

  subroutine model_clear_polarized (model)
    class(model_data_t), intent(inout), target :: model
    integer :: i
    type(field_data_t), pointer :: field
    do i = 1, model%get_n_field ()
      field => model%get_field_ptr_by_index (i)

```

```

        call field%set (p_polarized = .false.)
        if (field%has_antiparticle ()) then
            call field%set (a_polarized = .false.)
        end if
    end do
end subroutine model_clear_polarized

```

List all vertices, optionally also the hash table.

```

<Model data: model data: TBP>+≡
    procedure :: write_vertices => model_data_write_vertices

<Model data: procedures>+≡
    subroutine model_data_write_vertices (model, unit, verbose)
        class(model_data_t), intent(in) :: model
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: i, u
        u = given_output_unit (unit)
        do i = 1, size (model%vtx)
            call vertex_write (model%vtx(i), unit)
        end do
        if (present (verbose)) then
            if (verbose) then
                write (u, *)
                call vertex_table_write (model%vt, unit)
            end if
        end if
    end subroutine model_data_write_vertices

```

Vertex definition.

```

<Model data: model data: TBP>+≡
    generic :: set_vertex => &
        model_data_set_vertex_pdg, model_data_set_vertex_names
    procedure, private :: model_data_set_vertex_pdg
    procedure, private :: model_data_set_vertex_names

<Model data: procedures>+≡
    subroutine model_data_set_vertex_pdg (model, i, pdg)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: pdg
        call vertex_init (model%vtx(i), pdg, model)
    end subroutine model_data_set_vertex_pdg

    subroutine model_data_set_vertex_names (model, i, name)
        class(model_data_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(string_t), dimension(:), intent(in) :: name
        integer, dimension(size(name)) :: pdg
        integer :: j
        do j = 1, size (name)
            pdg(j) = model%get_pdg (name(j))
        end do
        call model%set_vertex (i, pdg)
    end subroutine model_data_set_vertex_names

```

```
end subroutine model_data_set_vertex_names
```

Finalize vertex definition: set up the hash table.

```
<Model data: model data: TBP>+≡
  procedure :: freeze_vertices => model_data_freeze_vertices

<Model data: procedures>+≡
  subroutine model_data_freeze_vertices (model)
    class(model_data_t), intent(inout) :: model
    call model%vt%init (model%field, model%vtx)
  end subroutine model_data_freeze_vertices
```

Number of vertices in model

```
<Model data: model data: TBP>+≡
  procedure :: get_n_vtx => model_data_get_n_vtx

<Model data: procedures>+≡
  function model_data_get_n_vtx (model) result (n)
    class(model_data_t), intent(in) :: model
    integer :: n
    n = size (model%vtx)
  end function model_data_get_n_vtx
```

Lookup functions

```
<Model data: model data: TBP>+≡
  procedure :: match_vertex => model_data_match_vertex

<Model data: procedures>+≡
  subroutine model_data_match_vertex (model, pdg1, pdg2, pdg3)
    class(model_data_t), intent(in) :: model
    integer, intent(in) :: pdg1, pdg2
    integer, dimension(:), allocatable, intent(out) :: pdg3
    call model%vt%match (pdg1, pdg2, pdg3)
  end subroutine model_data_match_vertex

<Model data: model data: TBP>+≡
  procedure :: check_vertex => model_data_check_vertex

<Model data: procedures>+≡
  function model_data_check_vertex (model, pdg1, pdg2, pdg3) result (flag)
    logical :: flag
    class(model_data_t), intent(in) :: model
    integer, intent(in) :: pdg1, pdg2, pdg3
    flag = model%vt%check (pdg1, pdg2, pdg3)
  end function model_data_check_vertex
```

11.1.6 Toy Models

This is a stripped-down version of the (already trivial) model 'Test'.

```
<Model data: model data: TBP>+≡
  procedure :: init_test => model_data_init_test
```

<Model data: procedures>+≡

```

subroutine model_data_init_test (model)
  class(model_data_t), intent(out) :: model
  type(field_data_t), pointer :: field
  integer, parameter :: n_real = 4
  integer, parameter :: n_field = 2
  integer, parameter :: n_vertex = 2
  integer :: i
  call model%init (var_str ("Test"), &
    n_real, 0, n_field, n_vertex)
  i = 0
  i = i + 1
  call model%init_par (i, var_str ("gy"), 1._default)
  i = i + 1
  call model%init_par (i, var_str ("ms"), 125._default)
  i = i + 1
  call model%init_par (i, var_str ("ff"), 1.5_default)
  i = i + 1
  call model%init_par (i, var_str ("mf"), 1.5_default * 125._default)
  i = 0
  i = i + 1
  field => model%get_field_ptr_by_index (i)
  call field%init (var_str ("SCALAR"), 25)
  call field%set (spin_type=1)
  call field%set (mass_data=model%get_par_real_ptr (2))
  call field%set (name = [var_str ("s")])
  i = i + 1
  field => model%get_field_ptr_by_index (i)
  call field%init (var_str ("FERMION"), 6)
  call field%set (spin_type=2)
  call field%set (mass_data=model%get_par_real_ptr (4))
  call field%set (name = [var_str ("f")], anti = [var_str ("fbar")])
  call model%freeze_fields ()
  i = 0
  i = i + 1
  call model%set_vertex (i, [var_str ("fbar"), var_str ("f"), var_str ("s")])
  i = i + 1
  call model%set_vertex (i, [var_str ("s"), var_str ("s"), var_str ("s")])
  call model%freeze_vertices ()
end subroutine model_data_init_test

```

This procedure prepares a subset of QED for testing purposes.

<Model data: model data: TBP>+≡

```

procedure :: init_qed_test => model_data_init_qed_test

```

<Model data: procedures>+≡

```

subroutine model_data_init_qed_test (model)
  class(model_data_t), intent(out) :: model
  type(field_data_t), pointer :: field
  integer, parameter :: n_real = 1
  integer, parameter :: n_field = 2
  integer :: i
  call model%init (var_str ("QED_test"), &
    n_real, 0, n_field, 0)

```

```

i = 0
i = i + 1
call model%init_par (i, var_str ("me"), 0.000510997_default)
i = 0
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_LEPTON"), 11)
call field%set (spin_type=2, charge_type=-4)
call field%set (mass_data=model%get_par_real_ptr (1))
call field%set (name = [var_str ("e-")], anti = [var_str ("e+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PHOTON"), 22)
call field%set (spin_type=3)
call field%set (name = [var_str ("A")])
call model%freeze_fields ()
call model%freeze_vertices ()
end subroutine model_data_init_qed_test

```

This procedure prepares a subset of the Standard Model for testing purposes. We can thus avoid dependencies on model I/O, which is not defined here.

(Model data: model data: TBP)+≡

```

procedure :: init_sm_test => model_data_init_sm_test

```

(Model data: procedures)+≡

```

subroutine model_data_init_sm_test (model)
class(model_data_t), intent(out) :: model
type(field_data_t), pointer :: field
integer, parameter :: n_real = 11
integer, parameter :: n_field = 19
integer, parameter :: n_vtx = 9
integer :: i
call model%init (var_str ("SM_test"), &
    n_real, 0, n_field, n_vtx)
i = 0
i = i + 1
call model%init_par (i, var_str ("mZ"), 91.1882_default)
i = i + 1
call model%init_par (i, var_str ("mW"), 80.419_default)
i = i + 1
call model%init_par (i, var_str ("me"), 0.000510997_default)
i = i + 1
call model%init_par (i, var_str ("mmu"), 0.105658389_default)
i = i + 1
call model%init_par (i, var_str ("mb"), 4.2_default)
i = i + 1
call model%init_par (i, var_str ("mtop"), 173.1_default)
i = i + 1
call model%init_par (i, var_str ("wZ"), 2.443_default)
i = i + 1
call model%init_par (i, var_str ("wW"), 2.049_default)
i = i + 1
call model%init_par (i, var_str ("ee"), 0.3079561542961_default)
i = i + 1

```

```

call model%init_par (i, var_str ("cw"), 8.819013863636E-01_default)
i = i + 1
call model%init_par (i, var_str ("sw"), 4.714339240339E-01_default)
i = 0
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("D_QUARK"), 1)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (name = [var_str ("d")], anti = [var_str ("dbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("U_QUARK"), 2)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (name = [var_str ("u")], anti = [var_str ("ubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("S_QUARK"), 3)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (name = [var_str ("s")], anti = [var_str ("sbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("C_QUARK"), 4)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (name = [var_str ("c")], anti = [var_str ("cbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("B_QUARK"), 5)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (mass_data=model%get_par_real_ptr (5))
call field%set (name = [var_str ("b")], anti = [var_str ("bbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("T_QUARK"), 6)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (mass_data=model%get_par_real_ptr (6))
call field%set (name = [var_str ("t")], anti = [var_str ("tbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_LEPTON"), 11)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (3))
call field%set (name = [var_str ("e-")], anti = [var_str ("e+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_NEUTRINO"), 12)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("nue")], anti = [var_str ("nuebar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("MU_LEPTON"), 13)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (4))
call field%set (name = [var_str ("mu-")], anti = [var_str ("mu+")])
i = i + 1

```



```

field => model%get_field_ptr_by_index (i)
call field%init (var_str ("MU_NEUTRINO"), 14)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("numu")], anti = [var_str ("numubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("GLUON"), 21)
call field%set (spin_type=3, color_type=8)
call field%set (name = [var_str ("gl")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PHOTON"), 22)
call field%set (spin_type=3)
call field%set (name = [var_str ("A")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("Z_BOSON"), 23)
call field%set (spin_type=3)
call field%set (mass_data=model%get_par_real_ptr (1))
call field%set (width_data=model%get_par_real_ptr (7))
call field%set (name = [var_str ("Z")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("W_BOSON"), 24)
call field%set (spin_type=3)
call field%set (mass_data=model%get_par_real_ptr (2))
call field%set (width_data=model%get_par_real_ptr (8))
call field%set (name = [var_str ("W+")], anti = [var_str ("W-")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HIGGS"), 25)
call field%set (spin_type=1)
!   call field%set (mass_data=model%get_par_real_ptr (2))
!   call field%set (width_data=model%get_par_real_ptr (8))
call field%set (name = [var_str ("H")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PROTON"), 2212)
call field%set (spin_type=2)
call field%set (name = [var_str ("p")], anti = [var_str ("pbar")])
!   call field%set (mass_data=model%get_par_real_ptr (12))
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_SINGLET"), 91)
call field%set (color_type=1)
call field%set (name = [var_str ("hr1")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_TRIPLET"), 92)
call field%set (color_type=3)
call field%set (name = [var_str ("hr3")], anti = [var_str ("hr3bar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_OCTET"), 93)

```

```

call field%set (color_type=8)
call field%set (name = [var_str ("hr8")])
call model%freeze_fields ()
i = 0
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("gl"), var_str ("gl"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("d"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("u"), var_str ("W-")])
call model%freeze_vertices ()
end subroutine model_data_init_sm_test

```

11.2 Model Testbed

The standard way of defining a model uses concrete variables and expressions to interpret the model file. Some of this is not available at the point of use. This is no problem for the WHIZARD program as a whole, but unit tests are kept local to their respective module and don't access all definitions.

Instead, we introduce a separate module that provides hooks, one for initializing a model and one for finalizing a model. The main program can assign real routines to the hooks (procedure pointers of abstract type) before unit tests are called. The unit tests can call the abstract routines without knowing about their implementation.

```
<model_testbed.f90>≡  
  <File header>  
  
  module model_testbed  
  
    <Use strings>  
    use model_data  
    use var_base  
  
    <Standard module head>  
  
    <Model testbed: public>  
  
    <Model testbed: variables>  
  
    <Model testbed: interfaces>  
  
  end module model_testbed
```

11.2.1 Abstract Model Handlers

Both routines take a polymorphic model (data) target, which is not allocated/deallocated inside the subroutine. The model constructor `prepare_model` requires the model name as input. It can, optionally, return a link to the variable list of the model.

```
<Model testbed: public>≡  
  public :: prepare_model  
  public :: cleanup_model  
  
<Model testbed: variables>≡  
  procedure (prepare_model_proc), pointer :: prepare_model => null ()  
  procedure (cleanup_model_proc), pointer :: cleanup_model => null ()  
  
<Model testbed: interfaces>≡  
  abstract interface  
    subroutine prepare_model_proc (model, name, vars)  
      import  
      class(model_data_t), intent(inout), pointer :: model  
      type(string_t), intent(in) :: name  
      class(vars_t), pointer, intent(out), optional :: vars  
    end subroutine prepare_model_proc  
  end interface
```

```
abstract interface
  subroutine cleanup_model_proc (model)
    import
    class(model_data_t), intent(inout), target :: model
  end subroutine cleanup_model_proc
end interface
```

11.3 Helicities

This module defines types and tools for dealing with helicity information.

```
(helicities.f90)≡  
  ⟨File header⟩
```

```
  module helicities  
  
    use io_units  
  
    ⟨Standard module head⟩  
  
    ⟨Helicities: public⟩  
  
    ⟨Helicities: types⟩  
  
    ⟨Helicities: interfaces⟩  
  
    contains  
  
    ⟨Helicities: procedures⟩  
  
  end module helicities
```

11.3.1 Helicity types

Helicities may be defined or undefined, corresponding to a polarized or unpolarized state. Each helicity is actually a pair of helicities, corresponding to an entry in the spin density matrix. Obviously, diagonal entries are distinguished.

```
⟨Helicities: public⟩≡  
  public :: helicity_t  
  
⟨Helicities: types⟩≡  
  type :: helicity_t  
    private  
    logical :: defined = .false.  
    integer :: h1, h2  
    contains  
    ⟨Helicities: helicity: TBP⟩  
  end type helicity_t
```

Constructor functions, for convenience:

```
⟨Helicities: public⟩+≡  
  public :: helicity  
  
⟨Helicities: interfaces⟩≡  
  interface helicity  
    module procedure helicity0, helicity1, helicity2  
  end interface helicity
```

```

<Helicities: procedures>≡
  pure function helicity0 () result (hel)
    type(helicity_t) :: hel
  end function helicity0

  elemental function helicity1 (h) result (hel)
    type(helicity_t) :: hel
    integer, intent(in) :: h
    call hel%init (h)
  end function helicity1

  elemental function helicity2 (h2, h1) result (hel)
    type(helicity_t) :: hel
    integer, intent(in) :: h1, h2
    call hel%init (h2, h1)
  end function helicity2

```

Initializers.

Note: conceptually, the argument to initializers should be INTENT(OUT). However, Interp. F08/0033 prohibited this. The reason is that, in principle, the call could result in the execution of an impure finalizer for a type extension of `hel` (ugh).

```

<Helicities: helicity: TBP>≡
  generic :: init => helicity_init_empty, helicity_init_same, helicity_init_different
  procedure, private :: helicity_init_empty
  procedure, private :: helicity_init_same
  procedure, private :: helicity_init_different

<Helicities: procedures>+≡
  elemental subroutine helicity_init_empty (hel)
    class(helicity_t), intent(inout) :: hel
    hel%defined = .false.
  end subroutine helicity_init_empty

  elemental subroutine helicity_init_same (hel, h)
    class(helicity_t), intent(inout) :: hel
    integer, intent(in) :: h
    hel%defined = .true.
    hel%h1 = h
    hel%h2 = h
  end subroutine helicity_init_same

  elemental subroutine helicity_init_different (hel, h2, h1)
    class(helicity_t), intent(inout) :: hel
    integer, intent(in) :: h1, h2
    hel%defined = .true.
    hel%h2 = h2
    hel%h1 = h1
  end subroutine helicity_init_different

```

Undefine:

```

<Helicities: helicity: TBP>+≡
  procedure :: undefine => helicity_undefine

```

```

<Helicities: procedures>+≡
  elemental subroutine helicity_undefine (hel)
    class(helicity_t), intent(inout) :: hel
    hel%defined = .false.
  end subroutine helicity_undefine

```

Diagonalize by removing the second entry (use with care!)

```

<Helicities: helicity: TBP>+≡
  procedure :: diagonalize => helicity_diagonalize

<Helicities: procedures>+≡
  elemental subroutine helicity_diagonalize (hel)
    class(helicity_t), intent(inout) :: hel
    hel%h2 = hel%h1
  end subroutine helicity_diagonalize

```

Flip helicity indices by sign.

```

<Helicities: helicity: TBP>+≡
  procedure :: flip => helicity_flip

<Helicities: procedures>+≡
  elemental subroutine helicity_flip (hel)
    class(helicity_t), intent(inout) :: hel
    hel%h1 = - hel%h1
    hel%h2 = - hel%h2
  end subroutine helicity_flip

```

```

<Helicities: helicity: TBP>+≡
  procedure :: get_indices => helicity_get_indices

<Helicities: procedures>+≡
  subroutine helicity_get_indices (hel, h1, h2)
    class(helicity_t), intent(in) :: hel
    integer, intent(out) :: h1, h2
    h1 = hel%h1; h2 = hel%h2
  end subroutine helicity_get_indices

```

Output (no linebreak). No output if undefined.

```

<Helicities: helicity: TBP>+≡
  procedure :: write => helicity_write

<Helicities: procedures>+≡
  subroutine helicity_write (hel, unit)
    class(helicity_t), intent(in) :: hel
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    if (hel%defined) then
      write (u, "(A)", advance="no") "h("
      write (u, "(IO)", advance="no") hel%h1
      if (hel%h1 /= hel%h2) then
        write (u, "(A)", advance="no") "|"
        write (u, "(IO)", advance="no") hel%h2
      end if
    end if
  end subroutine helicity_write

```

```

        end if
        write (u, "(A)", advance="no")  " ) "
    end if
end subroutine helicity_write

```

Binary I/O. Write contents only if defined.

```

<Helicities: helicity: TBP>+≡
    procedure :: write_raw => helicity_write_raw
    procedure :: read_raw => helicity_read_raw

<Helicities: procedures>+≡
    subroutine helicity_write_raw (hel, u)
        class(helicity_t), intent(in) :: hel
        integer, intent(in) :: u
        write (u) hel%defined
        if (hel%defined) then
            write (u) hel%h1, hel%h2
        end if
    end subroutine helicity_write_raw

    subroutine helicity_read_raw (hel, u, iostat)
        class(helicity_t), intent(out) :: hel
        integer, intent(in) :: u
        integer, intent(out), optional :: iostat
        read (u, iostat=iostat) hel%defined
        if (hel%defined) then
            read (u, iostat=iostat) hel%h1, hel%h2
        end if
    end subroutine helicity_read_raw

```

11.3.2 Predicates

Check if the helicity is defined:

```

<Helicities: helicity: TBP>+≡
    procedure :: is_defined => helicity_is_defined

<Helicities: procedures>+≡
    elemental function helicity_is_defined (hel) result (defined)
        logical :: defined
        class(helicity_t), intent(in) :: hel
        defined = hel%defined
    end function helicity_is_defined

```

Return true if the two helicities are equal or the particle is unpolarized:

```

<Helicities: helicity: TBP>+≡
    procedure :: is_diagonal => helicity_is_diagonal

<Helicities: procedures>+≡
    elemental function helicity_is_diagonal (hel) result (diagonal)
        logical :: diagonal
        class(helicity_t), intent(in) :: hel
        if (hel%defined) then

```



```

        diagonal = hel%h1 == hel%h2
    else
        diagonal = .true.
    end if
end function helicity_is_diagonal

```

11.3.3 Accessing contents

This returns a two-element array and thus cannot be elemental. The result is unpredictable if the helicity is undefined.

```

<Helicities: helicity: TBP>+≡
    procedure :: to_pair => helicity_to_pair

<Helicities: procedures>+≡
    pure function helicity_to_pair (hel) result (h)
        integer, dimension(2) :: h
        class(helicity_t), intent(in) :: hel
        h(1) = hel%h2
        h(2) = hel%h1
    end function helicity_to_pair

```

11.3.4 Comparisons

When comparing helicities, if either one is undefined, they are considered to match. In other words, an unpolarized particle matches any polarization. In the `dmatch` variant, it matches only diagonal helicity.

```

<Helicities: helicity: TBP>+≡
    generic :: operator(.match.) => helicity_match
    generic :: operator(.dmatch.) => helicity_match_diagonal
    generic :: operator(==) => helicity_eq
    generic :: operator(/=) => helicity_neq
    procedure, private :: helicity_match
    procedure, private :: helicity_match_diagonal
    procedure, private :: helicity_eq
    procedure, private :: helicity_neq

<Helicities: procedures>+≡
    elemental function helicity_match (hel1, hel2) result (eq)
        logical :: eq
        class(helicity_t), intent(in) :: hel1, hel2
        if (hel1%defined .and. hel2%defined) then
            eq = (hel1%h1 == hel2%h1) .and. (hel1%h2 == hel2%h2)
        else
            eq = .true.
        end if
    end function helicity_match

    elemental function helicity_match_diagonal (hel1, hel2) result (eq)
        logical :: eq
        class(helicity_t), intent(in) :: hel1, hel2
        if (hel1%defined .and. hel2%defined) then

```

```

        eq = (hel1%h1 == hel2%h1) .and. (hel1%h2 == hel2%h2)
    else if (hel1%defined) then
        eq = hel1%h1 == hel1%h2
    else if (hel2%defined) then
        eq = hel2%h1 == hel2%h2
    else
        eq = .true.
    end if
end function helicity_match_diagonal

```

<Helicities: procedures>+≡

```

elemental function helicity_eq (hel1, hel2) result (eq)
    logical :: eq
    class(helicity_t), intent(in) :: hel1, hel2
    if (hel1%defined .and. hel2%defined) then
        eq = (hel1%h1 == hel2%h1) .and. (hel1%h2 == hel2%h2)
    else if (.not. hel1%defined .and. .not. hel2%defined) then
        eq = .true.
    else
        eq = .false.
    end if
end function helicity_eq

```

<Helicities: procedures>+≡

```

elemental function helicity_neq (hel1, hel2) result (neq)
    logical :: neq
    class(helicity_t), intent(in) :: hel1, hel2
    if (hel1%defined .and. hel2%defined) then
        neq = (hel1%h1 /= hel2%h1) .or. (hel1%h2 /= hel2%h2)
    else if (.not. hel1%defined .and. .not. hel2%defined) then
        neq = .false.
    else
        neq = .true.
    end if
end function helicity_neq

```

11.3.5 Tools

Merge two helicity objects by taking the first entry from the first and the second entry from the second argument. Makes sense only if the input helicities were defined and diagonal. The handling of ghost flags is not well-defined; one should verify beforehand that they match.

<Helicities: helicity: TBP>+≡

```

generic :: operator(.merge.) => merge_helicities
procedure, private :: merge_helicities

```

<Helicities: procedures>+≡

```

elemental function merge_helicities (hel1, hel2) result (hel)
    type(helicity_t) :: hel
    class(helicity_t), intent(in) :: hel1, hel2
    if (hel1%defined .and. hel2%defined) then
        call hel%init (hel2%h1, hel1%h1)
    end if
end function merge_helicities

```

```
else if (hel1%defined) then
  call hel%init (hel1%h2, hel1%h1)
else if (hel2%defined) then
  call hel%init (hel2%h2, hel2%h1)
end if
end function merge_helicities
```

11.4 Colors

This module defines a type and tools for dealing with color information.

Each particle can have zero or more (in practice, usually not more than two) color indices. Color indices are positive; flow direction can be determined from the particle nature.

While parton shower matrix elements are diagonal in color, some special applications (e.g., subtractions for NLO matrix elements) require non-diagonal color matrices.

```
<colors.f90>≡  
  <File header>  
  
  module colors  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use diagnostics  
  
    <Standard module head>  
  
    <Colors: public>  
  
    <Colors: types>  
  
    <Colors: interfaces>  
  
    contains  
  
    <Colors: procedures>  
  
  end module colors
```

11.4.1 The color type

A particle may have an arbitrary number of color indices (in practice, from zero to two, but more are possible). This object acts as a container. (The current implementation has a fixed array of length two.)

The fact that color comes as an array prohibits elemental procedures in some places. (May add interfaces and multi versions where necessary.)

The color may be undefined.

NOTE: Due to a compiler bug in nagfor 5.2, we do not use allocatable but fixed-size arrays with dimension 2. Only nonzero entries count. This may be more efficient anyway, but gives up some flexibility. However, the squaring algorithm currently works only for singlets, (anti)triplets and octets anyway, so two components are enough.

This type has to be generalized (abstract type and specific implementations) when trying to pursue generalized color flows or Monte Carlo over continuous color.

```
<Colors: public>≡  
  public :: color_t
```

```

<Colors: types>≡
  type :: color_t
  private
    logical :: defined = .false.
    integer, dimension(2) :: c1 = 0, c2 = 0
    logical :: ghost = .false.
  contains
    <Colors: color: TBP>
  end type color_t

```

Initializers:

```

<Colors: color: TBP>≡
  generic :: init => &
    color_init_trivial, color_init_trivial_ghost, &
    color_init_array, color_init_array_ghost, &
    color_init_arrays, color_init_arrays_ghost
  procedure, private :: color_init_trivial
  procedure, private :: color_init_trivial_ghost
  procedure, private :: color_init_array
  procedure, private :: color_init_array_ghost
  procedure, private :: color_init_arrays
  procedure, private :: color_init_arrays_ghost

```

Undefined color: array remains unallocated

```

<Colors: procedures>≡
  pure subroutine color_init_trivial (col)
    class(color_t), intent(inout) :: col
    col%defined = .true.
    col%c1 = 0
    col%c2 = 0
    col%ghost = .false.
  end subroutine color_init_trivial

  pure subroutine color_init_trivial_ghost (col, ghost)
    class(color_t), intent(inout) :: col
    logical, intent(in) :: ghost
    col%defined = .true.
    col%c1 = 0
    col%c2 = 0
    col%ghost = ghost
  end subroutine color_init_trivial_ghost

```

This defines color from an arbitrary length color array, suitable for any representation. We may have two color arrays (non-diagonal matrix elements). This cannot be elemental. The third version assigns an array of colors, using a two-dimensional array as input.

```

<Colors: procedures>+≡
  pure subroutine color_init_array (col, c1)
    class(color_t), intent(inout) :: col
    integer, dimension(:), intent(in) :: c1
    col%defined = .true.
    col%c1 = pack (c1, c1 /= 0, [0,0])
    col%c2 = col%c1

```

```

        col%ghost = .false.
    end subroutine color_init_array

    pure subroutine color_init_array_ghost (col, c1, ghost)
        class(color_t), intent(inout) :: col
        integer, dimension(:), intent(in) :: c1
        logical, intent(in) :: ghost
        call color_init_array (col, c1)
        col%ghost = ghost
    end subroutine color_init_array_ghost

    pure subroutine color_init_arrays (col, c1, c2)
        class(color_t), intent(inout) :: col
        integer, dimension(:), intent(in) :: c1, c2
        col%defined = .true.
        if (size (c1) == size (c2)) then
            col%c1 = pack (c1, c1 /= 0, [0,0])
            col%c2 = pack (c2, c2 /= 0, [0,0])
        else if (size (c1) /= 0) then
            col%c1 = pack (c1, c1 /= 0, [0,0])
            col%c2 = col%c1
        else if (size (c2) /= 0) then
            col%c1 = pack (c2, c2 /= 0, [0,0])
            col%c2 = col%c1
        end if
        col%ghost = .false.
    end subroutine color_init_arrays

    pure subroutine color_init_arrays_ghost (col, c1, c2, ghost)
        class(color_t), intent(inout) :: col
        integer, dimension(:), intent(in) :: c1, c2
        logical, intent(in) :: ghost
        call color_init_arrays (col, c1, c2)
        col%ghost = ghost
    end subroutine color_init_arrays_ghost

```

This version is restricted to singlets, triplets, antitriplets, and octets: The input contains the color and anticolor index, each of the may be zero.

<Colors: color: TBP>+≡

```

    procedure :: init_col_acl => color_init_col_acl

```

<Colors: procedures>+≡

```

    elemental subroutine color_init_col_acl (col, col_in, acl_in)
        class(color_t), intent(inout) :: col
        integer, intent(in) :: col_in, acl_in
        integer, dimension(0) :: null_array
        select case (col_in)
        case (0)
            select case (acl_in)
            case (0)
                call color_init_array (col, null_array)
            case default
                call color_init_array (col, [-acl_in])
            end select
        end select
    end subroutine color_init_col_acl

```

```

case default
  select case (acl_in)
  case (0)
    call color_init_array (col, [col_in])
  case default
    call color_init_array (col, [col_in, -acl_in])
  end select
end select
end subroutine color_init_col_acl

```

This version is used for the external interface. We convert a fixed-size array of colors (for each particle) to the internal form by packing only the nonzero entries.

Some of these procedures produce an array, so they can't be all type-bound. We implement them as ordinary procedures.

<Colors: public>+≡

```
public :: color_init_from_array
```

<Colors: interfaces>≡

```

interface color_init_from_array
  module procedure color_init_from_array1
  module procedure color_init_from_array1g
  module procedure color_init_from_array2
  module procedure color_init_from_array2g
end interface color_init_from_array

```

<Colors: procedures>+≡

```

pure subroutine color_init_from_array1 (col, c1)
  type(color_t), intent(inout) :: col
  integer, dimension(:), intent(in) :: c1
  logical, dimension(size(c1)) :: mask
  mask = c1 /= 0
  col%defined = .true.
  col%c1 = pack (c1, mask, col%c1)
  col%c2 = col%c1
  col%ghost = .false.
end subroutine color_init_from_array1

pure subroutine color_init_from_array1g (col, c1, ghost)
  type(color_t), intent(inout) :: col
  integer, dimension(:), intent(in) :: c1
  logical, intent(in) :: ghost
  call color_init_from_array1 (col, c1)
  col%ghost = ghost
end subroutine color_init_from_array1g

pure subroutine color_init_from_array2 (col, c1)
  integer, dimension(:, :), intent(in) :: c1
  type(color_t), dimension(:), intent(inout) :: col
  integer :: i
  do i = 1, size (c1,2)
    call color_init_from_array1 (col(i), c1(:,i))
  end do

```

```

end subroutine color_init_from_array2

pure subroutine color_init_from_array2g (col, c1, ghost)
  integer, dimension(:,:), intent(in) :: c1
  type(color_t), dimension(:), intent(out) :: col
  logical, intent(in), dimension(:) :: ghost
  call color_init_from_array2 (col, c1)
  col%ghost = ghost
end subroutine color_init_from_array2g

```

Set the ghost property

```

<Colors: color: TBP>+≡
  procedure :: set_ghost => color_set_ghost

<Colors: procedures>+≡
  elemental subroutine color_set_ghost (col, ghost)
    class(color_t), intent(inout) :: col
    logical, intent(in) :: ghost
    col%ghost = ghost
  end subroutine color_set_ghost

```

Undefine the color state:

```

<Colors: color: TBP>+≡
  procedure :: undefine => color_undefine

<Colors: procedures>+≡
  elemental subroutine color_undefine (col, undefine_ghost)
    class(color_t), intent(inout) :: col
    logical, intent(in), optional :: undefine_ghost
    col%defined = .false.
    if (present (undefine_ghost)) then
      if (undefine_ghost) col%ghost = .false.
    else
      col%ghost = .false.
    end if
  end subroutine color_undefine

```

Output. As dense as possible, no linebreak. If color is undefined, no output.

The separate version for a color array suggest two distinct interfaces.

```

<Colors: public>+≡
  public :: color_write

<Colors: interfaces>+≡
  interface color_write
    module procedure color_write_single
    module procedure color_write_array
  end interface color_write

<Colors: color: TBP>+≡
  procedure :: write => color_write_single

```


<Colors: procedures>+≡

```

subroutine color_write_single (col, unit)
  class(color_t), intent(in) :: col
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  if (col%ghost) then
    write (u, "(A)", advance="no") "c*"
  else if (col%defined) then
    write (u, "(A)", advance="no") "c("
    if (col%c1(1) /= 0) write (u, "(I0)", advance="no") col%c1(1)
    if (any (col%c1 /= 0)) write (u, "(1x)", advance="no")
    if (col%c1(2) /= 0) write (u, "(I0)", advance="no") col%c1(2)
    if (.not. col%is_diagonal ()) then
      write (u, "(A)", advance="no") "|"
      if (col%c2(1) /= 0) write (u, "(I0)", advance="no") col%c2(1)
      if (any (col%c2 /= 0)) write (u, "(1x)", advance="no")
      if (col%c2(2) /= 0) write (u, "(I0)", advance="no") col%c2(2)
    end if
    write (u, "(A)", advance="no") ")"
  end if
end subroutine color_write_single

subroutine color_write_array (col, unit)
  type(color_t), dimension(:), intent(in) :: col
  integer, intent(in), optional :: unit
  integer :: u
  integer :: i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(A)", advance="no") "["
  do i = 1, size (col)
    if (i > 1) write (u, "(1x)", advance="no")
    call color_write_single (col(i), u)
  end do
  write (u, "(A)", advance="no") "]"
end subroutine color_write_array

```

Binary I/O. For allocatable colors, this would have to be modified.

<Colors: color: TBP>+≡

```

procedure :: write_raw => color_write_raw
procedure :: read_raw => color_read_raw

```

<Colors: procedures>+≡

```

subroutine color_write_raw (col, u)
  class(color_t), intent(in) :: col
  integer, intent(in) :: u
  logical :: defined
  defined = col%is_defined () .or. col%is_ghost ()
  write (u) defined
  if (defined) then
    write (u) col%c1, col%c2
    write (u) col%ghost
  end if
end subroutine color_write_raw

```

```

subroutine color_read_raw (col, u, iostat)
  class(color_t), intent(inout) :: col
  integer, intent(in) :: u
  integer, intent(out), optional :: iostat
  logical :: defined
  read (u, iostat=iostat) col%defined
  if (col%defined) then
    read (u, iostat=iostat) col%c1, col%c2
    read (u, iostat=iostat) col%ghost
  end if
end subroutine color_read_raw

```

11.4.2 Predicates

Return the definition status. A color state may be defined but trivial.

```

<Colors: color: TBP>+≡
  procedure :: is_defined => color_is_defined
  procedure :: is_nonzero => color_is_nonzero

<Colors: procedures>+≡
  elemental function color_is_defined (col) result (defined)
    logical :: defined
    class(color_t), intent(in) :: col
    defined = col%defined
  end function color_is_defined

  elemental function color_is_nonzero (col) result (flag)
    logical :: flag
    class(color_t), intent(in) :: col
    flag = col%defined &
      .and. .not. col%ghost &
      .and. any (col%c1 /= 0 .or. col%c2 /= 0)
  end function color_is_nonzero

```

Diagonal color objects have only one array allocated:

```

<Colors: color: TBP>+≡
  procedure :: is_diagonal => color_is_diagonal

<Colors: procedures>+≡
  elemental function color_is_diagonal (col) result (diagonal)
    logical :: diagonal
    class(color_t), intent(in) :: col
    if (col%defined) then
      diagonal = all (col%c1 == col%c2)
    else
      diagonal = .true.
    end if
  end function color_is_diagonal

```

Return the ghost flag

```

<Colors: color: TBP>+≡
  procedure :: is_ghost => color_is_ghost

```

```

<Colors: procedures>+≡
  elemental function color_is_ghost (col) result (ghost)
    logical :: ghost
    class(color_t), intent(in) :: col
    ghost = col%ghost
  end function color_is_ghost

```

The ghost parity: true if the color-ghost flag is set. Again, no TBP since this is an array.

```

<Colors: procedures>+≡
  pure function color_ghost_parity (col) result (parity)
    type(color_t), dimension(:), intent(in) :: col
    logical :: parity
    parity = mod (count (col%ghost), 2) == 1
  end function color_ghost_parity

```

Determine the color representation, given a color object. We allow only singlet (1), (anti)triplet (± 3), and octet states (8). A color ghost must not have color assigned, but the color type is 8. For non-diagonal color, representations must match. If the color type is undefined, return 0. If it is invalid or unsupported, return -1 .

Assumption: nonzero entries precede nonzero ones.

```

<Colors: color: TBP>+≡
  procedure :: get_type => color_get_type

<Colors: procedures>+≡
  elemental function color_get_type (col) result (ctype)
    class(color_t), intent(in) :: col
    integer :: ctype
    if (col%defined) then
      ctype = -1
      if (col%ghost) then
        if (all (col%c1 == 0 .and. col%c2 == 0)) then
          ctype = 8
        end if
      else
        if (all ((col%c1 == 0 .and. col%c2 == 0) &
          & .or. (col%c1 > 0 .and. col%c2 > 0) &
          & .or. (col%c1 < 0 .and. col%c2 < 0))) then
          if (all (col%c1 == 0)) then
            ctype = 1
          else if ((col%c1(1) > 0 .and. col%c1(2) == 0)) then
            ctype = 3
          else if ((col%c1(1) < 0 .and. col%c1(2) == 0)) then
            ctype = -3
          else if ((col%c1(1) > 0 .and. col%c1(2) < 0) &
            .or. (col%c1(1) < 0 .and. col%c1(2) > 0)) then
            ctype = 8
          end if
        end if
      end if
    else
      ctype = 0
    end if
  end function color_get_type

```

```

        end if
    end function color_get_type

```

11.4.3 Accessing contents

Return the number of color indices. We assume that it is identical for both arrays.

```

<Colors: color: TBP>+≡
    procedure, private :: get_number_of_indices => color_get_number_of_indices

<Colors: procedures>+≡
    elemental function color_get_number_of_indices (col) result (n)
        integer :: n
        class(color_t), intent(in) :: col
        if (col%defined .and. .not. col%ghost) then
            n = count (col%c1 /= 0)
        else
            n = 0
        end if
    end function color_get_number_of_indices

```

Return the (first) color/anticolor entry (assuming that color is diagonal). The result is a positive color index.

```

<Colors: color: TBP>+≡
    procedure :: get_col => color_get_col
    procedure :: get_acl => color_get_acl

<Colors: procedures>+≡
    elemental function color_get_col (col) result (c)
        integer :: c
        class(color_t), intent(in) :: col
        integer :: i
        if (col%defined .and. .not. col%ghost) then
            do i = 1, size (col%c1)
                if (col%c1(i) > 0) then
                    c = col%c1(i)
                    return
                end if
            end do
        end if
        c = 0
    end function color_get_col

    elemental function color_get_acl (col) result (c)
        integer :: c
        class(color_t), intent(in) :: col
        integer :: i
        if (col%defined .and. .not. col%ghost) then
            do i = 1, size (col%c1)
                if (col%c1(i) < 0) then
                    c = - col%c1(i)
                    return
                end if
            end do
        end if
        c = 0
    end function color_get_acl

```

```

        end if
    end do
end if
c = 0
end function color_get_acl

```

Return the color index with highest absolute value

```

<Colors: public>+≡
    public :: color_get_max_value

<Colors: interfaces>+≡
    interface color_get_max_value
        module procedure color_get_max_value0
        module procedure color_get_max_value1
        module procedure color_get_max_value2
    end interface color_get_max_value

<Colors: procedures>+≡
    elemental function color_get_max_value0 (col) result (cmax)
        integer :: cmax
        type(color_t), intent(in) :: col
        if (col%defined .and. .not. col%ghost) then
            cmax = maxval (abs (col%c1))
        else
            cmax = 0
        end if
    end function color_get_max_value0

    pure function color_get_max_value1 (col) result (cmax)
        integer :: cmax
        type(color_t), dimension(:), intent(in) :: col
        cmax = maxval (color_get_max_value0 (col))
    end function color_get_max_value1

    pure function color_get_max_value2 (col) result (cmax)
        integer :: cmax
        type(color_t), dimension(:, :), intent(in) :: col
        integer, dimension(size(col, 2)) :: cm
        integer :: i
        forall (i = 1:size(col, 2))
            cm(i) = color_get_max_value1 (col(:,i))
        end forall
        cmax = maxval (cm)
    end function color_get_max_value2

```

11.4.4 Comparisons

Similar to helicities, colors match if they are equal, or if either one is undefined.

```

<Colors: color: TBP>+≡
    generic :: operator(.match.) => color_match
    generic :: operator(==) => color_eq
    generic :: operator(/=) => color_neq

```

```

procedure, private :: color_match
procedure, private :: color_eq
procedure, private :: color_neq

(Colors: procedures) +=
  elemental function color_match (col1, col2) result (eq)
    logical :: eq
    class(color_t), intent(in) :: col1, col2
    if (col1%defined .and. col2%defined) then
      if (col1%ghost .and. col2%ghost) then
        eq = .true.
      else if (.not. col1%ghost .and. .not. col2%ghost) then
        eq = all (col1%c1 == col2%c1) .and. all (col1%c2 == col2%c2)
      else
        eq = .false.
      end if
    else
      eq = .true.
    end if
  end function color_match

  elemental function color_eq (col1, col2) result (eq)
    logical :: eq
    class(color_t), intent(in) :: col1, col2
    if (col1%defined .and. col2%defined) then
      if (col1%ghost .and. col2%ghost) then
        eq = .true.
      else if (.not. col1%ghost .and. .not. col2%ghost) then
        eq = all (col1%c1 == col2%c1) .and. all (col1%c2 == col2%c2)
      else
        eq = .false.
      end if
    else if (.not. col1%defined &
      .and. .not. col2%defined) then
      eq = col1%ghost .eqv. col2%ghost
    else
      eq = .false.
    end if
  end function color_eq

(Colors: procedures) +=
  elemental function color_neq (col1, col2) result (neq)
    logical :: neq
    class(color_t), intent(in) :: col1, col2
    if (col1%defined .and. col2%defined) then
      if (col1%ghost .and. col2%ghost) then
        neq = .false.
      else if (.not. col1%ghost .and. .not. col2%ghost) then
        neq = any (col1%c1 /= col2%c1) .or. any (col1%c2 /= col2%c2)
      else
        neq = .true.
      end if
    else if (.not. col1%defined &
      .and. .not. col2%defined) then

```

```

        neq = col1%ghost .neqv. col2%ghost
    else
        neq = .true.
    end if
end function color_neq

```

11.4.5 Tools

Shift color indices by a common offset.

```

<Colors: color: TBP>+≡
    procedure :: add_offset => color_add_offset

<Colors: procedures>+≡
    elemental subroutine color_add_offset (col, offset)
        class(color_t), intent(inout) :: col
        integer, intent(in) :: offset
        if (col%defined .and. .not. col%ghost) then
            where (col%c1 /= 0) col%c1 = col%c1 + sign (offset, col%c1)
            where (col%c2 /= 0) col%c2 = col%c2 + sign (offset, col%c2)
        end if
    end subroutine color_add_offset

```

Reassign color indices for an array of colored particle in canonical order. The allocated size of the color map is such that two colors per particle can be accommodated.

The algorithm works directly on the contents of the color objects, it

```

<Colors: public>+≡
    public :: color_canonicalize

<Colors: procedures>+≡
    subroutine color_canonicalize (col)
        type(color_t), dimension(:), intent(inout) :: col
        integer, dimension(2*size(col)) :: map
        integer :: n_col, i, j, k
        n_col = 0
        do i = 1, size (col)
            if (col(i)%defined .and. .not. col(i)%ghost) then
                do j = 1, size (col(i)%c1)
                    if (col(i)%c1(j) /= 0) then
                        k = find (abs (col(i)%c1(j)), map(:n_col))
                        if (k == 0) then
                            n_col = n_col + 1
                            map(n_col) = abs (col(i)%c1(j))
                            k = n_col
                        end if
                        col(i)%c1(j) = sign (k, col(i)%c1(j))
                    end if
                end do
                if (col(i)%c2(j) /= 0) then
                    k = find (abs (col(i)%c2(j)), map(:n_col))
                    if (k == 0) then
                        n_col = n_col + 1
                        map(n_col) = abs (col(i)%c2(j))
                    end if
                end if
            end if
        end do
    end subroutine color_canonicalize

```

```

        k = n_col
    end if
    col(i)%c2(j) = sign (k, col(i)%c2(j))
end if
end do
end if
end do
contains
function find (c, array) result (k)
    integer :: k
    integer, intent(in) :: c
    integer, dimension(:), intent(in) :: array
    integer :: i
    k = 0
    do i = 1, size (array)
        if (c == array (i)) then
            k = i
            return
        end if
    end do
end function find
end subroutine color_canonicalize

```

Return an array of different color indices from an array of colors. The last argument is a pseudo-color array, where the color entries correspond to the position of the corresponding index entry in the index array. The colors are assumed to be diagonal.

The algorithm works directly on the contents of the color objects.

(Colors: procedures)+≡

```

subroutine extract_color_line_indices (col, c_index, col_pos)
    type(color_t), dimension(:), intent(in) :: col
    integer, dimension(:), intent(out), allocatable :: c_index
    type(color_t), dimension(size(col)), intent(out) :: col_pos
    integer, dimension(:), allocatable :: c_tmp
    integer :: i, j, k, n, c
    allocate (c_tmp (sum (col%get_number_of_indices ())), source=0)
    n = 0
    SCAN1: do i = 1, size (col)
        if (col(i)%defined .and. .not. col(i)%ghost) then
            SCAN2: do j = 1, 2
                c = abs (col(i)%c1(j))
                if (c /= 0) then
                    do k = 1, n
                        if (c_tmp(k) == c) then
                            col_pos(i)%c1(j) = k
                            cycle SCAN2
                        end if
                    end do
                    n = n + 1
                    c_tmp(n) = c
                    col_pos(i)%c1(j) = n
                end if
            end do SCAN2
        end do SCAN1
    end do SCAN1

```



```

        end if
    end do SCAN1
    allocate (c_index (n))
    c_index = c_tmp(1:n)
end subroutine extract_color_line_indices

```

Given a color array, pairwise contract the color lines in all possible ways and return the resulting array of arrays. The input color array must be diagonal, and each color should occur exactly twice, once as color and once as anticolor.

Gluon entries with equal color and anticolor are explicitly excluded.

This algorithm is generic, but for long arrays it is neither efficient, nor does it avoid duplicates. It is intended for small arrays, in particular for the state matrix of a structure-function pair.

The algorithm works directly on the contents of the color objects, it thus depends on the implementation.

```

<Colors: public>+≡
    public :: color_array_make_contractions

<Colors: procedures>+≡
    subroutine color_array_make_contractions (col_in, col_out)
        type(color_t), dimension(:), intent(in) :: col_in
        type(color_t), dimension(:,:), intent(out), allocatable :: col_out
        type :: entry_t
            integer, dimension(:), allocatable :: map
            type(color_t), dimension(:), allocatable :: col
            type(entry_t), pointer :: next => null ()
            logical :: nlo_event = .false.
        end type entry_t
        type :: list_t
            integer :: n = 0
            type(entry_t), pointer :: first => null ()
            type(entry_t), pointer :: last => null ()
        end type list_t
        type(list_t) :: list
        type(entry_t), pointer :: entry
        integer, dimension(:), allocatable :: c_index
        type(color_t), dimension(size(col_in)) :: col_pos
        integer :: n_prt, n_c_index
        integer, dimension(:), allocatable :: map
        integer :: i, j, c
        n_prt = size (col_in)
        call extract_color_line_indices (col_in, c_index, col_pos)
        n_c_index = size (c_index)
        allocate (map (n_c_index))
        map = 0
        call list_append_if_valid (list, map)
        entry => list%first
        do while (associated (entry))
            do i = 1, n_c_index
                if (entry%map(i) == 0) then
                    c = c_index(i)
                    do j = i + 1, n_c_index
                        if (entry%map(j) == 0) then

```

```

        map = entry%map
        map(i) = c
        map(j) = c
        call list_append_if_valid (list, map)
    end if
end do
end if
end do
entry => entry%next
end do
call list_to_array (list, col_out)
contains
subroutine list_append_if_valid (list, map)
    type(list_t), intent(inout) :: list
    integer, dimension(:), intent(in) :: map
    type(entry_t), pointer :: entry
    integer :: i, j, c, p
    entry => list%first
    do while (associated (entry))
        if (all (map == entry%map)) return
        entry => entry%next
    end do
    allocate (entry)
    allocate (entry%map (n_c_index))
    entry%map = map
    allocate (entry%col (n_prt))
    do i = 1, n_prt
        do j = 1, 2
            c = col_in(i)%c1(j)
            if (c /= 0) then
                p = col_pos(i)%c1(j)
                entry%col(i)%defined = .true.
                if (map(p) /= 0) then
                    entry%col(i)%c1(j) = sign (map(p), c)
                else
                    entry%col(i)%c1(j) = c
                endif
            endif
            entry%col(i)%c2(j) = entry%col(i)%c1(j)
        end if
    end do
    if (any (entry%col(i)%c1 /= 0) .and. &
        entry%col(i)%c1(1) == - entry%col(i)%c1(2)) return
end do
    if (associated (list%last)) then
        list%last%next => entry
    else
        list%first => entry
    end if
    list%last => entry
    list%n = list%n + 1
end subroutine list_append_if_valid
subroutine list_to_array (list, col)
    type(list_t), intent(inout) :: list
    type(color_t), dimension(:,:), intent(out), allocatable :: col

```

```

    type(entry_t), pointer :: entry
    integer :: i
    allocate (col (n_prt, list%n - 1))
    do i = 0, list%n - 1
        entry => list%first
        list%first => list%first%next
        if (i /= 0) col(:,i) = entry%col
        deallocate (entry)
    end do
    list%last => null ()
end subroutine list_to_array
end subroutine color_array_make_contractions

```

Invert the color index, switching from particle to antiparticle. For gluons, we have to swap the order of color entries.

```

<Colors: color: TBP>+≡
    procedure :: invert => color_invert

<Colors: procedures>+≡
    elemental subroutine color_invert (col)
        class(color_t), intent(inout) :: col
        if (col%defined .and. .not. col%ghost) then
            col%c1 = - col%c1
            col%c2 = - col%c2
            if (col%c1(1) < 0 .and. col%c1(2) > 0) then
                col%c1 = col%c1(2:1:-1)
                col%c2 = col%c2(2:1:-1)
            end if
        end if
    end subroutine color_invert

```

Make a color map for two matching color arrays. The result is an array of integer pairs.

```

<Colors: public>+≡
    public :: make_color_map

<Colors: interfaces>+≡
    interface make_color_map
        module procedure color_make_color_map
    end interface make_color_map

<Colors: procedures>+≡
    subroutine color_make_color_map (map, col1, col2)
        integer, dimension(:,:), intent(out), allocatable :: map
        type(color_t), dimension(:), intent(in) :: col1, col2
        integer, dimension(:,:), allocatable :: map1
        integer :: i, j, k
        allocate (map1 (2, 2 * sum (col1%get_number_of_indices ())))
        k = 0
        do i = 1, size (col1)
            if (col1(i)%defined .and. .not. col1(i)%ghost) then
                do j = 1, size (col1(i)%c1)
                    if (col1(i)%c1(j) /= 0 &

```

```

        .and. all (map1(1,:k) /= abs (col1(i)%c1(j)))) then
        k = k + 1
        map1(1,k) = abs (col1(i)%c1(j))
        map1(2,k) = abs (col2(i)%c1(j))
    end if
    if (col1(i)%c2(j) /= 0 &
        .and. all (map1(1,:k) /= abs (col1(i)%c2(j)))) then
        k = k + 1
        map1(1,k) = abs (col1(i)%c2(j))
        map1(2,k) = abs (col2(i)%c2(j))
    end if
end do
end if
end do
allocate (map (2, k))
map(:, :) = map1(:, :k)
end subroutine color_make_color_map

```

Translate colors which have a match in the translation table (an array of integer pairs). Color that do not match an entry are simply transferred; this is done by first transferring all components, then modifying entries where appropriate.

```

<Colors: public>+≡
    public :: color_translate

<Colors: interfaces>+≡
    interface color_translate
        module procedure color_translate0
        module procedure color_translate0_offset
        module procedure color_translate1
    end interface color_translate

<Colors: procedures>+≡
    subroutine color_translate0 (col, map)
        type(color_t), intent(inout) :: col
        integer, dimension(:, :), intent(in) :: map
        type(color_t) :: col_tmp
        integer :: i
        if (col%defined .and. .not. col%ghost) then
            col_tmp = col
            do i = 1, size (map,2)
                where (abs (col%c1) == map(1,i))
                    col_tmp%c1 = sign (map(2,i), col%c1)
                end where
                where (abs (col%c2) == map(1,i))
                    col_tmp%c2 = sign (map(2,i), col%c2)
                end where
            end do
            col = col_tmp
        end if
    end subroutine color_translate0

    subroutine color_translate0_offset (col, map, offset)
        type(color_t), intent(inout) :: col

```

```

integer, dimension(:, :), intent(in) :: map
integer, intent(in) :: offset
logical, dimension(size(col%c1)) :: mask1, mask2
type(color_t) :: col_tmp
integer :: i
if (col%defined .and. .not. col%ghost) then
    col_tmp = col
    mask1 = col%c1 /= 0
    mask2 = col%c2 /= 0
    do i = 1, size (map,2)
        where (abs (col%c1) == map(1,i))
            col_tmp%c1 = sign (map(2,i), col%c1)
            mask1 = .false.
        end where
        where (abs (col%c2) == map(1,i))
            col_tmp%c2 = sign (map(2,i), col%c2)
            mask2 = .false.
        end where
    end do
    col = col_tmp
    where (mask1) col%c1 = sign (abs (col%c1) + offset, col%c1)
    where (mask2) col%c2 = sign (abs (col%c2) + offset, col%c2)
end if
end subroutine color_translate0_offset

subroutine color_translate1 (col, map, offset)
type(color_t), dimension(:), intent(inout) :: col
integer, dimension(:, :), intent(in) :: map
integer, intent(in), optional :: offset
integer :: i
if (present (offset)) then
    do i = 1, size (col)
        call color_translate0_offset (col(i), map, offset)
    end do
else
    do i = 1, size (col)
        call color_translate0 (col(i), map)
    end do
end if
end subroutine color_translate1

```

Merge two color objects by taking the first entry from the first and the first entry from the second argument. Makes sense only if the input colors are defined (and diagonal). If either one is undefined, transfer the defined one.

```

<Colors: color: TBP>+≡
    generic :: operator(.merge.) => merge_colors
    procedure, private :: merge_colors

<Colors: procedures>+≡
    elemental function merge_colors (col1, col2) result (col)
    type(color_t) :: col
    class(color_t), intent(in) :: col1, col2
    if (color_is_defined (col1) .and. color_is_defined (col2)) then
        if (color_is_ghost (col1) .and. color_is_ghost (col2)) then

```

```

        call color_init_trivial_ghost (col, .true.)
    else
        call color_init_arrays (col, col1%c1, col2%c1)
    end if
    else if (color_is_defined (col1)) then
        call color_init_array (col, col1%c1)
    else if (color_is_defined (col2)) then
        call color_init_array (col, col2%c1)
    end if
end function merge_colors

```

Merge up to two (diagonal!) color objects. The result inherits the unmatched color lines of the input colors. If one of the input colors is undefined, the output is undefined as well. It must be in a supported color representation.

A color-ghost object should not actually occur in real-particle events, but for completeness we define its behavior. For simplicity, it is identified as a color-octet with zero color/anticolor. It can only couple to a triplet or antitriplet. A fusion of triplet with matching antitriplet will yield a singlet, not a ghost, however.

If the fusion fails, the result is undefined.

```

<Colors: color: TBP>+=
    generic :: operator (.fuse.) => color_fusion
    procedure, private :: color_fusion

<Colors: procedures>+=
    function color_fusion (col1, col2) result (col)
        class(color_t), intent(in) :: col1, col2
        type(color_t) :: col
        integer, dimension(2) :: ctype
        if (col1%is_defined () .and. col2%is_defined ()) then
            if (col1%is_diagonal () .and. col2%is_diagonal ()) then
                ctype = [col1%get_type (), col2%get_type ()]
                select case (ctype(1))
                    case (1)
                        select case (ctype(2))
                            case (1,3,-3,8)
                                col = col2
                            end select
                        end select
                    case (3)
                        select case (ctype(2))
                            case (1)
                                col = col1
                            case (-3)
                                call t_a (col1%get_col (), col2%get_acl ())
                            case (8)
                                call t_o (col1%get_col (), col2%get_acl (), &
                                    & col2%get_col ())
                            end select
                        end select
                    case (-3)
                        select case (ctype(2))
                            case (1)
                                col = col1
                            case (3)

```

```

        call t_a (col2%get_col (), col1%get_acl ())
    case (8)
        call a_o (col1%get_acl (), col2%get_col (), &
            & col2%get_acl ())
    end select
case (8)
    select case (ctype(2))
    case (1)
        col = col1
    case (3)
        call t_o (col2%get_col (), col1%get_acl (), &
            & col1%get_col ())
    case (-3)
        call a_o (col2%get_acl (), col1%get_col (), &
            & col1%get_acl ())
    case (8)
        call o_o (col1%get_col (), col1%get_acl (), &
            & col2%get_col (), col2%get_acl ())
    end select
    end select
end if
end if
contains
subroutine t_a (c1, c2)
    integer, intent(in) :: c1, c2
    if (c1 == c2) then
        call col%init_col_acl (0, 0)
    else
        call col%init_col_acl (c1, c2)
    end if
end subroutine t_a
subroutine t_o (c1, c2, c3)
    integer, intent(in) :: c1, c2, c3
    if (c1 == c2) then
        call col%init_col_acl (c3, 0)
    else if (c2 == 0 .and. c3 == 0) then
        call col%init_col_acl (c1, 0)
    end if
end subroutine t_o
subroutine a_o (c1, c2, c3)
    integer, intent(in) :: c1, c2, c3
    if (c1 == c2) then
        call col%init_col_acl (0, c3)
    else if (c2 == 0 .and. c3 == 0) then
        call col%init_col_acl (0, c1)
    end if
end subroutine a_o
subroutine o_o (c1, c2, c3, c4)
    integer, intent(in) :: c1, c2, c3, c4
    if (all ([c1,c2,c3,c4] /= 0)) then
        if (c2 == c3 .and. c4 == c1) then
            call col%init_col_acl (0, 0)
        else if (c2 == c3) then
            call col%init_col_acl (c1, c4)
        end if
    end if
end subroutine o_o

```

```

        else if (c4 == c1) then
            call col%init_col_acl (c3, c2)
        end if
    end if
end subroutine o_o
end function color_fusion

```

Compute the color factor, given two interfering color arrays.

```

<Colors: public>+≡
    public :: compute_color_factor

<Colors: procedures>+≡
    function compute_color_factor (col1, col2, nc) result (factor)
        real(default) :: factor
        type(color_t), dimension(:), intent(in) :: col1, col2
        integer, intent(in), optional :: nc
        type(color_t), dimension(size(col1)) :: col
        integer :: ncol, nloops, nghost
        ncol = 3; if (present (nc)) ncol = nc
        col = col1 .merge. col2
        nloops = count_color_loops (col)
        nghost = count (col%is_ghost ())
        factor = real (ncol, default) ** (nloops - nghost)
        if (color_ghost_parity (col)) factor = - factor
    end function compute_color_factor

```

We have a pair of color index arrays which corresponds to a squared matrix element. We want to determine the number of color loops in this square matrix element. So we first copy the colors (stored in a single color array with a pair of color lists in each entry) to a temporary where the color indices are shifted by some offset. We then recursively follow each loop, starting at the first color that has the offset, resetting the first color index to the loop index and each further index to zero as we go. We check that (a) each color index occurs twice within the left (right) color array, (b) the loops are closed, so we always come back to a line which has the loop index.

In order for the algorithm to work we have to conjugate the colors of initial state particles (one for decays, two for scatterings) into their corresponding anticolors of outgoing particles.

```

<Colors: public>+≡
    public :: count_color_loops

<Colors: procedures>+≡
    function count_color_loops (col) result (count)
        integer :: count
        type(color_t), dimension(:), intent(in) :: col
        type(color_t), dimension(size(col)) :: cc
        integer :: i, n, offset
        cc = col
        n = size (cc)
        offset = n
        call color_add_offset (cc, offset)
        count = 0
        SCAN_LOOPS: do

```



```

do i = 1, n
  if (color_is_nonzero (cc(i))) then
    if (any (cc(i)%c1 > offset)) then
      count = count + 1
      call follow_line1 (pick_new_line (cc(i)%c1, count, 1))
      cycle SCAN_LOOPS
    end if
  end if
end do
exit SCAN_LOOPS
end do SCAN_LOOPS
contains
function pick_new_line (c, reset_val, sgn) result (line)
  integer :: line
  integer, dimension(:), intent(inout) :: c
  integer, intent(in) :: reset_val
  integer, intent(in) :: sgn
  integer :: i
  if (any (c == count)) then
    line = count
  else
    do i = 1, size (c)
      if (sign (1, c(i)) == sgn .and. abs (c(i)) > offset) then
        line = c(i)
        c(i) = reset_val
        return
      end if
    end do
    call color_mismatch
  end if
end function pick_new_line

subroutine reset_line (c, line)
  integer, dimension(:), intent(inout) :: c
  integer, intent(in) :: line
  integer :: i
  do i = 1, size (c)
    if (c(i) == line) then
      c(i) = 0
      return
    end if
  end do
end subroutine reset_line

recursive subroutine follow_line1 (line)
  integer, intent(in) :: line
  integer :: i
  if (line == count) return
  do i = 1, n
    if (any (cc(i)%c1 == -line)) then
      call reset_line (cc(i)%c1, -line)
      call follow_line2 (pick_new_line (cc(i)%c2, 0, sign (1, -line)))
      return
    end if
  end do
end if

```

```

        end do
        call color_mismatch ()
    end subroutine follow_line1

recursive subroutine follow_line2 (line)
    integer, intent(in) :: line
    integer :: i
    do i = 1, n
        if (any (cc(i)%c2 == -line)) then
            call reset_line (cc(i)%c2, -line)
            call follow_line1 (pick_new_line (cc(i)%c1, 0, sign (1, -line)))
            return
        end if
    end do
    call color_mismatch ()
end subroutine follow_line2

subroutine color_mismatch ()
    call color_write (col)
    print *
    call msg_fatal ("Color flow mismatch: Non-closed color lines appear during ", &
        [var_str ("the evaluation of color correlations. This can happen if there "), &
        var_str ("are different color structures in the initial or final state of "), &
        var_str ("the process definition. If so, please use separate processes for "), &
        var_str ("the different initial / final states. In a future WHIZARD version "), &
        var_str ("this will be fixed.")])
end subroutine color_mismatch
end function count_color_loops

```

11.4.6 Unit tests

Test module, followed by the corresponding implementation module.

```

(colors_ut.f90)≡
    <File header>

```

```

module colors_ut
    use unit_tests
    use colors_uti

```

```

    <Standard module head>

```

```

    <Colors: public test>

```

```

contains

```

```

    <Colors: test driver>

```

```

end module colors_ut

```

```

(colors_uti.f90)≡
    <File header>

```

```

module colors_uti

```

```

    use colors

    <Standard module head>

    <Colors: test declarations>

contains

    <Colors: tests>

end module colors_util
API: driver for the unit tests below.
<Colors: public test>≡
    public :: color_test
<Colors: test driver>≡
    subroutine color_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Colors: execute tests>
    end subroutine color_test

```

This is a color counting test.

```

<Colors: execute tests>≡
    call test (color_1, "color_1", &
        "check color counting", &
        u, results)
<Colors: test declarations>≡
    public :: color_1
<Colors: tests>≡
    subroutine color_1 (u)
        integer, intent(in) :: u
        type(color_t), dimension(4) :: col1, col2, col
        type(color_t), dimension(:), allocatable :: col3
        type(color_t), dimension(:,:), allocatable :: col_array
        integer :: count, i
        call col1%init_col_acl ([1, 0, 2, 3], [0, 1, 3, 2])
        col2 = col1
        call color_write (col1, u)
        write (u, "(A)")
        call color_write (col2, u)
        write (u, "(A)")
        col = col1 .merge. col2
        call color_write (col, u)
        write (u, "(A)")
        count = count_color_loops (col)
        write (u, "(A,I1)") "Number of color loops (3): ", count
        call col2%init_col_acl ([1, 0, 2, 3], [0, 2, 3, 1])
        call color_write (col1, u)
        write (u, "(A)")
        call color_write (col2, u)
        write (u, "(A)")
    end subroutine color_1

```

```

col = col1 .merge. col2
call color_write (col, u)
write (u, "(A)")
count = count_color_loops (col)
write (u, "(A,I1)") "Number of color loops (2): ", count
write (u, "(A)")
allocate (col3 (4))
call color_init_from_array (col3, &
    reshape ([1, 0, 0, -1, 2, -3, 3, -2], &
        [2, 4]))
call color_write (col3, u)
write (u, "(A)")
call color_array_make_contractions (col3, col_array)
write (u, "(A)") "Contractions:"
do i = 1, size (col_array, 2)
    call color_write (col_array(:,i), u)
    write (u, "(A)")
end do
deallocate (col3)
write (u, "(A)")
allocate (col3 (6))
call color_init_from_array (col3, &
    reshape ([1, -2, 3, 0, 0, -1, 2, -4, -3, 0, 4, 0], &
        [2, 6]))
call color_write (col3, u)
write (u, "(A)")
call color_array_make_contractions (col3, col_array)
write (u, "(A)") "Contractions:"
do i = 1, size (col_array, 2)
    call color_write (col_array(:,i), u)
    write (u, "(A)")
end do
end subroutine color_1

```

A color fusion test.

```

<Colors: execute tests>+≡
    call test (color_2, "color_2", &
        "color fusion", &
        u, results)

<Colors: test declarations>+≡
    public :: color_2

<Colors: tests>+≡
    subroutine color_2 (u)
        integer, intent(in) :: u
        type(color_t) :: s1, t1, t2, a1, a2, o1, o2, o3, o4, g1

        write (u, "(A)") "* Test output: color_2"
        write (u, "(A)") "* Purpose: test all combinations for color-object fusion"
        write (u, "(A)")

        call s1%init_col_acl (0,0)
        call t1%init_col_acl (1,0)
        call t2%init_col_acl (2,0)
    end subroutine color_2

```

```

call a1%init_col_acl (0,1)
call a2%init_col_acl (0,2)
call o1%init_col_acl (1,2)
call o2%init_col_acl (1,3)
call o3%init_col_acl (2,3)
call o4%init_col_acl (2,1)
call g1%init (ghost=.true.)

call wrt ("s1", s1)
call wrt ("t1", t1)
call wrt ("t2", t2)
call wrt ("a1", a1)
call wrt ("a2", a2)
call wrt ("o1", o1)
call wrt ("o2", o2)
call wrt ("o3", o3)
call wrt ("o4", o4)
call wrt ("g1", g1)

write (u, *)

call wrt ("s1 * s1", s1 .fuse. s1)

write (u, *)

call wrt ("s1 * t1", s1 .fuse. t1)
call wrt ("s1 * a1", s1 .fuse. a1)
call wrt ("s1 * o1", s1 .fuse. o1)

write (u, *)

call wrt ("t1 * s1", t1 .fuse. s1)
call wrt ("a1 * s1", a1 .fuse. s1)
call wrt ("o1 * s1", o1 .fuse. s1)

write (u, *)

call wrt ("t1 * t1", t1 .fuse. t1)

write (u, *)

call wrt ("t1 * t2", t1 .fuse. t2)
call wrt ("t1 * a1", t1 .fuse. a1)
call wrt ("t1 * a2", t1 .fuse. a2)
call wrt ("t1 * o1", t1 .fuse. o1)
call wrt ("t2 * o1", t2 .fuse. o1)

write (u, *)

call wrt ("t2 * t1", t2 .fuse. t1)
call wrt ("a1 * t1", a1 .fuse. t1)
call wrt ("a2 * t1", a2 .fuse. t1)
call wrt ("o1 * t1", o1 .fuse. t1)
call wrt ("o1 * t2", o1 .fuse. t2)

```

```

write (u, *)

call wrt ("a1 * a1", a1 .fuse. a1)

write (u, *)

call wrt ("a1 * a2", a1 .fuse. a2)
call wrt ("a1 * o1", a1 .fuse. o1)
call wrt ("a2 * o2", a2 .fuse. o2)

write (u, *)

call wrt ("a2 * a1", a2 .fuse. a1)
call wrt ("o1 * a1", o1 .fuse. a1)
call wrt ("o2 * a2", o2 .fuse. a2)

write (u, *)

call wrt ("o1 * o1", o1 .fuse. o1)

write (u, *)

call wrt ("o1 * o2", o1 .fuse. o2)
call wrt ("o1 * o3", o1 .fuse. o3)
call wrt ("o1 * o4", o1 .fuse. o4)

write (u, *)

call wrt ("o2 * o1", o2 .fuse. o1)
call wrt ("o3 * o1", o3 .fuse. o1)
call wrt ("o4 * o1", o4 .fuse. o1)

write (u, *)

call wrt ("g1 * g1", g1 .fuse. g1)

write (u, *)

call wrt ("g1 * s1", g1 .fuse. s1)
call wrt ("g1 * t1", g1 .fuse. t1)
call wrt ("g1 * a1", g1 .fuse. a1)
call wrt ("g1 * o1", g1 .fuse. o1)

write (u, *)

call wrt ("s1 * g1", s1 .fuse. g1)
call wrt ("t1 * g1", t1 .fuse. g1)
call wrt ("a1 * g1", a1 .fuse. g1)
call wrt ("o1 * g1", o1 .fuse. g1)

write (u, "(A)")
write (u, "(A)")  "* Test output end: color_2"

```

```

contains

subroutine wrt (s, col)
  character(*), intent(in) :: s
  class(color_t), intent(in) :: col
  write (u, "(A,1x,'=',1x)", advance="no") s
  call col%write (u)
  write (u, *)
end subroutine wrt

end subroutine color_2

```

11.4.7 The Madgraph color model

This section describes the method for matrix element and color flow calculation within Madgraph.

For each Feynman diagram, the colorless amplitude for a specified helicity and momentum configuration (in- and out- combined) is computed:

$$A_d(p, h) \quad (11.1)$$

Inserting color, the squared matrix element for definite helicity and momentum is

$$M^2(p, h) = \sum_{dd'} A_d(p, h) C_{dd'} A_{d'}^*(p, h) \quad (11.2)$$

where $C_{dd'}$ describes the color interference of the two diagrams A_d and $A_{d'}$, which is independent of momentum and helicity and can be calculated for each Feynman diagram pair by reducing it to the corresponding color graph. Obviously, one could combine all diagrams with identical color structure, such that the index d runs only over different color graphs. For colorless diagrams all elements of $C_{dd'}$ are equal to unity.

The hermitian matrix $C_{dd'}$ is diagonalized once and for all, such that it can be written in the form

$$C_{dd'} = \sum_{\lambda} c_d^{\lambda} \lambda c_d^{\lambda*}, \quad (11.3)$$

where the eigenvectors c_d are normalized,

$$\sum_d |c_d^{\lambda}|^2 = 1, \quad (11.4)$$

and the λ values are the corresponding eigenvalues. In the colorless case, this means $c_d = 1/\sqrt{N_d}$ for all diagrams (N_d = number of diagrams), and $\lambda = N_d$ is the only nonzero eigenvalue.

Consequently, the squared matrix element for definite helicity and momentum can also be written as

$$M^2(p, h) = \sum_{\lambda} A_{\lambda}(p, h) \lambda A_{\lambda}(p, h)^* \quad (11.5)$$

with

$$A_{\lambda}(p, h) = \sum_d c_d^{\lambda} A_d(p, h). \quad (11.6)$$

For generic spin density matrices, this is easily generalized to

$$M^2(p, h, h') = \sum_{\lambda} A_{\lambda}(p, h) \lambda A_{\lambda}(p, h')^* \quad (11.7)$$

To determine the color flow probabilities of a given momentum-helicity configuration, the color flow amplitudes are calculated as

$$a_f(p, h) = \sum_d \beta_d^f A_d(p, h), \quad (11.8)$$

where the coefficients β_d^f describe the amplitude for a given Feynman diagram (or color graph) d to correspond to a definite color flow f . They are computed from $C_{dd'}$ by transforming this matrix into the color flow basis and neglecting all off-diagonal elements. Again, these coefficients do not depend on momentum or helicity and can therefore be calculated in advance. This gives the color flow transition matrix

$$F^f(p, h, h') = a_f(p, h) a_f^*(p, h') \quad (11.9)$$

which is assumed diagonal in color flow space and is separate from the color-summed transition matrix M^2 . They are, however, equivalent (up to a factor) to leading order in $1/N_c$, and using the color flow transition matrix is appropriate for matching to hadronization.

Note that the color flow transition matrix is not normalized at this stage. To make use of it, we have to fold it with the in-state density matrix to get a pseudo density matrix

$$\hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h'_{\text{out}}) = \sum_{h_{\text{in}} h'_{\text{in}}} F^f(p, h, h') \rho_{\text{in}}(p, h_{\text{in}}, h'_{\text{in}}) \quad (11.10)$$

which gets a meaning only after contracted with projections on the outgoing helicity states k_{out} , given as linear combinations of helicity states with the unitary coefficient matrix $c(k_{\text{out}}, h_{\text{out}})$. Then the probability of finding color flow f when the helicity state k_{out} is measured is given by

$$P^f(p, k_{\text{out}}) = Q^f(p, k_{\text{out}}) / \sum_f Q^f(p, k_{\text{out}}) \quad (11.11)$$

where

$$Q^f(p, k_{\text{out}}) = \sum_{h_{\text{out}} h'_{\text{out}}} c(k_{\text{out}}, h_{\text{out}}) \hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h'_{\text{out}}) c^*(k_{\text{out}}, h'_{\text{out}}) \quad (11.12)$$

However, if we can assume that the out-state helicity basis is the canonical one, we can throw away the off diagonal elements in the color flow density matrix and normalize the ones on the diagonal to obtain

$$P^f(p, h_{\text{out}}) = \hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h_{\text{out}}) / \sum_f \hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h_{\text{out}}) \quad (11.13)$$

Finally, the color-summed out-state density matrix is computed by the scattering formula

$$\rho_{\text{out}}(p, h_{\text{out}}, h'_{\text{out}}) = \sum_{h_{\text{in}} h'_{\text{in}}} M^2(p, h, h') \rho_{\text{in}}(p, h_{\text{in}}, h'_{\text{in}}) \quad (11.14)$$

$$= \sum_{h_{\text{in}} h'_{\text{in}} \lambda} A_{\lambda}(p, h) \lambda A_{\lambda}(p, h')^* \rho_{\text{in}}(p, h_{\text{in}}, h'_{\text{in}}), \quad (11.15)$$

The trace of ρ_{out} is the squared matrix element, summed over all internal degrees of freedom. To get the squared matrix element for a definite helicity k_{out} and color flow f , one has to project the density matrix onto the given helicity state and multiply with $P^f(p, k_{\text{out}})$.

For diagonal helicities the out-state density reduces to

$$\rho_{\text{out}}(p, h_{\text{out}}) = \sum_{h_{\text{in}} \lambda} \lambda |A_\lambda(p, h)|^2 \rho_{\text{in}}(p, h_{\text{in}}). \quad (11.16)$$

Since no basis transformation is involved, we can use the normalized color flow probability $P^f(p, h_{\text{out}})$ and express the result as

$$\rho_{\text{out}}^f(p, h_{\text{out}}) = \rho_{\text{out}}(p, h_{\text{out}}) P^f(p, h_{\text{out}}) \quad (11.17)$$

$$= \sum_{h_{\text{in}} \lambda} \frac{|a^f(p, h)|^2}{\sum_f |a^f(p, h)|^2} \lambda |A_\lambda(p, h)|^2 \rho_{\text{in}}(p, h_{\text{in}}). \quad (11.18)$$

From these considerations, the following calculation strategy can be derived:

- Before the first event is generated, the color interference matrix $C_{dd'}$ is computed and diagonalized, so the eigenvectors c_d^λ , eigenvalues λ and color flow coefficients β_d^f are obtained. In practice, these calculations are done when the matrix element code is generated, and the results are hardcoded in the matrix element subroutine as `DATA` statements.
- For each event, one loops over helicities once and stores the matrices $A_\lambda(p, h)$ and $a^f(p, h)$. The allowed color flows, helicity combinations and eigenvalues are each labeled by integer indices, so one has to store complex matrices of dimension $N_\lambda \times N_h$ and $N_f \times N_h$, respectively.
- The further strategy depends on the requested information.
 1. If colorless diagonal helicity amplitudes are required, the eigenvalues $A_\lambda(p, h)$ are squared, summed with weight λ , and the result contracted with the in-state probability vector $\rho_{\text{in}}(p, h_{\text{in}})$. The result is a probability vector $\rho_{\text{out}}(p, h_{\text{out}})$.
 2. For colored diagonal helicity amplitudes, the color coefficients $a^f(p, h)$ are also squared and used as weights to obtain the color-flow probability vector $\rho_{\text{out}}^f(p, h_{\text{out}})$.
 3. For colorless non-diagonal helicity amplitudes, we contract the tensor product of $A_\lambda(p, h)$ with $A_\lambda(p, h')$, weighted with λ , with the correlated in-state density matrix, to obtain a correlated out-state density matrix.
 4. In the general (colored, non-diagonal) case, we do the same as in the colorless case, but return the un-normalized color flow density matrix $\hat{\rho}_{\text{out}}^f(p, h_{\text{out}}, h'_{\text{out}})$ in addition. When the relevant helicity basis is known, the latter can be used by the caller program to determine flow probabilities. (In reality, we assume the canonical basis and reduce the correlated out-state density to its diagonal immediately.)

11.5 Flavors: Particle properties

This module contains a type for holding the flavor code, and all functions that depend on the model, i.e., that determine particle properties.

The PDG code is packed in a special **flavor** type. (This prohibits meaningless operations, and it allows for a different implementation, e.g., some non-PDG scheme internally, if appropriate at some point.)

There are lots of further particle properties that depend on the model. Implementing a flyweight pattern, the associated field data object is to be stored in a central area, the **flavor** object just receives a pointer to this, so all queries can be delegated.

`<flavors.f90>`≡
<File header>

module flavors

<Use kinds>

<Use strings>

use io_units

use diagnostics

use physics_defs, only: UNDEFINED

use physics_defs, only: INVALID

use physics_defs, only: HADRON_REMNANT

use physics_defs, only: HADRON_REMNANT_SINGLET

use physics_defs, only: HADRON_REMNANT_TRIPLET

use physics_defs, only: HADRON_REMNANT_OCTET

use model_data

use colors, only: color_t

<Standard module head>

<Flavors: public>

<Flavors: types>

<Flavors: interfaces>

contains

<Flavors: procedures>

end module flavors

11.5.1 The flavor type

The flavor type is an integer representing the PDG code, or undefined (zero). Negative codes represent ant flavors. They should be used only for particles which do have a distinct antiparticle.

The **hard_process** flag can be set for particles that are participating in the hard interaction.

The **radiated** flag can be set for particles that are the result of a beam-structure interaction (hadron beam remnant, ISR photon, etc.), not of the hard

interaction itself.

Further properties of the given flavor can be retrieved via the particle-data pointer, if it is associated.

```

<Flavors: public>≡
    public :: flavor_t

<Flavors: types>≡
    type :: flavor_t
    private
    integer :: f = UNDEFINED
    logical :: hard_process = .false.
    logical :: radiated = .false.
    type(field_data_t), pointer :: field_data => null ()
    contains
    <Flavors: flavor: TBP>
    end type flavor_t

```

Initializer form. If the model is assigned, the procedure is impure, therefore we have to define a separate array version.

Note: The pure elemental subroutines can't have an intent(out) CLASS argument (because of the potential for an impure finalizer in a type extension), so we stick to intent(inout) and (re)set all components explicitly.

```

<Flavors: flavor: TBP>≡
    generic :: init => &
        flavor_init_empty, &
        flavor_init, &
        flavor_init_field_data, &
        flavor_init_model, &
        flavor_init_model_alt, &
        flavor_init_name_model
    procedure, private :: flavor_init_empty
    procedure, private :: flavor_init
    procedure, private :: flavor_init_field_data
    procedure, private :: flavor_init_model
    procedure, private :: flavor_init_model_alt
    procedure, private :: flavor_init_name_model

<Flavors: procedures>≡
    elemental subroutine flavor_init_empty (flv)
        class(flavor_t), intent(inout) :: flv
        flv%f = UNDEFINED
        flv%hard_process = .false.
        flv%radiated = .false.
        flv%field_data => null ()
    end subroutine flavor_init_empty

    elemental subroutine flavor_init (flv, f)
        class(flavor_t), intent(inout) :: flv
        integer, intent(in) :: f
        flv%f = f
        flv%hard_process = .false.
        flv%radiated = .false.
        flv%field_data => null ()
    end subroutine flavor_init

```

```

impure elemental subroutine flavor_init_field_data (flv, field_data)
  class(flavor_t), intent(inout) :: flv
  type(field_data_t), intent(in), target :: field_data
  flv%f = field_data%get_pdg ()
  flv%hard_process = .false.
  flv%radiated = .false.
  flv%field_data => field_data
end subroutine flavor_init_field_data

impure elemental subroutine flavor_init_model (flv, f, model)
  class(flavor_t), intent(inout) :: flv
  integer, intent(in) :: f
  class(model_data_t), intent(in), target :: model
  flv%f = f
  flv%hard_process = .false.
  flv%radiated = .false.
  flv%field_data => model%get_field_ptr (f, check=.true.)
end subroutine flavor_init_model

impure elemental subroutine flavor_init_model_alt (flv, f, model, alt_model)
  class(flavor_t), intent(inout) :: flv
  integer, intent(in) :: f
  class(model_data_t), intent(in), target :: model, alt_model
  flv%f = f
  flv%hard_process = .false.
  flv%radiated = .false.
  flv%field_data => model%get_field_ptr (f, check=.false.)
  if (.not. associated (flv%field_data)) then
    flv%field_data => alt_model%get_field_ptr (f, check=.false.)
    if (.not. associated (flv%field_data)) then
      write (msg_buffer, "(A,1x,I0,1x,A,1x,A,1x,A,1x,A)") &
        "Particle with code", f, &
        "found neither in model", char (model%get_name ()), &
        "nor in model", char (alt_model%get_name ())
      call msg_fatal ()
    end if
  end if
end subroutine flavor_init_model_alt

impure elemental subroutine flavor_init_name_model (flv, name, model)
  class(flavor_t), intent(inout) :: flv
  type(string_t), intent(in) :: name
  class(model_data_t), intent(in), target :: model
  flv%f = model%get_pdg (name)
  flv%hard_process = .false.
  flv%radiated = .false.
  flv%field_data => model%get_field_ptr (name, check=.true.)
end subroutine flavor_init_name_model

```

Set the radiated flag.

(Flavors: flavor: TBP)+≡

```

procedure :: tag_radiated => flavor_tag_radiated

```

```

<Flavors: procedures>+≡
  elemental subroutine flavor_tag_radiated (flv)
    class(flavor_t), intent(inout) :: flv
    flv%radiated = .true.
  end subroutine flavor_tag_radiated

```

Set the `hard_process` flag.

```

<Flavors: flavor: TBP>+≡
  procedure :: tag_hard_process => flavor_tag_hard_process

<Flavors: procedures>+≡
  elemental subroutine flavor_tag_hard_process (flv, hard)
    class(flavor_t), intent(inout) :: flv
    logical, intent(in), optional :: hard
    if (present (hard)) then
      flv%hard_process = hard
    else
      flv%hard_process = .true.
    end if
  end subroutine flavor_tag_hard_process

```

Undefine the flavor state:

```

<Flavors: flavor: TBP>+≡
  procedure :: undefine => flavor_undefine

<Flavors: procedures>+≡
  elemental subroutine flavor_undefine (flv)
    class(flavor_t), intent(inout) :: flv
    flv%f = UNDEFINED
    flv%field_data => null ()
  end subroutine flavor_undefine

```

Output: dense, no linebreak

A hard-process tag is only shown if debugging is on.

```

<Flavors: flavor: TBP>+≡
  procedure :: write => flavor_write

<Flavors: procedures>+≡
  subroutine flavor_write (flv, unit)
    class(flavor_t), intent(in) :: flv
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    if (associated (flv%field_data)) then
      write (u, "(A)", advance="no") "f("
    else
      write (u, "(A)", advance="no") "p("
    end if
    write (u, "(IO)", advance="no") flv%f
    if (flv%radiated) then
      write (u, "('*)", advance="no")
    end if
    if (msg_level (D_FLAVOR) >= DEBUG) then

```

```

        if (flv%hard_process) then
            write (u, "(' #')", advance="no")
        end if
    end if
    write (u, "(A)", advance="no")  ")"
end subroutine flavor_write

```

<Flavors: public>+≡

```
public :: flavor_write_array
```

<Flavors: procedures>+≡

```

subroutine flavor_write_array (flv, unit)
    type(flavor_t), intent(in), dimension(:) :: flv
    integer, intent(in), optional :: unit
    integer :: u, i_flv
    u = given_output_unit (unit); if (u < 0) return
    do i_flv = 1, size (flv)
        call flv(i_flv)%write (u)
        if (i_flv /= size (flv)) write (u,"(A)", advance = "no") " / "
    end do
    write (u,"(A)")
end subroutine flavor_write_array

```

Binary I/O. Currently, the model information is not written/read, so after reading the particle-data pointer is empty.

<Flavors: flavor: TBP>+≡

```

procedure :: write_raw => flavor_write_raw
procedure :: read_raw => flavor_read_raw

```

<Flavors: procedures>+≡

```

subroutine flavor_write_raw (flv, u)
    class(flavor_t), intent(in) :: flv
    integer, intent(in) :: u
    write (u) flv%f
    write (u) flv%radiated
    write (u) flv%hard_process
end subroutine flavor_write_raw

subroutine flavor_read_raw (flv, u, iostat)
    class(flavor_t), intent(out) :: flv
    integer, intent(in) :: u
    integer, intent(out), optional :: iostat
    read (u, iostat=iostat) flv%f
    if (present (iostat)) then
        if (iostat /= 0) return
    end if
    read (u, iostat=iostat) flv%radiated
    read (u, iostat=iostat) flv%hard_process
end subroutine flavor_read_raw

```

Assignment

Default assignment of flavor objects is possible, but cannot be used in pure procedures, because a pointer assignment is involved.

Assign the particle pointer separately. This cannot be elemental, so we define a scalar and an array version explicitly. We refer to an array of flavors, not an array of models.

```
<Flavors: flavor: TBP>+≡
  procedure :: set_model => flavor_set_model_single

<Flavors: procedures>+≡
  impure elemental subroutine flavor_set_model_single (flv, model)
    class(flavor_t), intent(inout) :: flv
    class(model_data_t), intent(in), target :: model
    if (flv%f /= UNDEFINED) &
      flv%field_data => model%get_field_ptr (flv%f)
  end subroutine flavor_set_model_single
```

Predicates

Return the definition status. By definition, the flavor object is defined if the flavor PDG code is nonzero.

```
<Flavors: flavor: TBP>+≡
  procedure :: is_defined => flavor_is_defined

<Flavors: procedures>+≡
  elemental function flavor_is_defined (flv) result (defined)
    class(flavor_t), intent(in) :: flv
    logical :: defined
    defined = flv%f /= UNDEFINED
  end function flavor_is_defined
```

Check for valid flavor (including undefined). This is distinct from the `is_defined` status. Invalid flavor is actually a specific PDG code.

```
<Flavors: flavor: TBP>+≡
  procedure :: is_valid => flavor_is_valid

<Flavors: procedures>+≡
  elemental function flavor_is_valid (flv) result (valid)
    class(flavor_t), intent(in) :: flv
    logical :: valid
    valid = flv%f /= INVALID
  end function flavor_is_valid
```

Return true if the particle-data pointer is associated. (Debugging aid)

```
<Flavors: flavor: TBP>+≡
  procedure :: is_associated => flavor_is_associated

<Flavors: procedures>+≡
  elemental function flavor_is_associated (flv) result (flag)
    class(flavor_t), intent(in) :: flv
    logical :: flag
    flag = associated (flv%field_data)
```

```
end function flavor_is_associated
```

Check the **radiated** flag. A radiated particle has a definite PDG flavor status, but it is actually a pseudoparticle (a beam remnant) which may be subject to fragmentation.

```
<Flavors: flavor: TBP>+=
  procedure :: is_radiated => flavor_is_radiated

<Flavors: procedures>+=
  elemental function flavor_is_radiated (flv) result (flag)
    class(flavor_t), intent(in) :: flv
    logical :: flag
    flag = flv%radiated
  end function flavor_is_radiated
```

Check the **hard_process** flag. A particle is tagged with this flag if it participates in the hard interaction and is not a beam remnant.

```
<Flavors: flavor: TBP>+=
  procedure :: is_hard_process => flavor_is_hard_process

<Flavors: procedures>+=
  elemental function flavor_is_hard_process (flv) result (flag)
    class(flavor_t), intent(in) :: flv
    logical :: flag
    flag = flv%hard_process
  end function flavor_is_hard_process
```

Accessing contents

With the exception of the PDG code, all particle property enquiries are delegated to the **field_data** pointer. If this is unassigned, some access function will crash.

Return the flavor as an integer

```
<Flavors: flavor: TBP>+=
  procedure :: get_pdg => flavor_get_pdg

<Flavors: procedures>+=
  elemental function flavor_get_pdg (flv) result (f)
    integer :: f
    class(flavor_t), intent(in) :: flv
    f = flv%f
  end function flavor_get_pdg
```

Return the flavor of the antiparticle

```
<Flavors: flavor: TBP>+=
  procedure :: get_pdg_anti => flavor_get_pdg_anti

<Flavors: procedures>+=
  elemental function flavor_get_pdg_anti (flv) result (f)
    integer :: f
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
```



```

        if (flv%field_data%has_antiparticle ()) then
            f = -flv%f
        else
            f = flv%f
        end if
    else
        f = 0
    end if
end function flavor_get_pdg_anti

```

Absolute value:

```

<Flavors: flavor: TBP>+≡
    procedure :: get_pdg_abs => flavor_get_pdg_abs

<Flavors: procedures>+≡
    elemental function flavor_get_pdg_abs (flv) result (f)
        integer :: f
        class(flavor_t), intent(in) :: flv
        f = abs (flv%f)
    end function flavor_get_pdg_abs

```

Generic properties

```

<Flavors: flavor: TBP>+≡
    procedure :: is_visible => flavor_is_visible
    procedure :: is_parton => flavor_is_parton
    procedure :: is_beam_remnant => flavor_is_beam_remnant
    procedure :: is_gauge => flavor_is_gauge
    procedure :: is_left_handed => flavor_is_left_handed
    procedure :: is_right_handed => flavor_is_right_handed
    procedure :: is_antiparticle => flavor_is_antiparticle
    procedure :: has_antiparticle => flavor_has_antiparticle
    procedure :: is_stable => flavor_is_stable
    procedure :: get_decays => flavor_get_decays
    procedure :: decays_isotropically => flavor_decays_isotropically
    procedure :: decays_diagonal => flavor_decays_diagonal
    procedure :: has_decay_helicity => flavor_has_decay_helicity
    procedure :: get_decay_helicity => flavor_get_decay_helicity
    procedure :: is_polarized => flavor_is_polarized

<Flavors: procedures>+≡
    elemental function flavor_is_visible (flv) result (flag)
        logical :: flag
        class(flavor_t), intent(in) :: flv
        if (associated (flv%field_data)) then
            flag = flv%field_data%is_visible ()
        else
            flag = .false.
        end if
    end function flavor_is_visible

    elemental function flavor_is_parton (flv) result (flag)
        logical :: flag
        class(flavor_t), intent(in) :: flv
        if (associated (flv%field_data)) then

```

```

        flag = flv%field_data%is_parton ()
    else
        flag = .false.
    end if
end function flavor_is_parton

elemental function flavor_is_beam_remnant (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    select case (abs (flv%f))
    case (HADRON_REMNANT, &
         HADRON_REMNANT_SINGLET, HADRON_REMNANT_TRIPLET, HADRON_REMNANT_OCTET)
        flag = .true.
    case default
        flag = .false.
    end select
end function flavor_is_beam_remnant

elemental function flavor_is_gauge (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        flag = flv%field_data%is_gauge ()
    else
        flag = .false.
    end if
end function flavor_is_gauge

elemental function flavor_is_left_handed (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        if (flv%f > 0) then
            flag = flv%field_data%is_left_handed ()
        else
            flag = flv%field_data%is_right_handed ()
        end if
    else
        flag = .false.
    end if
end function flavor_is_left_handed

elemental function flavor_is_right_handed (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        if (flv%f > 0) then
            flag = flv%field_data%is_right_handed ()
        else
            flag = flv%field_data%is_left_handed ()
        end if
    else
        flag = .false.
    end if
end if

```

```

end function flavor_is_right_handed

elemental function flavor_is_antiparticle (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  flag = flv%f < 0
end function flavor_is_antiparticle

elemental function flavor_has_antiparticle (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%has_antiparticle ()
  else
    flag = .false.
  end if
end function flavor_has_antiparticle

elemental function flavor_is_stable (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%is_stable (anti = flv%f < 0)
  else
    flag = .true.
  end if
end function flavor_is_stable

subroutine flavor_get_decays (flv, decay)
  class(flavor_t), intent(in) :: flv
  type(string_t), dimension(:), intent(out), allocatable :: decay
  logical :: anti
  anti = flv%f < 0
  if (.not. flv%field_data%is_stable (anti)) then
    call flv%field_data%get_decays (decay, anti)
  end if
end subroutine flavor_get_decays

elemental function flavor_decays_isotropically (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%decays_isotropically (anti = flv%f < 0)
  else
    flag = .true.
  end if
end function flavor_decays_isotropically

elemental function flavor_decays_diagonal (flv) result (flag)
  logical :: flag
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    flag = flv%field_data%decays_diagonal (anti = flv%f < 0)
  else

```

```

        flag = .true.
    end if
end function flavor_decays_diagonal

elemental function flavor_has_decay_helicity (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        flag = flv%field_data%has_decay_helicity (anti = flv%f < 0)
    else
        flag = .false.
    end if
end function flavor_has_decay_helicity

elemental function flavor_get_decay_helicity (flv) result (hel)
    integer :: hel
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        hel = flv%field_data%decay_helicity (anti = flv%f < 0)
    else
        hel = 0
    end if
end function flavor_get_decay_helicity

elemental function flavor_is_polarized (flv) result (flag)
    logical :: flag
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        flag = flv%field_data%is_polarized (anti = flv%f < 0)
    else
        flag = .false.
    end if
end function flavor_is_polarized

```

Names:

(Flavors: flavor: TBP)+≡

```

    procedure :: get_name => flavor_get_name
    procedure :: get_tex_name => flavor_get_tex_name

```

(Flavors: procedures)+≡

```

    elemental function flavor_get_name (flv) result (name)
        type(string_t) :: name
        class(flavor_t), intent(in) :: flv
        if (associated (flv%field_data)) then
            name = flv%field_data%get_name (flv%f < 0)
        else
            name = "?"
        end if
    end function flavor_get_name

```

```

    elemental function flavor_get_tex_name (flv) result (name)
        type(string_t) :: name
        class(flavor_t), intent(in) :: flv
        if (associated (flv%field_data)) then

```

```

        name = flv%field_data%get_tex_name (flv%f < 0)
    else
        name = "?"
    end if
end function flavor_get_tex_name

```

(Flavors: flavor: TBP)+≡

```

procedure :: get_spin_type => flavor_get_spin_type
procedure :: get_multiplicity => flavor_get_multiplicity
procedure :: get_isospin_type => flavor_get_isospin_type
procedure :: get_charge_type => flavor_get_charge_type
procedure :: get_color_type => flavor_get_color_type

```

(Flavors: procedures)+≡

```

elemental function flavor_get_spin_type (flv) result (type)
    integer :: type
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        type = flv%field_data%get_spin_type ()
    else
        type = 1
    end if
end function flavor_get_spin_type

```

```

elemental function flavor_get_multiplicity (flv) result (type)
    integer :: type
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        type = flv%field_data%get_multiplicity ()
    else
        type = 1
    end if
end function flavor_get_multiplicity

```

```

elemental function flavor_get_isospin_type (flv) result (type)
    integer :: type
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        type = flv%field_data%get_isospin_type ()
    else
        type = 1
    end if
end function flavor_get_isospin_type

```

```

elemental function flavor_get_charge_type (flv) result (type)
    integer :: type
    class(flavor_t), intent(in) :: flv
    if (associated (flv%field_data)) then
        type = flv%field_data%get_charge_type ()
    else
        type = 1
    end if
end function flavor_get_charge_type

```

```

elemental function flavor_get_color_type (flv) result (type)
  integer :: type
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    if (flavor_is_antiparticle (flv)) then
      type = - flv%field_data%get_color_type ()
    else
      type = flv%field_data%get_color_type ()
    end if
    select case (type)
      case (-1,-8); type = abs (type)
    end select
  else
    type = 1
  end if
end function flavor_get_color_type

```

These functions return real values:

$\langle \text{Flavors: flavor: TBP} \rangle + \equiv$

```

procedure :: get_charge => flavor_get_charge
procedure :: get_mass => flavor_get_mass
procedure :: get_width => flavor_get_width
procedure :: get_isospin => flavor_get_isospin

```

$\langle \text{Flavors: procedures} \rangle + \equiv$

```

elemental function flavor_get_charge (flv) result (charge)
  real(default) :: charge
  class(flavor_t), intent(in) :: flv
  integer :: charge_type
  if (associated (flv%field_data)) then
    charge_type = flv%get_charge_type ()
    if (charge_type == 0 .or. charge_type == 1) then
      charge = 0
    else
      if (flavor_is_antiparticle (flv)) then
        charge = - flv%field_data%get_charge ()
      else
        charge = flv%field_data%get_charge ()
      end if
    end if
  else
    charge = 0
  end if
end function flavor_get_charge

```

```

elemental function flavor_get_mass (flv) result (mass)
  real(default) :: mass
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    mass = flv%field_data%get_mass ()
  else
    mass = 0
  end if
end function flavor_get_mass

```

```

elemental function flavor_get_width (flv) result (width)
  real(default) :: width
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    width = flv%field_data%get_width ()
  else
    width = 0
  end if
end function flavor_get_width

elemental function flavor_get_isospin (flv) result (isospin)
  real(default) :: isospin
  class(flavor_t), intent(in) :: flv
  if (associated (flv%field_data)) then
    if (flavor_is_antiparticle (flv)) then
      isospin = - flv%field_data%get_isospin ()
    else
      isospin = flv%field_data%get_isospin ()
    end if
  else
    isospin = 0
  end if
end function flavor_get_isospin

```

Comparisons

If one of the flavors is undefined, the other defined, they match.

```

<Flavors: flavor: TBP>+≡
  generic :: operator(.match.) => flavor_match
  generic :: operator(==) => flavor_eq
  generic :: operator(/=) => flavor_neq
  procedure, private :: flavor_match
  procedure, private :: flavor_eq
  procedure, private :: flavor_neq

<Flavors: procedures>+≡
  elemental function flavor_match (flv1, flv2) result (eq)
    logical :: eq
    class(flavor_t), intent(in) :: flv1, flv2
    if (flv1%f /= UNDEFINED .and. flv2%f /= UNDEFINED) then
      eq = flv1%f == flv2%f
    else
      eq = .true.
    end if
  end function flavor_match

  elemental function flavor_eq (flv1, flv2) result (eq)
    logical :: eq
    class(flavor_t), intent(in) :: flv1, flv2
    if (flv1%f /= UNDEFINED .and. flv2%f /= UNDEFINED) then
      eq = flv1%f == flv2%f
    else if (flv1%f == UNDEFINED .and. flv2%f == UNDEFINED) then

```

```

        eq = .true.
    else
        eq = .false.
    end if
end function flavor_eq

```

```

<Flavors: procedures>+≡
elemental function flavor_neq (flv1, flv2) result (neq)
    logical :: neq
    class(flavor_t), intent(in) :: flv1, flv2
    if (flv1%f /= UNDEFINED .and. flv2%f /= UNDEFINED) then
        neq = flv1%f /= flv2%f
    else if (flv1%f == UNDEFINED .and. flv2%f == UNDEFINED) then
        neq = .false.
    else
        neq = .true.
    end if
end function flavor_neq

```

Tools

Merge two flavor indices. This works only if both are equal or either one is undefined, because we have no off-diagonal flavor entries. Otherwise, generate an invalid flavor.

We cannot use elemental procedures because of the pointer component.

```

<Flavors: public>+≡
    public :: operator(.merge.)

<Flavors: interfaces>≡
interface operator(.merge.)
    module procedure merge_flavors0
    module procedure merge_flavors1
end interface

```

```

<Flavors: procedures>+≡
function merge_flavors0 (flv1, flv2) result (flv)
    type(flavor_t) :: flv
    type(flavor_t), intent(in) :: flv1, flv2
    if (flavor_is_defined (flv1) .and. flavor_is_defined (flv2)) then
        if (flv1 == flv2) then
            flv = flv1
        else
            flv%f = INVALID
        end if
    else if (flavor_is_defined (flv1)) then
        flv = flv1
    else if (flavor_is_defined (flv2)) then
        flv = flv2
    end if
end function merge_flavors0

function merge_flavors1 (flv1, flv2) result (flv)

```



```

type(flavor_t), dimension(:), intent(in) :: flv1, flv2
type(flavor_t), dimension(size(flv1)) :: flv
integer :: i
do i = 1, size (flv1)
    flv(i) = flv1(i) .merge. flv2(i)
end do
end function merge_flavors1

```

Generate consecutive color indices for a given flavor. The indices are counted starting with the stored value of *c*, so new indices are created each time this (impure) function is called. The counter can be reset by the optional argument *c_seed* if desired. The optional flag *reverse* is used only for octets. If set, the color and anticolor entries of the octet particle are exchanged.

```

<Flavors: public>+≡
    public :: color_from_flavor

<Flavors: interfaces>+≡
    interface color_from_flavor
        module procedure color_from_flavor0
        module procedure color_from_flavor1
    end interface

<Flavors: procedures>+≡
    function color_from_flavor0 (flv, c_seed, reverse) result (col)
        type(color_t) :: col
        type(flavor_t), intent(in) :: flv
        integer, intent(in), optional :: c_seed
        logical, intent(in), optional :: reverse
        integer, save :: c = 1
        logical :: rev
        if (present (c_seed)) c = c_seed
        rev = .false.; if (present (reverse)) rev = reverse
        select case (flavor_get_color_type (flv))
        case (1)
            call col%init ()
        case (3)
            call col%init ([c]); c = c + 1
        case (-3)
            call col%init ([-c]); c = c + 1
        case (8)
            if (rev) then
                call col%init ([c+1, -c]); c = c + 2
            else
                call col%init ([c, -(c+1)]); c = c + 2
            end if
        end select
    end function color_from_flavor0

    function color_from_flavor1 (flv, c_seed, reverse) result (col)
        type(flavor_t), dimension(:), intent(in) :: flv
        integer, intent(in), optional :: c_seed
        logical, intent(in), optional :: reverse
        type(color_t), dimension(size(flv)) :: col
        integer :: i

```

```

col(1) = color_from_flavor0 (flv(1), c_seed, reverse)
do i = 2, size (flv)
    col(i) = color_from_flavor0 (flv(i), reverse=reverse)
end do
end function color_from_flavor1

```

This procedure returns the flavor object for the antiparticle. The antiparticle code may either be the same code or its negative.

```

<Flavors: flavor: TBP>+≡
    procedure :: anti => flavor_anti

<Flavors: procedures>+≡
    function flavor_anti (flv) result (aflv)
        type(flavor_t) :: aflv
        class(flavor_t), intent(in) :: flv
        if (flavor_has_antiparticle (flv)) then
            aflv%f = - flv%f
        else
            aflv%f = flv%f
        end if
        aflv%field_data => flv%field_data
    end function flavor_anti

```

11.6 Quantum numbers

This module collects helicity, color, and flavor in a single type and defines procedures

```
<quantum_numbers.f90>≡  
  <File header>  
  
  module quantum_numbers  
  
    use io_units  
    use model_data  
    use helicities  
    use colors  
    use flavors  
  
    <Standard module head>  
  
    <Quantum numbers: public>  
  
    <Quantum numbers: types>  
  
    <Quantum numbers: interfaces>  
  
    contains  
  
    <Quantum numbers: procedures>  
  
  end module quantum_numbers
```

11.6.1 The quantum number type

```
<Quantum numbers: public>≡  
  public :: quantum_numbers_t  
  
<Quantum numbers: types>≡  
  type :: quantum_numbers_t  
    private  
    type(flavor_t) :: f  
    type(color_t) :: c  
    type(helicity_t) :: h  
    integer :: sub = 0  
    contains  
    <Quantum numbers: quantum numbers: TBP>  
  end type quantum_numbers_t
```

Define quantum numbers: Initializer form. All arguments may be present or absent.

Some elemental initializers are impure because they set the `flv` component. This implies transfer of a pointer behind the scenes.

```
<Quantum numbers: quantum numbers: TBP>≡  
  generic :: init => &  
    quantum_numbers_init_f, &  
    quantum_numbers_init_c, &
```

```

        quantum_numbers_init_h, &
        quantum_numbers_init_fc, &
        quantum_numbers_init_fh, &
        quantum_numbers_init_ch, &
        quantum_numbers_init_fch, &
        quantum_numbers_init_fs, &
        quantum_numbers_init_fhs, &
        quantum_numbers_init_fcs, &
        quantum_numbers_init_fhcs
    procedure, private :: quantum_numbers_init_f
    procedure, private :: quantum_numbers_init_c
    procedure, private :: quantum_numbers_init_h
    procedure, private :: quantum_numbers_init_fc
    procedure, private :: quantum_numbers_init_fh
    procedure, private :: quantum_numbers_init_ch
    procedure, private :: quantum_numbers_init_fch
    procedure, private :: quantum_numbers_init_fs
    procedure, private :: quantum_numbers_init_fhs
    procedure, private :: quantum_numbers_init_fcs
    procedure, private :: quantum_numbers_init_fhcs
<Quantum numbers: procedures>≡
    impure elemental subroutine quantum_numbers_init_f (qn, flv)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        qn%f = flv
        call qn%c%undefine ()
        call qn%h%undefine ()
        qn%sub = 0
    end subroutine quantum_numbers_init_f

    impure elemental subroutine quantum_numbers_init_c (qn, col)
        class(quantum_numbers_t), intent(out) :: qn
        type(color_t), intent(in) :: col
        call qn%f%undefine ()
        qn%c = col
        call qn%h%undefine ()
        qn%sub = 0
    end subroutine quantum_numbers_init_c

    impure elemental subroutine quantum_numbers_init_h (qn, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(helicity_t), intent(in) :: hel
        call qn%f%undefine ()
        call qn%c%undefine ()
        qn%h = hel
        qn%sub = 0
    end subroutine quantum_numbers_init_h

    impure elemental subroutine quantum_numbers_init_fc (qn, flv, col)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(color_t), intent(in) :: col
        qn%f = flv
        qn%c = col

```

```

        call qn%h%undefine ()
        qn%sub = 0
    end subroutine quantum_numbers_init_fc

    impure elemental subroutine quantum_numbers_init_fh (qn, flv, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(in) :: hel
        qn%f = flv
        call qn%c%undefine ()
        qn%h = hel
        qn%sub = 0
    end subroutine quantum_numbers_init_fh

    impure elemental subroutine quantum_numbers_init_ch (qn, col, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(color_t), intent(in) :: col
        type(helicity_t), intent(in) :: hel
        call qn%f%undefine ()
        qn%c = col
        qn%h = hel
        qn%sub = 0
    end subroutine quantum_numbers_init_ch

    impure elemental subroutine quantum_numbers_init_fch (qn, flv, col, hel)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(color_t), intent(in) :: col
        type(helicity_t), intent(in) :: hel
        qn%f = flv
        qn%c = col
        qn%h = hel
        qn%sub = 0
    end subroutine quantum_numbers_init_fch

    impure elemental subroutine quantum_numbers_init_fs (qn, flv, sub)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        integer, intent(in) :: sub
        qn%f = flv; qn%sub = sub
    end subroutine quantum_numbers_init_fs

    impure elemental subroutine quantum_numbers_init_fhs (qn, flv, hel, sub)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(in) :: hel
        integer, intent(in) :: sub
        qn%f = flv; qn%h = hel; qn%sub = sub
    end subroutine quantum_numbers_init_fhs

    impure elemental subroutine quantum_numbers_init_fcs (qn, flv, col, sub)
        class(quantum_numbers_t), intent(out) :: qn
        type(flavor_t), intent(in) :: flv
        type(color_t), intent(in) :: col

```

```

integer, intent(in) :: sub
qn%f = flv; qn%c = col; qn%sub = sub
end subroutine quantum_numbers_init_fcs

impure elemental subroutine quantum_numbers_init_fhcs (qn, flv, hel, col, sub)
class(quantum_numbers_t), intent(out) :: qn
type(flavor_t), intent(in) :: flv
type(helicity_t), intent(in) :: hel
type(color_t), intent(in) :: col
integer, intent(in) :: sub
qn%f = flv; qn%h = hel; qn%c = col; qn%sub = sub
end subroutine quantum_numbers_init_fhcs

```

11.6.2 I/O

Write the quantum numbers in condensed form, enclosed by square brackets. Color is written only if nontrivial. For convenience, introduce also an array version.

If the `col_verbose` option is set, show the quantum number color also if it is zero, but defined. Otherwise, suppress zero color.

```

<Quantum numbers: public>+≡
public :: quantum_numbers_write

<Quantum numbers: quantum numbers: TBP>+≡
procedure :: write => quantum_numbers_write_single

<Quantum numbers: interfaces>≡
interface quantum_numbers_write
module procedure quantum_numbers_write_single
module procedure quantum_numbers_write_array
end interface

<Quantum numbers: procedures>+≡
subroutine quantum_numbers_write_single (qn, unit, col_verbose)
class(quantum_numbers_t), intent(in) :: qn
integer, intent(in), optional :: unit
logical, intent(in), optional :: col_verbose
integer :: u
logical :: col_verb
u = given_output_unit (unit); if (u < 0) return
col_verb = .false.; if (present (col_verbose)) col_verb = col_verbose
write (u, "(A)", advance = "no") "["
if (qn%f%is_defined ()) then
call qn%f%write (u)
if (qn%c%is_nonzero () .or. qn%h%is_defined ()) &
write (u, "(1x)", advance = "no")
end if
if (col_verb) then
if (qn%c%is_defined () .or. qn%c%is_ghost ()) then
call color_write (qn%c, u)
if (qn%h%is_defined ()) write (u, "(1x)", advance = "no")
end if
else
if (qn%c%is_nonzero () .or. qn%c%is_ghost ()) then

```

```

        call color_write (qn%c, u)
        if (qn%h%is_defined ()) write (u, "(1x)", advance = "no")
    end if
end if
if (qn%h%is_defined ()) then
    call qn%h%write (u)
end if
if (qn%sub > 0) &
    write (u, "(A,I0)", advance = "no") " SUB = ", qn%sub
write (u, "(A)", advance="no") "]"
end subroutine quantum_numbers_write_single

subroutine quantum_numbers_write_array (qn, unit, col_verbose)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: col_verbose
    integer :: i
    integer :: u
    logical :: col_verb
    u = given_output_unit (unit); if (u < 0) return
    col_verb = .false.; if (present (col_verbose)) col_verb = col_verbose
    write (u, "(A)", advance="no") "["
    do i = 1, size (qn)
        if (i > 1) write (u, "(A)", advance="no") " / "
        if (qn(i)%f%is_defined ()) then
            call qn(i)%f%write (u)
            if (qn(i)%c%is_nonzero () .or. qn(i)%h%is_defined ()) &
                write (u, "(1x)", advance="no")
        end if
        if (col_verb) then
            if (qn(i)%c%is_defined () .or. qn(i)%c%is_ghost ()) then
                call color_write (qn(i)%c, u)
                if (qn(i)%h%is_defined ()) write (u, "(1x)", advance="no")
            end if
        else
            if (qn(i)%c%is_nonzero () .or. qn(i)%c%is_ghost ()) then
                call color_write (qn(i)%c, u)
                if (qn(i)%h%is_defined ()) write (u, "(1x)", advance="no")
            end if
        end if
        if (qn(i)%h%is_defined ()) then
            call qn(i)%h%write (u)
        end if
        if (qn(i)%sub > 0) &
            write (u, "(A,I2)", advance = "no") " SUB = ", qn(i)%sub
    end do
    write (u, "(A)", advance = "no") "]"
end subroutine quantum_numbers_write_array

```

Binary I/O.

\langle Quantum numbers: quantum numbers: TBP $\rangle + \equiv$

```

    procedure :: write_raw => quantum_numbers_write_raw
    procedure :: read_raw => quantum_numbers_read_raw

```

```

<Quantum numbers: procedures>+≡
subroutine quantum_numbers_write_raw (qn, u)
  class(quantum_numbers_t), intent(in) :: qn
  integer, intent(in) :: u
  call qn%f%write_raw (u)
  call qn%c%write_raw (u)
  call qn%h%write_raw (u)
end subroutine quantum_numbers_write_raw

subroutine quantum_numbers_read_raw (qn, u, iostat)
  class(quantum_numbers_t), intent(out) :: qn
  integer, intent(in) :: u
  integer, intent(out), optional :: iostat
  call qn%f%read_raw (u, iostat=iostat)
  call qn%c%read_raw (u, iostat=iostat)
  call qn%h%read_raw (u, iostat=iostat)
end subroutine quantum_numbers_read_raw

```

11.6.3 Accessing contents

Color and helicity can be done by elemental functions. Flavor needs impure elemental. We export also the functions directly, this allows us to avoid temporaries in some places.

```

<Quantum numbers: public>+≡
public :: quantum_numbers_get_flavor
public :: quantum_numbers_get_color
public :: quantum_numbers_get_helicity

<Quantum numbers: quantum numbers: TBP>+≡
procedure :: get_flavor => quantum_numbers_get_flavor
procedure :: get_color => quantum_numbers_get_color
procedure :: get_helicity => quantum_numbers_get_helicity
procedure :: get_sub => quantum_numbers_get_sub

<Quantum numbers: procedures>+≡
impure elemental function quantum_numbers_get_flavor (qn) result (flv)
  type(flavor_t) :: flv
  class(quantum_numbers_t), intent(in) :: qn
  flv = qn%f
end function quantum_numbers_get_flavor

elemental function quantum_numbers_get_color (qn) result (col)
  type(color_t) :: col
  class(quantum_numbers_t), intent(in) :: qn
  col = qn%c
end function quantum_numbers_get_color

elemental function quantum_numbers_get_helicity (qn) result (hel)
  type(helicity_t) :: hel
  class(quantum_numbers_t), intent(in) :: qn
  hel = qn%h
end function quantum_numbers_get_helicity

```



```

elemental function quantum_numbers_get_sub (qn) result (sub)
  integer :: sub
  class(quantum_numbers_t), intent(in) :: qn
  sub = qn%sub
end function quantum_numbers_get_sub

```

This just resets the ghost property of the color part:

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: set_color_ghost => quantum_numbers_set_color_ghost

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_set_color_ghost (qn, ghost)
    class(quantum_numbers_t), intent(inout) :: qn
    logical, intent(in) :: ghost
    call qn%c%set_ghost (ghost)
  end subroutine quantum_numbers_set_color_ghost

```

Assign a model to the flavor part of quantum numbers.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: set_model => quantum_numbers_set_model

<Quantum numbers: procedures>+≡
  impure elemental subroutine quantum_numbers_set_model (qn, model)
    class(quantum_numbers_t), intent(inout) :: qn
    class(model_data_t), intent(in), target :: model
    call qn%f%set_model (model)
  end subroutine quantum_numbers_set_model

```

Set the radiated flag for the flavor component.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: tag_radiated => quantum_numbers_tag_radiated

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_tag_radiated (qn)
    class(quantum_numbers_t), intent(inout) :: qn
    call qn%f%tag_radiated ()
  end subroutine quantum_numbers_tag_radiated

```

Set the hard_process flag for the flavor component.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: tag_hard_process => quantum_numbers_tag_hard_process

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_tag_hard_process (qn, hard)
    class(quantum_numbers_t), intent(inout) :: qn
    logical, intent(in), optional :: hard
    call qn%f%tag_hard_process (hard)
  end subroutine quantum_numbers_tag_hard_process

```

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: set_subtraction_index => quantum_numbers_set_subtraction_index

```

```

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_set_subtraction_index (qn, i)
    class(quantum_numbers_t), intent(inout) :: qn
    integer, intent(in) :: i
    qn%sub = i
  end subroutine quantum_numbers_set_subtraction_index

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: get_subtraction_index => quantum_numbers_get_subtraction_index

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_get_subtraction_index (qn) result (sub)
    integer :: sub
    class(quantum_numbers_t), intent(in) :: qn
    sub = qn%sub
  end function quantum_numbers_get_subtraction_index

```

This is a convenience function: return the color type for the flavor (array).

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: get_color_type => quantum_numbers_get_color_type

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_get_color_type (qn) result (color_type)
    integer :: color_type
    class(quantum_numbers_t), intent(in) :: qn
    color_type = qn%f%get_color_type ()
  end function quantum_numbers_get_color_type

```

11.6.4 Predicates

Check if the flavor index is valid (including UNDEFINED).

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: are_valid => quantum_numbers_are_valid

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_are_valid (qn) result (valid)
    logical :: valid
    class(quantum_numbers_t), intent(in) :: qn
    valid = qn%f%is_valid ()
  end function quantum_numbers_are_valid

```

Check if the flavor part has its particle-data pointer associated (debugging aid).

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: are_associated => quantum_numbers_are_associated

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_are_associated (qn) result (flag)
    logical :: flag
    class(quantum_numbers_t), intent(in) :: qn
    flag = qn%f%is_associated ()
  end function quantum_numbers_are_associated

```

Check if the helicity and color quantum numbers are diagonal. (Unpolarized/colorless also counts as diagonal.) Flavor is diagonal by definition.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: are_diagonal => quantum_numbers_are_diagonal

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_are_diagonal (qn) result (diagonal)
    logical :: diagonal
    class(quantum_numbers_t), intent(in) :: qn
    diagonal = qn%h%is_diagonal () .and. qn%c%is_diagonal ()
  end function quantum_numbers_are_diagonal

```

Check if the color part has the ghost property.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: is_color_ghost => quantum_numbers_is_color_ghost

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_is_color_ghost (qn) result (ghost)
    logical :: ghost
    class(quantum_numbers_t), intent(in) :: qn
    ghost = qn%c%is_ghost ()
  end function quantum_numbers_is_color_ghost

```

Check if the flavor participates in the hard interaction.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: are_hard_process => quantum_numbers_are_hard_process

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_are_hard_process (qn) result (hard_process)
    logical :: hard_process
    class(quantum_numbers_t), intent(in) :: qn
    hard_process = qn%f%is_hard_process ()
  end function quantum_numbers_are_hard_process

```

11.6.5 Comparisons

Matching and equality is derived from the individual quantum numbers. The variant `fhmatch` matches only flavor and helicity. The variant `dhmatch` matches only diagonal helicity, if the matching helicity is undefined.

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_eq_wo_sub

<Quantum numbers: quantum numbers: TBP>+≡
  generic :: operator(.match.) => quantum_numbers_match
  generic :: operator(.fmatch.) => quantum_numbers_match_f
  generic :: operator(.hmatch.) => quantum_numbers_match_h
  generic :: operator(.fhmatch.) => quantum_numbers_match_fh
  generic :: operator(.dhmatch.) => quantum_numbers_match_hel_diag
  generic :: operator(==) => quantum_numbers_eq
  generic :: operator(/=) => quantum_numbers_neq
  procedure, private :: quantum_numbers_match
  procedure, private :: quantum_numbers_match_f

```

```

procedure, private :: quantum_numbers_match_h
procedure, private :: quantum_numbers_match_fh
procedure, private :: quantum_numbers_match_hel_diag
procedure, private :: quantum_numbers_eq
procedure, private :: quantum_numbers_neq

<Quantum numbers: procedures>+≡
elemental function quantum_numbers_match (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%f .match. qn2%f) .and. &
           (qn1%c .match. qn2%c) .and. &
           (qn1%h .match. qn2%h)
end function quantum_numbers_match

elemental function quantum_numbers_match_f (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%f .match. qn2%f)
end function quantum_numbers_match_f

elemental function quantum_numbers_match_h (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%h .match. qn2%h)
end function quantum_numbers_match_h

elemental function quantum_numbers_match_fh (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%f .match. qn2%f) .and. &
           (qn1%h .match. qn2%h)
end function quantum_numbers_match_fh

elemental function quantum_numbers_match_hel_diag (qn1, qn2) result (match)
  logical :: match
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  match = (qn1%f .match. qn2%f) .and. &
           (qn1%c .match. qn2%c) .and. &
           (qn1%h .dmatch. qn2%h)
end function quantum_numbers_match_hel_diag

elemental function quantum_numbers_eq_wo_sub (qn1, qn2) result (eq)
  logical :: eq
  type(quantum_numbers_t), intent(in) :: qn1, qn2
  eq = (qn1%f == qn2%f) .and. &
        (qn1%c == qn2%c) .and. &
        (qn1%h == qn2%h)
end function quantum_numbers_eq_wo_sub

elemental function quantum_numbers_eq (qn1, qn2) result (eq)
  logical :: eq
  class(quantum_numbers_t), intent(in) :: qn1, qn2
  eq = (qn1%f == qn2%f) .and. &
        (qn1%c == qn2%c) .and. &

```

```

        (qn1%h == qn2%h) .and. &
        (qn1%sub == qn2%sub)
end function quantum_numbers_eq

elemental function quantum_numbers_neq (qn1, qn2) result (neq)
    logical :: neq
    class(quantum_numbers_t), intent(in) :: qn1, qn2
    neq = (qn1%f /= qn2%f) .or. &
        (qn1%c /= qn2%c) .or. &
        (qn1%h /= qn2%h) .or. &
        (qn1%sub /= qn2%sub)
end function quantum_numbers_neq

<Quantum numbers: public>+≡
    public :: assignment(=)

<Quantum numbers: interfaces>+≡
    interface assignment(=)
        module procedure quantum_numbers_assign
    end interface

<Quantum numbers: procedures>+≡
    subroutine quantum_numbers_assign (qn_out, qn_in)
        type(quantum_numbers_t), intent(out) :: qn_out
        type(quantum_numbers_t), intent(in) :: qn_in
        qn_out%f = qn_in%f
        qn_out%c = qn_in%c
        qn_out%h = qn_in%h
        qn_out%sub = qn_in%sub
    end subroutine quantum_numbers_assign

```

Two sets of quantum numbers are compatible if the individual quantum numbers are compatible, depending on the mask. Flavor has to match, regardless of the flavor mask.

If the color flag is set, color is compatible if the ghost property is identical. If the color flag is unset, color has to be identical. I.e., if the flag is set, the color amplitudes can interfere. If it is not set, they must be identical, and there must be no ghost. The latter property is used for expanding physical color flows.

Helicity is compatible if the mask is unset, otherwise it has to match. This determines if two amplitudes can be multiplied (no mask) or traced (mask).

```

<Quantum numbers: public>+≡
    public :: quantum_numbers_are_compatible

<Quantum numbers: procedures>+≡
    elemental function quantum_numbers_are_compatible (qn1, qn2, mask) &
        result (flag)
        logical :: flag
        type(quantum_numbers_t), intent(in) :: qn1, qn2
        type(quantum_numbers_mask_t), intent(in) :: mask
        if (mask%h .or. mask%hd) then
            flag = (qn1%f .match. qn2%f) .and. (qn1%h .match. qn2%h)
        else
            flag = (qn1%f .match. qn2%f)
        end if
    end function quantum_numbers_are_compatible

```

```

end if
if (mask%c) then
  flag = flag .and. (qn1%c%is_ghost () .eqv. qn2%c%is_ghost ())
else
  flag = flag .and. &
    .not. (qn1%c%is_ghost () .or. qn2%c%is_ghost ()) .and. &
    (qn1%c == qn2%c)
end if
end function quantum_numbers_are_compatible

```

This is the analog for a single quantum-number set. We just check for color ghosts; they are excluded if the color mask is unset (color-flow expansion).

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_are_physical

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_are_physical (qn, mask) result (flag)
    logical :: flag
    type(quantum_numbers_t), intent(in) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    if (mask%c) then
      flag = .true.
    else
      flag = .not. qn%c%is_ghost ()
    end if
  end function quantum_numbers_are_physical

```

11.6.6 Operations

Inherited from the color component: reassign color indices in canonical order.

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_canonicalize_color

<Quantum numbers: procedures>+≡
  subroutine quantum_numbers_canonicalize_color (qn)
    type(quantum_numbers_t), dimension(:), intent(inout) :: qn
    call color_canonicalize (qn%c)
  end subroutine quantum_numbers_canonicalize_color

```

Inherited from the color component: make a color map for two matching quantum-number arrays.

```

<Quantum numbers: public>+≡
  public :: make_color_map

<Quantum numbers: interfaces>+≡
  interface make_color_map
    module procedure quantum_numbers_make_color_map
  end interface make_color_map

```

```

<Quantum numbers: procedures>+≡
  subroutine quantum_numbers_make_color_map (map, qn1, qn2)
    integer, dimension(:,:), intent(out), allocatable :: map
    type(quantum_numbers_t), dimension(:), intent(in) :: qn1, qn2
    call make_color_map (map, qn1%c, qn2%c)
  end subroutine quantum_numbers_make_color_map

```

Inherited from the color component: translate the color part using a color-map array

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_translate_color

<Quantum numbers: interfaces>+≡
  interface quantum_numbers_translate_color
    module procedure quantum_numbers_translate_color0
    module procedure quantum_numbers_translate_color1
  end interface

```

```

<Quantum numbers: procedures>+≡
  subroutine quantum_numbers_translate_color0 (qn, map, offset)
    type(quantum_numbers_t), intent(inout) :: qn
    integer, dimension(:,:), intent(in) :: map
    integer, intent(in), optional :: offset
    call color_translate (qn%c, map, offset)
  end subroutine quantum_numbers_translate_color0

  subroutine quantum_numbers_translate_color1 (qn, map, offset)
    type(quantum_numbers_t), dimension(:), intent(inout) :: qn
    integer, dimension(:,:), intent(in) :: map
    integer, intent(in), optional :: offset
    call color_translate (qn%c, map, offset)
  end subroutine quantum_numbers_translate_color1

```

Inherited from the color component: return the color index with highest absolute value.

Since the algorithm is not elemental, we keep the separate procedures for different array rank.

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_get_max_color_value

<Quantum numbers: interfaces>+≡
  interface quantum_numbers_get_max_color_value
    module procedure quantum_numbers_get_max_color_value0
    module procedure quantum_numbers_get_max_color_value1
    module procedure quantum_numbers_get_max_color_value2
  end interface

<Quantum numbers: procedures>+≡
  pure function quantum_numbers_get_max_color_value0 (qn) result (cmax)
    integer :: cmax
    type(quantum_numbers_t), intent(in) :: qn
    cmax = color_get_max_value (qn%c)
  end function quantum_numbers_get_max_color_value0

```

```

pure function quantum_numbers_get_max_color_value1 (qn) result (cmax)
  integer :: cmax
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  cmax = color_get_max_value (qn%c)
end function quantum_numbers_get_max_color_value1

pure function quantum_numbers_get_max_color_value2 (qn) result (cmax)
  integer :: cmax
  type(quantum_numbers_t), dimension(:,:), intent(in) :: qn
  cmax = color_get_max_value (qn%c)
end function quantum_numbers_get_max_color_value2

```

Inherited from the color component: add an offset to the indices of the color part

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: add_color_offset => quantum_numbers_add_color_offset

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_add_color_offset (qn, offset)
    class(quantum_numbers_t), intent(inout) :: qn
    integer, intent(in) :: offset
    call qn%c%add_offset (offset)
  end subroutine quantum_numbers_add_color_offset

```

Given a quantum number array, return all possible color contractions, leaving the other quantum numbers intact.

```

<Quantum numbers: public>+≡
  public :: quantum_number_array_make_color_contractions

<Quantum numbers: procedures>+≡
  subroutine quantum_number_array_make_color_contractions (qn_in, qn_out)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
    type(quantum_numbers_t), dimension(:,:), intent(out), allocatable :: qn_out
    type(color_t), dimension(:,:), allocatable :: col
    integer :: i
    call color_array_make_contractions (qn_in%c, col)
    allocate (qn_out (size (col, 1), size (col, 2)))
    do i = 1, size (qn_out, 2)
      qn_out(:,i)%f = qn_in%f
      qn_out(:,i)%c = col(:,i)
      qn_out(:,i)%h = qn_in%h
    end do
  end subroutine quantum_number_array_make_color_contractions

```

Inherited from the color component: invert the color, switching particle/antiparticle.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: invert_color => quantum_numbers_invert_color

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_invert_color (qn)
    class(quantum_numbers_t), intent(inout) :: qn
    call qn%c%invert ()

```



```
end subroutine quantum_numbers_invert_color
```

Flip helicity.

```
<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: flip_helicity => quantum_numbers_flip_helicity

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_flip_helicity (qn)
    class(quantum_numbers_t), intent(inout) :: qn
    call qn%h%flip ()
  end subroutine quantum_numbers_flip_helicity
```

Merge two quantum number sets: for each entry, if both are defined, combine them to an off-diagonal entry (meaningful only if the input was diagonal). If either entry is undefined, take the defined one.

For flavor, off-diagonal entries are invalid, so both flavors must be equal, otherwise an invalid flavor is inserted.

```
<Quantum numbers: public>+≡
  public :: operator(.merge.)

<Quantum numbers: interfaces>+≡
  interface operator(.merge.)
    module procedure merge_quantum_numbers0
    module procedure merge_quantum_numbers1
  end interface

<Quantum numbers: procedures>+≡
  function merge_quantum_numbers0 (qn1, qn2) result (qn3)
    type(quantum_numbers_t) :: qn3
    type(quantum_numbers_t), intent(in) :: qn1, qn2
    qn3%f = qn1%f .merge. qn2%f
    qn3%c = qn1%c .merge. qn2%c
    qn3%h = qn1%h .merge. qn2%h
    qn3%sub = merge_subtraction_index (qn1%sub, qn2%sub)
  end function merge_quantum_numbers0

  function merge_quantum_numbers1 (qn1, qn2) result (qn3)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn1, qn2
    type(quantum_numbers_t), dimension(size(qn1)) :: qn3
    qn3%f = qn1%f .merge. qn2%f
    qn3%c = qn1%c .merge. qn2%c
    qn3%h = qn1%h .merge. qn2%h
    qn3%sub = merge_subtraction_index (qn1%sub, qn2%sub)
  end function merge_quantum_numbers1

<Quantum numbers: procedures>+≡
  elemental function merge_subtraction_index (sub1, sub2) result (sub3)
    integer :: sub3
    integer, intent(in) :: sub1, sub2
    if (sub1 > 0 .and. sub2 > 0) then
      if (sub1 == sub2) then
        sub3 = sub1
```

```

        else
            sub3 = 0
        end if
    else if (sub1 > 0) then
        sub3 = sub1
    else if (sub2 > 0) then
        sub3 = sub2
    else
        sub3 = 0
    end if
end function merge_subtraction_index

```

11.6.7 The quantum number mask

The quantum numbers mask is true for quantum numbers that should be ignored or summed over. The three mandatory entries correspond to flavor, color, and helicity, respectively.

There is an additional entry `cg`: If false, the color-ghosts property should be kept even if color is ignored. This is relevant only if `c` is set, otherwise it is always false.

The flag `hd` tells that only diagonal entries in helicity should be kept. If `h` is set, `hd` is irrelevant and will be kept `.false`.

```

<Quantum numbers: public>+≡
    public :: quantum_numbers_mask_t

<Quantum numbers: types>+≡
    type :: quantum_numbers_mask_t
        private
            logical :: f = .false.
            logical :: c = .false.
            logical :: cg = .false.
            logical :: h = .false.
            logical :: hd = .false.
            integer :: sub = 0
        contains
            <Quantum numbers: quantum numbers mask: TBP>
        end type quantum_numbers_mask_t

```

Define a quantum number mask: Constructor form

```

<Quantum numbers: public>+≡
    public :: quantum_numbers_mask

<Quantum numbers: procedures>+≡
    elemental function quantum_numbers_mask &
        (mask_f, mask_c, mask_h, mask_cg, mask_hd) result (mask)
        type(quantum_numbers_mask_t) :: mask
        logical, intent(in) :: mask_f, mask_c, mask_h
        logical, intent(in), optional :: mask_cg
        logical, intent(in), optional :: mask_hd
        call quantum_numbers_mask_init &
            (mask, mask_f, mask_c, mask_h, mask_cg, mask_hd)
    end function quantum_numbers_mask

```

Define quantum numbers: Initializer form

```

<Quantum numbers: quantum numbers mask: TBP>≡
  procedure :: init => quantum_numbers_mask_init

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_mask_init &
    (mask, mask_f, mask_c, mask_h, mask_cg, mask_hd)
    class(quantum_numbers_mask_t), intent(inout) :: mask
    logical, intent(in) :: mask_f, mask_c, mask_h
    logical, intent(in), optional :: mask_cg, mask_hd
    mask%f = mask_f
    mask%c = mask_c
    mask%h = mask_h
    mask%cg = .false.
    if (present (mask_cg)) then
      if (mask%c) mask%cg = mask_cg
    else
      mask%cg = mask_c
    end if
    mask%hd = .false.
    if (present (mask_hd)) then
      if (.not. mask%h) mask%hd = mask_hd
    end if
  end subroutine quantum_numbers_mask_init

```

Write a quantum numbers mask. We need the stand-alone subroutine for the array case.

```

<Quantum numbers: public>+≡
  public :: quantum_numbers_mask_write

<Quantum numbers: interfaces>+≡
  interface quantum_numbers_mask_write
    module procedure quantum_numbers_mask_write_single
    module procedure quantum_numbers_mask_write_array
  end interface

<Quantum numbers: quantum numbers mask: TBP>+≡
  procedure :: write => quantum_numbers_mask_write_single

<Quantum numbers: procedures>+≡
  subroutine quantum_numbers_mask_write_single (mask, unit)
    class(quantum_numbers_mask_t), intent(in) :: mask
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(A)", advance="no") "["
    write (u, "(L1)", advance="no") mask%f
    write (u, "(L1)", advance="no") mask%c
    if (.not.mask%cg) write (u, "('g')", advance="no")
    write (u, "(L1)", advance="no") mask%h
    if (mask%hd) write (u, "('d')", advance="no")
    write (u, "(A)", advance="no") "]"
  end subroutine quantum_numbers_mask_write_single

  subroutine quantum_numbers_mask_write_array (mask, unit)

```

```

type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit); if (u < 0) return
write (u, "(A)", advance="no") "["
do i = 1, size (mask)
  if (i > 1) write (u, "(A)", advance="no") "/"
  write (u, "(L1)", advance="no") mask(i)%f
  write (u, "(L1)", advance="no") mask(i)%c
  if (.not.mask(i)%cg) write (u, "('g')", advance="no")
  write (u, "(L1)", advance="no") mask(i)%h
  if (mask(i)%hd) write (u, "('d')", advance="no")
end do
write (u, "(A)", advance="no") "]"
end subroutine quantum_numbers_mask_write_array

```

11.6.8 Setting mask components

(Quantum numbers: quantum numbers mask: TBP)+≡

```

procedure :: set_flavor => quantum_numbers_mask_set_flavor
procedure :: set_color => quantum_numbers_mask_set_color
procedure :: set_helicity => quantum_numbers_mask_set_helicity
procedure :: set_sub => quantum_numbers_mask_set_sub

```

(Quantum numbers: procedures)+≡

```

elemental subroutine quantum_numbers_mask_set_flavor (mask, mask_f)
  class(quantum_numbers_mask_t), intent(inout) :: mask
  logical, intent(in) :: mask_f
  mask%f = mask_f
end subroutine quantum_numbers_mask_set_flavor

elemental subroutine quantum_numbers_mask_set_color (mask, mask_c, mask_cg)
  class(quantum_numbers_mask_t), intent(inout) :: mask
  logical, intent(in) :: mask_c
  logical, intent(in), optional :: mask_cg
  mask%c = mask_c
  if (present (mask_cg)) then
    if (mask%c) mask%cg = mask_cg
  else
    mask%cg = mask_c
  end if
end subroutine quantum_numbers_mask_set_color

elemental subroutine quantum_numbers_mask_set_helicity (mask, mask_h, mask_hd)
  class(quantum_numbers_mask_t), intent(inout) :: mask
  logical, intent(in) :: mask_h
  logical, intent(in), optional :: mask_hd
  mask%h = mask_h
  if (present (mask_hd)) then
    if (.not. mask%h) mask%hd = mask_hd
  end if
end subroutine quantum_numbers_mask_set_helicity

```

```

elemental subroutine quantum_numbers_mask_set_sub (mask, sub)
  class(quantum_numbers_mask_t), intent(inout) :: mask
  integer, intent(in) :: sub
  mask%sub = sub
end subroutine quantum_numbers_mask_set_sub

```

The following routines assign part of a mask, depending on the flags given.

```

<Quantum numbers: quantum numbers mask: TBP>+≡
  procedure :: assign => quantum_numbers_mask_assign

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_mask_assign &
    (mask, mask_in, flavor, color, helicity)
    class(quantum_numbers_mask_t), intent(inout) :: mask
    class(quantum_numbers_mask_t), intent(in) :: mask_in
    logical, intent(in), optional :: flavor, color, helicity
    if (present (flavor)) then
      if (flavor) then
        mask%f = mask_in%f
      end if
    end if
    if (present (color)) then
      if (color) then
        mask%c = mask_in%c
        mask%cg = mask_in%cg
      end if
    end if
    if (present (helicity)) then
      if (helicity) then
        mask%h = mask_in%h
        mask%hd = mask_in%hd
      end if
    end if
  end subroutine quantum_numbers_mask_assign

```

11.6.9 Mask predicates

Return true if either one of the entries is set:

```

<Quantum numbers: public>+≡
  public :: any

<Quantum numbers: interfaces>+≡
  interface any
    module procedure quantum_numbers_mask_any
  end interface

<Quantum numbers: procedures>+≡
  function quantum_numbers_mask_any (mask) result (match)
    logical :: match
    type(quantum_numbers_mask_t), intent(in) :: mask
    match = mask%f .or. mask%c .or. mask%h .or. mask%hd
  end function quantum_numbers_mask_any

```

11.6.10 Operators

The OR operation is applied to all components.

```
<Quantum numbers: quantum numbers mask: TBP>+≡
  generic :: operator(.or.) => quantum_numbers_mask_or
  procedure, private :: quantum_numbers_mask_or

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_mask_or (mask1, mask2) result (mask)
    type(quantum_numbers_mask_t) :: mask
    class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
    mask%f = mask1%f .or. mask2%f
    mask%c = mask1%c .or. mask2%c
    if (mask%c) mask%cg = mask1%cg .or. mask2%cg
    mask%h = mask1%h .or. mask2%h
    if (.not. mask%h) mask%hd = mask1%hd .or. mask2%hd
  end function quantum_numbers_mask_or
```

11.6.11 Mask comparisons

Return true if the two masks are equivalent / differ:

```
<Quantum numbers: quantum numbers mask: TBP>+≡
  generic :: operator(.eqv.) => quantum_numbers_mask_eqv
  generic :: operator(.neqv.) => quantum_numbers_mask_neqv
  procedure, private :: quantum_numbers_mask_eqv
  procedure, private :: quantum_numbers_mask_neqv

<Quantum numbers: procedures>+≡
  elemental function quantum_numbers_mask_eqv (mask1, mask2) result (eqv)
    logical :: eqv
    class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
    eqv = (mask1%f .eqv. mask2%f) .and. &
           (mask1%c .eqv. mask2%c) .and. &
           (mask1%cg .eqv. mask2%cg) .and. &
           (mask1%h .eqv. mask2%h) .and. &
           (mask1%hd .eqv. mask2%hd)
  end function quantum_numbers_mask_eqv

  elemental function quantum_numbers_mask_neqv (mask1, mask2) result (neqv)
    logical :: neqv
    class(quantum_numbers_mask_t), intent(in) :: mask1, mask2
    neqv = (mask1%f .neqv. mask2%f) .or. &
           (mask1%c .neqv. mask2%c) .or. &
           (mask1%cg .neqv. mask2%cg) .or. &
           (mask1%h .neqv. mask2%h) .or. &
           (mask1%hd .neqv. mask2%hd)
  end function quantum_numbers_mask_neqv
```

11.6.12 Apply a mask

Applying a mask to the quantum number object means undefining those entries where the mask is set. The others remain unaffected.

The `hd` mask has the special property that it “diagonalizes” helicity, i.e., the second helicity entry is dropped and the result is a diagonal helicity quantum number.

```

<Quantum numbers: quantum numbers: TBP>+≡
  procedure :: undefine => quantum_numbers_undefine
  procedure :: undefined => quantum_numbers_undefined0

<Quantum numbers: public>+≡
  public :: quantum_numbers_undefined

<Quantum numbers: interfaces>+≡
  interface quantum_numbers_undefined
    module procedure quantum_numbers_undefined0
    module procedure quantum_numbers_undefined1
    module procedure quantum_numbers_undefined11
  end interface

<Quantum numbers: procedures>+≡
  elemental subroutine quantum_numbers_undefine (qn, mask)
    class(quantum_numbers_t), intent(inout) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    if (mask%f) call qn%f%undefine ()
    if (mask%c) call qn%c%undefine (undefine_ghost = mask%cg)
    if (mask%h) then
      call qn%h%undefine ()
    else if (mask%hd) then
      if (.not. qn%h%is_diagonal ()) then
        call qn%h%diagonalize ()
      end if
    end if
    if (mask%sub > 0) qn%sub = 0
  end subroutine quantum_numbers_undefine

  function quantum_numbers_undefined0 (qn, mask) result (qn_new)
    class(quantum_numbers_t), intent(in) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    type(quantum_numbers_t) :: qn_new
    select type (qn)
      type is (quantum_numbers_t); qn_new = qn
    end select
    call quantum_numbers_undefine (qn_new, mask)
  end function quantum_numbers_undefined0

  function quantum_numbers_undefined1 (qn, mask) result (qn_new)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    type(quantum_numbers_mask_t), intent(in) :: mask
    type(quantum_numbers_t), dimension(size(qn)) :: qn_new
    qn_new = qn
    call quantum_numbers_undefine (qn_new, mask)
  end function quantum_numbers_undefined1

  function quantum_numbers_undefined11 (qn, mask) result (qn_new)
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    type(quantum_numbers_t), dimension(size(qn)) :: qn_new

```

```

    qn_new = qn
    call quantum_numbers_undefine (qn_new, mask)
end function quantum_numbers_undefined11

```

Return true if the input quantum number set has entries that would be removed by the applied mask, e.g., if polarization is defined but `mask%h` is set:

```

<Quantum numbers: quantum numbers: TBP>+≡
    procedure :: are_redundant => quantum_numbers_are_redundant

<Quantum numbers: procedures>+≡
    elemental function quantum_numbers_are_redundant (qn, mask) &
        result (redundant)
        logical :: redundant
        class(quantum_numbers_t), intent(in) :: qn
        type(quantum_numbers_mask_t), intent(in) :: mask
        redundant = .false.
        if (mask%f) then
            redundant = qn%f%is_defined ()
        end if
        if (mask%c) then
            redundant = qn%c%is_defined ()
        end if
        if (mask%h) then
            redundant = qn%h%is_defined ()
        else if (mask%hd) then
            redundant = .not. qn%h%is_diagonal ()
        end if
        if (mask%sub > 0) redundant = qn%sub >= mask%sub
    end function quantum_numbers_are_redundant

```

Return true if the helicity flag is set or the diagonal-helicity flag is set.

```

<Quantum numbers: quantum numbers mask: TBP>+≡
    procedure :: diagonal_helicity => quantum_numbers_mask_diagonal_helicity

<Quantum numbers: procedures>+≡
    elemental function quantum_numbers_mask_diagonal_helicity (mask) &
        result (flag)
        logical :: flag
        class(quantum_numbers_mask_t), intent(in) :: mask
        flag = mask%h .or. mask%hd
    end function quantum_numbers_mask_diagonal_helicity

```


Chapter 12

Transition Matrices and Evaluation

The modules in this chapter implement transition matrices and calculations. The functionality is broken down in three modules

state_matrices represent state and transition density matrices built from particle quantum numbers (helicity, color, flavor)

interactions extend state matrices with the record of particle momenta. They also distinguish in- and out-particles and store parent-child relations.

evaluators These objects extend interaction objects by the information how to calculate matrix elements from products and squares of other interactions. They implement the methods to actually compute those matrix elements.

12.1 State matrices

This module deals with the internal state of a particle system, i.e., with its density matrix in flavor, color, and helicity space.

```
<state_matrices.f90>≡  
<File header>  
  
module state_matrices  
  
  <Use kinds>  
  use constants, only: zero  
  use io_units  
  use format_utils, only: pac_fmt  
  use format_defs, only: FMT_17, FMT_19  
  use diagnostics  
  use sorting  
  use model_data  
  use flavors  
  use colors  
  use helicities  
  use quantum_numbers  
  
  <Standard module head>  
  
  <State matrices: public>  
  
  <State matrices: parameters>  
  
  <State matrices: types>  
  
  <State matrices: interfaces>  
  
contains  
  
  <State matrices: procedures>  
  
end module state_matrices
```

12.1.1 Nodes of the quantum state trie

A quantum state object represents an unnormalized density matrix, i.e., an array of possibilities for flavor, color, and helicity indices with associated complex values. Physically, the trace of this matrix is the summed squared matrix element for an interaction, and the matrix elements divided by this value correspond to the flavor-color-helicity density matrix. (Flavor and color are diagonal.)

We store density matrices as tries, that is, as trees where each branching represents the possible quantum numbers of a particle. The first branching is the first particle in the system. A leaf (the node corresponding to the last particle) contains the value of the matrix element.

Each node contains a flavor, color, and helicity entry. Note that each of those entries may be actually undefined, so we can also represent, e.g., unpolarized particles.

The value is meaningful only for leaves, which have no child nodes. There is a pointer to the parent node which allows for following the trie downwards from a leaf, it is null for a root node. The child nodes are implemented as a list, so there is a pointer to the first and last child, and each node also has a **next** pointer to the next sibling.

The root node does not correspond to a particle, only its children do. The quantum numbers of the root node are irrelevant and will not be set. However, we use a common type for the three classes (root, branch, leaf); they may easily be distinguished by the association status of parent and child.

Node type

The node is linked in all directions: the parent, the first and last in the list of children, and the previous and next sibling. This allows us for adding and removing nodes and whole branches anywhere in the trie. (Circular links are not allowed, however.). The node holds its associated set of quantum numbers. The integer index, which is set only for leaf nodes, is the index of the corresponding matrix element value within the state matrix.

Temporarily, matrix-element values may be stored within a leaf node. This is used during state-matrix factorization. When the state matrix is **frozen**, these values are transferred to the matrix-element array within the host state matrix.

```

(State matrices: types)≡
  type :: node_t
  private
  type(quantum_numbers_t) :: qn
  type(node_t), pointer :: parent => null ()
  type(node_t), pointer :: child_first => null ()
  type(node_t), pointer :: child_last => null ()
  type(node_t), pointer :: next => null ()
  type(node_t), pointer :: previous => null ()
  integer :: me_index = 0
  integer, dimension(:), allocatable :: me_count
  complex(default) :: me = 0
end type node_t

```

Operations on nodes

Recursively deallocate all children of the current node. This includes any values associated with the children.

```

(State matrices: procedures)≡
  pure recursive subroutine node_delete_offspring (node)
  type(node_t), pointer :: node
  type(node_t), pointer :: child
  child => node%child_first
  do while (associated (child))
    node%child_first => node%child_first%next
    call node_delete_offspring (child)
    deallocate (child)
    child => node%child_first
  end do

```

```

        node%child_last => null ()
    end subroutine node_delete_offspring

```

Remove a node including its offspring. Adjust the pointers of parent and siblings, if necessary.

(State matrices: procedures)+≡

```

    pure subroutine node_delete (node)
        type(node_t), pointer :: node
        call node_delete_offspring (node)
        if (associated (node%previous)) then
            node%previous%next => node%next
        else if (associated (node%parent)) then
            node%parent%child_first => node%next
        end if
        if (associated (node%next)) then
            node%next%previous => node%previous
        else if (associated (node%parent)) then
            node%parent%child_last => node%previous
        end if
        deallocate (node)
    end subroutine node_delete

```

Append a child node

(State matrices: procedures)+≡

```

    subroutine node_append_child (node, child)
        type(node_t), target, intent(inout) :: node
        type(node_t), pointer :: child
        allocate (child)
        if (associated (node%child_last)) then
            node%child_last%next => child
            child%previous => node%child_last
        else
            node%child_first => child
        end if
        node%child_last => child
        child%parent => node
    end subroutine node_append_child

```

I/O

Output of a single node, no recursion. We print the quantum numbers in square brackets, then the value (if any).

(State matrices: procedures)+≡

```

    subroutine node_write (node, me_array, verbose, unit, col_verbose, testflag)
        type(node_t), intent(in) :: node
        complex(default), dimension(:), intent(in), optional :: me_array
        logical, intent(in), optional :: verbose, col_verbose, testflag
        integer, intent(in), optional :: unit
        logical :: verb
        integer :: u
        character(len=7) :: fmt

```

```

call pac_fmt (fmt, FMT_19, FMT_17, testflag)
verb = .false.; if (present (verbose)) verb = verbose
u = given_output_unit (unit); if (u < 0) return
call node%qn%write (u, col_verbose)
if (node%me_index /= 0) then
  write (u, "(A,I0,A)", advance="no") " => ME(", node%me_index, ")"
  if (present (me_array)) then
    write (u, "(A)", advance="no") " = "
    write (u, "('(', " // fmt // ",',', " // fmt // ",')')'", &
      advance="no") pacify_complex (me_array(node%me_index))
  end if
end if
write (u, *)
if (verb) then
  call ptr_write ("parent      ", node%parent)
  call ptr_write ("child_first", node%child_first)
  call ptr_write ("child_last ", node%child_last)
  call ptr_write ("next       ", node%next)
  call ptr_write ("previous   ", node%previous)
end if
contains
subroutine ptr_write (label, node)
  character(*), intent(in) :: label
  type(node_t), pointer :: node
  if (associated (node)) then
    write (u, "(10x,A,1x,'->',1x)", advance="no") label
    call node%qn%write (u, col_verbose)
    write (u, *)
  end if
end subroutine ptr_write
end subroutine node_write

```

Recursive output of a node:

(State matrices: procedures)+≡

```

recursive subroutine node_write_rec (node, me_array, verbose, &
  indent, unit, col_verbose, testflag)
  type(node_t), intent(in), target :: node
  complex(default), dimension(:), intent(in), optional :: me_array
  logical, intent(in), optional :: verbose, col_verbose, testflag
  integer, intent(in), optional :: indent
  integer, intent(in), optional :: unit
  type(node_t), pointer :: current
  logical :: verb
  integer :: i, u
  verb = .false.; if (present (verbose)) verb = verbose
  i = 0; if (present (indent)) i = indent
  u = given_output_unit (unit); if (u < 0) return
  current => node%child_first
  do while (associated (current))
    write (u, "(A)", advance="no") repeat (" ", i)
    call node_write (current, me_array, verbose = verb, &
      unit = u, col_verbose = col_verbose, testflag = testflag)
    call node_write_rec (current, me_array, verbose = verb, &
      indent = i + 2, unit = u, col_verbose = col_verbose, testflag = testflag)
  end do

```

```

        current => current%next
    end do
end subroutine node_write_rec

```

Binary I/O. Matrix elements are written only for leaf nodes.

<State matrices: procedures>+≡

```

recursive subroutine node_write_raw_rec (node, u)
    type(node_t), intent(in), target :: node
    integer, intent(in) :: u
    logical :: associated_child_first, associated_next
    call node%qn%write_raw (u)
    associated_child_first = associated (node%child_first)
    write (u) associated_child_first
    associated_next = associated (node%next)
    write (u) associated_next
    if (associated_child_first) then
        call node_write_raw_rec (node%child_first, u)
    else
        write (u) node%me_index
        write (u) node%me
    end if
    if (associated_next) then
        call node_write_raw_rec (node%next, u)
    end if
end subroutine node_write_raw_rec

recursive subroutine node_read_raw_rec (node, u, parent, iostat)
    type(node_t), intent(out), target :: node
    integer, intent(in) :: u
    type(node_t), intent(in), optional, target :: parent
    integer, intent(out), optional :: iostat
    logical :: associated_child_first, associated_next
    type(node_t), pointer :: child
    call node%qn%read_raw (u, iostat=iostat)
    read (u, iostat=iostat) associated_child_first
    read (u, iostat=iostat) associated_next
    if (present (parent)) node%parent => parent
    if (associated_child_first) then
        allocate (child)
        node%child_first => child
        node%child_last => null ()
        call node_read_raw_rec (child, u, node, iostat=iostat)
        do while (associated (child))
            child%previous => node%child_last
            node%child_last => child
            child => child%next
        end do
    else
        read (u, iostat=iostat) node%me_index
        read (u, iostat=iostat) node%me
    end if
    if (associated_next) then
        allocate (node%next)
        call node_read_raw_rec (node%next, u, parent, iostat=iostat)
    end if
end subroutine node_read_raw_rec

```

```

        end if
    end subroutine node_read_raw_rec

```

12.1.2 State matrix

Definition

The quantum state object is a container that keeps and hides the root node. For direct accessibility of values, they are stored in a separate array. The leaf nodes of the quantum-number tree point to those values, once the state matrix is finalized.

The `norm` component is redefined if a common factor is extracted from all nodes.

```

<State matrices: public>≡
    public :: state_matrix_t

<State matrices: types>+=
    type :: state_matrix_t
    private
        type(node_t), pointer :: root => null ()
        integer :: depth = 0
        integer :: n_matrix_elements = 0
        logical :: leaf_nodes_store_values = .false.
        integer :: n_counters = 0
        complex(default), dimension(:), allocatable :: me
        real(default) :: norm = 1
        integer :: n_sub = -1
    contains
        <State matrices: state matrix: TBP>
    end type state_matrix_t

```

This initializer allocates the root node but does not fill anything. We declare whether values are stored within the nodes during state-matrix construction, and how many counters should be maintained (default: none).

```

<State matrices: state matrix: TBP>≡
    procedure :: init => state_matrix_init

<State matrices: procedures>+=
    subroutine state_matrix_init (state, store_values, n_counters)
        class(state_matrix_t), intent(out) :: state
        logical, intent(in), optional :: store_values
        integer, intent(in), optional :: n_counters
        allocate (state%root)
        if (present (store_values)) &
            state%leaf_nodes_store_values = store_values
        if (present (n_counters)) state%n_counters = n_counters
    end subroutine state_matrix_init

```

This recursively deletes all children of the root node, restoring the initial state. The matrix element array is not finalized, since it does not contain physical entries, just pointers.

```

<State matrices: state matrix: TBP>+=

```

```

        procedure :: final => state_matrix_final
    <State matrices: procedures>+≡
        subroutine state_matrix_final (state)
            class(state_matrix_t), intent(inout) :: state
            if (allocated (state%me)) deallocate (state%me)
            if (associated (state%root)) call node_delete (state%root)
            state%depth = 0
            state%n_matrix_elements = 0
        end subroutine state_matrix_final

```

Output: Present the tree as a nested list with appropriate indentation.

```

    <State matrices: state matrix: TBP>+≡
        procedure :: write => state_matrix_write
    <State matrices: procedures>+≡
        subroutine state_matrix_write (state, unit, write_value_list, &
            verbose, col_verbose, testflag)
            class(state_matrix_t), intent(in) :: state
            logical, intent(in), optional :: write_value_list, verbose, col_verbose
            logical, intent(in), optional :: testflag
            integer, intent(in), optional :: unit
            complex(default) :: me_dum
            character(len=7) :: fmt
            integer :: u
            integer :: i
            call pac_fmt (fmt, FMT_19, FMT_17, testflag)
            u = given_output_unit (unit); if (u < 0) return
            write (u, "(1x,A," // fmt // ")") "State matrix: norm = ", state%norm
            if (associated (state%root)) then
                if (allocated (state%me)) then
                    call node_write_rec (state%root, state%me, verbose = verbose, &
                        indent = 1, unit = u, col_verbose = col_verbose, &
                        testflag = testflag)
                else
                    call node_write_rec (state%root, verbose = verbose, indent = 1, &
                        unit = u, col_verbose = col_verbose, testflag = testflag)
                end if
            end if
            if (present (write_value_list)) then
                if (write_value_list .and. allocated (state%me)) then
                    do i = 1, size (state%me)
                        write (u, "(1x,I0,A)", advance="no") i, ":"
                        me_dum = state%me(i)
                        if (real(state%me(i)) == -real(state%me(i))) then
                            me_dum = &
                                cmplx (0._default, aimag(me_dum), kind=default)
                        end if
                        if (aimag(me_dum) == -aimag(me_dum)) then
                            me_dum = &
                                cmplx (real(me_dum), 0._default, kind=default)
                        end if
                        write (u, "('(', " // fmt // ",','," // fmt // &
                            ",')'") me_dum
                    end do
                end if
            end if

```



```

        end if
    end if
end subroutine state_matrix_write

```

Binary I/O. The auxiliary matrix-element array is not written, but reconstructed after reading the tree.

Note: To be checked. Might be broken, don't use (unless trivial).

(State matrices: state matrix: TBP)+≡

```

    procedure :: write_raw => state_matrix_write_raw
    procedure :: read_raw => state_matrix_read_raw

```

(State matrices: procedures)+≡

```

subroutine state_matrix_write_raw (state, u)
    class(state_matrix_t), intent(in), target :: state
    integer, intent(in) :: u
    logical :: is_defined
    integer :: depth, j
    type(state_iterator_t) :: it
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    is_defined = state%is_defined ()
    write (u) is_defined
    if (is_defined) then
        write (u) state%get_norm ()
        write (u) state%get_n_leaves ()
        depth = state%get_depth ()
        write (u) depth
        allocate (qn (depth))
        call it%init (state)
        do while (it%is_valid ())
            qn = it%get_quantum_numbers ()
            do j = 1, depth
                call qn(j)%write_raw (u)
            end do
            write (u) it%get_me_index ()
            write (u) it%get_matrix_element ()
            call it%advance ()
        end do
    end if
end subroutine state_matrix_write_raw

```

```

subroutine state_matrix_read_raw (state, u, iostat)
    class(state_matrix_t), intent(out) :: state
    integer, intent(in) :: u
    integer, intent(out) :: iostat
    logical :: is_defined
    real(default) :: norm
    integer :: n_leaves, depth, i, j
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: me_index
    complex(default) :: me
    read (u, iostat=iostat) is_defined
    if (iostat /= 0) goto 1
    if (is_defined) then
        call state%init (store_values = .true.)
    end if
1
end subroutine state_matrix_read_raw

```

```

        read (u, iostat=iostat) norm
        if (iostat /= 0) goto 1
        call state_matrix_set_norm (state, norm)
        read (u) n_leaves
        if (iostat /= 0) goto 1
        read (u) depth
        if (iostat /= 0) goto 1
        allocate (qn (depth))
        do i = 1, n_leaves
            do j = 1, depth
                call qn(j)%read_raw (u, iostat=iostat)
                if (iostat /= 0) goto 1
            end do
            read (u, iostat=iostat) me_index
            if (iostat /= 0) goto 1
            read (u, iostat=iostat) me
            if (iostat /= 0) goto 1
            call state%add_state (qn, index = me_index, value = me)
        end do
        call state_matrix_freeze (state)
    end if
    return

    ! Clean up on error
1    continue
    call state%final ()
end subroutine state_matrix_read_raw

```

Assign a model pointer to all flavor entries. This will become necessary when we have read a state matrix from file.

```

<State matrices: state matrix: TBP>+≡
    procedure :: set_model => state_matrix_set_model

<State matrices: procedures>+≡
    subroutine state_matrix_set_model (state, model)
        class(state_matrix_t), intent(inout), target :: state
        class(model_data_t), intent(in), target :: model
        type(state_iterator_t) :: it
        call it%init (state)
        do while (it%is_valid ())
            call it%set_model (model)
            call it%advance ()
        end do
    end subroutine state_matrix_set_model

```

Iterate over **state**, get the quantum numbers array **qn** for each iteration, and tag all array elements of **qn** with the indices given by **tag** as part of the hard interaction. Then add them to **tagged_state** and return it. If no **tag** is given, tag all **qn** as part of the hard process.

```

<State matrices: state matrix: TBP>+≡
    procedure :: tag_hard_process => state_matrix_tag_hard_process

<State matrices: procedures>+≡

```

```

subroutine state_matrix_tag_hard_process (state, tagged_state, tag)
  class(state_matrix_t), intent(in), target :: state
  type(state_matrix_t), intent(out) :: tagged_state
  integer, dimension(:), intent(in), optional :: tag
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  complex(default) :: value
  integer :: i
  call tagged_state%init (store_values = .true.)
  call it%init (state)
  do while (it%is_valid ())
    qn = it%get_quantum_numbers ()
    value = it%get_matrix_element ()
    if (present (tag)) then
      do i = 1, size (tag)
        call qn(tag(i))%tag_hard_process ()
      end do
    else
      call qn%tag_hard_process ()
    end if
    call tagged_state%add_state (qn, index = it%get_me_index (), value = value)
    call it%advance ()
  end do
  call tagged_state%freeze ()
end subroutine state_matrix_tag_hard_process

```

Properties of the quantum state

A state is defined if its root is allocated:

```

<State matrices: state matrix: TBP>+≡
  procedure :: is_defined => state_matrix_is_defined

<State matrices: procedures>+≡
  elemental function state_matrix_is_defined (state) result (defined)
    logical :: defined
    class(state_matrix_t), intent(in) :: state
    defined = associated (state%root)
  end function state_matrix_is_defined

```

A state is empty if its depth is zero:

```

<State matrices: state matrix: TBP>+≡
  procedure :: is_empty => state_matrix_is_empty

<State matrices: procedures>+≡
  elemental function state_matrix_is_empty (state) result (flag)
    logical :: flag
    class(state_matrix_t), intent(in) :: state
    flag = state%depth == 0
  end function state_matrix_is_empty

```

Return the number of matrix-element values.

```

<State matrices: state matrix: TBP>+≡
generic :: get_n_matrix_elements => get_n_matrix_elements_all, get_n_matrix_elements_mask
procedure :: get_n_matrix_elements_all => state_matrix_get_n_matrix_elements_all
procedure :: get_n_matrix_elements_mask => state_matrix_get_n_matrix_elements_mask

```

```

<State matrices: procedures>+≡
pure function state_matrix_get_n_matrix_elements_all (state) result (n)
  integer :: n
  class(state_matrix_t), intent(in) :: state
  n = state%n_matrix_elements
end function state_matrix_get_n_matrix_elements_all

```

```

<State matrices: procedures>+≡
function state_matrix_get_n_matrix_elements_mask (state, qn_mask) result (n)
  integer :: n
  class(state_matrix_t), intent(in) :: state
  type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(size(qn_mask)) :: qn
  type(state_matrix_t) :: state_tmp
  call state_tmp%init ()
  call it%init (state)
  do while (it%is_valid ())
    qn = it%get_quantum_numbers ()
    call qn%undefine (qn_mask)
    call state_tmp%add_state (qn)
    call it%advance ()
  end do
  n = state_tmp%n_matrix_elements
  call state_tmp%final ()
end function state_matrix_get_n_matrix_elements_mask

```

Return the size of the me-array for debugging purposes.

```

<State matrices: state matrix: TBP>+≡
procedure :: get_me_size => state_matrix_get_me_size

```

```

<State matrices: procedures>+≡
pure function state_matrix_get_me_size (state) result (n)
  integer :: n
  class(state_matrix_t), intent(in) :: state
  if (allocated (state%me)) then
    n = size (state%me)
  else
    n = 0
  end if
end function state_matrix_get_me_size

```

```

<State matrices: state matrix: TBP>+≡
procedure :: compute_n_sub => state_matrix_compute_n_sub

```

```

<State matrices: procedures>+≡
function state_matrix_compute_n_sub (state) result (n_sub)
  integer :: n_sub

```

```

class(state_matrix_t), intent(in) :: state
type(state_iterator_t) :: it
type(quantum_numbers_t), dimension(state%depth) :: qn
integer :: sub, sub_pos
n_sub = 0
call it%init (state)
do while (it%is_valid ())
  qn = it%get_quantum_numbers ()
  sub = 0
  sub_pos = qn_array_sub_pos ()
  if (sub_pos > 0) sub = qn(sub_pos)%get_sub ()
  if (sub > n_sub) n_sub = sub
  call it%advance ()
end do
contains
function qn_array_sub_pos () result (pos)
  integer :: pos
  integer :: i
  pos = 0
  do i = 1, state%depth
    if (qn(i)%get_sub () > 0) then
      pos = i
      exit
    end if
  end do
end function qn_array_sub_pos
end function state_matrix_compute_n_sub

```

<State matrices: state matrix: TBP>+≡
 procedure :: set_n_sub => state_matrix_set_n_sub

<State matrices: procedures>+≡
 subroutine state_matrix_set_n_sub (state)
 class(state_matrix_t), intent(inout) :: state
 state%n_sub = state%compute_n_sub ()
end subroutine state_matrix_set_n_sub

Return number of subtractions.

<State matrices: state matrix: TBP>+≡
 procedure :: get_n_sub => state_matrix_get_n_sub

<State matrices: procedures>+≡
 function state_matrix_get_n_sub (state) result (n_sub)
 integer :: n_sub
 class(state_matrix_t), intent(in) :: state
 if (state%n_sub < 0) then
 call msg_bug ("[state_matrix_get_n_sub] number of subtractions not set.")
 end if
 n_sub = state%n_sub
end function state_matrix_get_n_sub

Return the number of leaves. This can be larger than the number of independent matrix elements.

<State matrices: state matrix: TBP>+≡

```

    procedure :: get_n_leaves => state_matrix_get_n_leaves
<State matrices: procedures>+≡
    function state_matrix_get_n_leaves (state) result (n)
        integer :: n
        class(state_matrix_t), intent(in) :: state
        type(state_iterator_t) :: it
        n = 0
        call it%init (state)
        do while (it%is_valid ())
            n = n + 1
            call it%advance ()
        end do
    end function state_matrix_get_n_leaves

```

Return the depth:

```

<State matrices: state matrix: TBP>+≡
    procedure :: get_depth => state_matrix_get_depth
<State matrices: procedures>+≡
    pure function state_matrix_get_depth (state) result (depth)
        integer :: depth
        class(state_matrix_t), intent(in) :: state
        depth = state%depth
    end function state_matrix_get_depth

```

Return the norm:

```

<State matrices: state matrix: TBP>+≡
    procedure :: get_norm => state_matrix_get_norm
<State matrices: procedures>+≡
    pure function state_matrix_get_norm (state) result (norm)
        real(default) :: norm
        class(state_matrix_t), intent(in) :: state
        norm = state%norm
    end function state_matrix_get_norm

```

Retrieving contents

Return the quantum number array, using an index. We have to scan the state matrix since there is no shortcut.

```

<State matrices: state matrix: TBP>+≡
    procedure :: get_quantum_number => &
        state_matrix_get_quantum_number
<State matrices: procedures>+≡
    function state_matrix_get_quantum_number (state, i, by_me_index) result (qn)
        class(state_matrix_t), intent(in), target :: state
        integer, intent(in) :: i
        logical, intent(in), optional :: by_me_index
        logical :: opt_by_me_index
        type(quantum_numbers_t), dimension(state%depth) :: qn
        type(state_iterator_t) :: it

```

```

integer :: k
opt_by_me_index = .false.
if (present (by_me_index)) opt_by_me_index = by_me_index
k = 0
call it%init (state)
do while (it%is_valid ())
  if (opt_by_me_index) then
    k = it%get_me_index ()
  else
    k = k + 1
  end if
  if (k == i) then
    qn = it%get_quantum_numbers ()
    exit
  end if
  call it%advance ()
end do
end function state_matrix_get_quantum_number

```

<State matrices: state matrix: TBP>+≡

```

generic :: get_quantum_numbers => get_quantum_numbers_all, get_quantum_numbers_mask
procedure :: get_quantum_numbers_all => state_matrix_get_quantum_numbers_all
procedure :: get_quantum_numbers_mask => state_matrix_get_quantum_numbers_mask

```

<State matrices: procedures>+≡

```

subroutine state_matrix_get_quantum_numbers_all (state, qn)
  class(state_matrix_t), intent(in), target :: state
  type(quantum_numbers_t), intent(out), dimension(:,:), allocatable :: qn
  integer :: i
  allocate (qn (state%get_n_matrix_elements (), &
    state%get_depth()))
  do i = 1, state%get_n_matrix_elements ()
    qn (i, :) = state%get_quantum_number (i)
  end do
end subroutine state_matrix_get_quantum_numbers_all

```

<State matrices: procedures>+≡

```

subroutine state_matrix_get_quantum_numbers_mask (state, qn_mask, qn)
  class(state_matrix_t), intent(in), target :: state
  type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
  type(quantum_numbers_t), intent(out), dimension(:,:), allocatable :: qn
  type(quantum_numbers_t), dimension(:), allocatable :: qn_tmp
  type(state_matrix_t) :: state_tmp
  type(state_iterator_t) :: it
  integer :: i, n
  n = state%get_n_matrix_elements (qn_mask)
  allocate (qn (n, state%get_depth ()))
  allocate (qn_tmp (state%get_depth ()))
  call it%init (state)
  call state_tmp%init ()
  do while (it%is_valid ())
    qn_tmp = it%get_quantum_numbers ()
    call qn_tmp%undefine (qn_mask)
    call state_tmp%add_state (qn_tmp)
  end do
end subroutine state_matrix_get_quantum_numbers_mask

```

```

        call it%advance ()
    end do
    do i = 1, n
        qn (i, :) = state_tmp%get_quantum_number (i)
    end do
    call state_tmp%final ()
end subroutine state_matrix_get_quantum_numbers_mask

```

<State matrices: state matrix: TBP>+≡

```

    procedure :: get_flavors => state_matrix_get_flavors

```

<State matrices: procedures>+≡

```

subroutine state_matrix_get_flavors (state, only_elementary, qn_mask, flv)
    class(state_matrix_t), intent(in), target :: state
    logical, intent(in) :: only_elementary
    type(quantum_numbers_mask_t), intent(in), dimension(:), optional :: qn_mask
    integer, intent(out), dimension(:,:), allocatable :: flv
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    integer :: i_flv, n_partons
    type(flavor_t), dimension(:), allocatable :: flv_flv
    if (present (qn_mask)) then
        call state%get_quantum_numbers (qn_mask, qn)
    else
        call state%get_quantum_numbers (qn)
    end if
    allocate (flv_flv (size (qn, dim=2)))
    if (only_elementary) then
        flv_flv = qn(1, :)%get_flavor ()
        n_partons = count (is_elementary (flv_flv%get_pdg ()))
    end if
    allocate (flv (n_partons, size (qn, dim=1)))
    associate (n_flv => size (qn, dim=1))
        do i_flv = 1, size (qn, dim=1)
            flv_flv = qn(i_flv, :)%get_flavor ()
            flv(:, i_flv) = pack (flv_flv%get_pdg (), is_elementary(flv_flv%get_pdg()))
        end do
    end associate
contains
    elemental function is_elementary (pdg)
        logical :: is_elementary
        integer, intent(in) :: pdg
        is_elementary = abs(pdg) /= 2212 .and. abs(pdg) /= 92 .and. abs(pdg) /= 93
    end function is_elementary
end subroutine state_matrix_get_flavors

```

Return a single matrix element using its index. Works only if the shortcut array is allocated.

<State matrices: state matrix: TBP>+≡

```

generic :: get_matrix_element => get_matrix_element_single
generic :: get_matrix_element => get_matrix_element_array
procedure :: get_matrix_element_single => &
    state_matrix_get_matrix_element_single
procedure :: get_matrix_element_array => &
    state_matrix_get_matrix_element_array

```



```

<State matrices: procedures>+≡
elemental function state_matrix_get_matrix_element_single (state, i) result (me)
  complex(default) :: me
  class(state_matrix_t), intent(in) :: state
  integer, intent(in) :: i
  if (allocated (state%me)) then
    me = state%me(i)
  else
    me = 0
  end if
end function state_matrix_get_matrix_element_single

```

```

<State matrices: procedures>+≡
function state_matrix_get_matrix_element_array (state) result (me)
  complex(default), dimension(:), allocatable :: me
  class(state_matrix_t), intent(in) :: state
  if (allocated (state%me)) then
    allocate (me (size (state%me)))
    me = state%me
  else
    me = 0
  end if
end function state_matrix_get_matrix_element_array

```

Return the color index with maximum absolute value that is present within the state matrix.

```

<State matrices: state matrix: TBP>+≡
procedure :: get_max_color_value => state_matrix_get_max_color_value

```

```

<State matrices: procedures>+≡
function state_matrix_get_max_color_value (state) result (cmax)
  integer :: cmax
  class(state_matrix_t), intent(in) :: state
  if (associated (state%root)) then
    cmax = node_get_max_color_value (state%root)
  else
    cmax = 0
  end if
contains
  recursive function node_get_max_color_value (node) result (cmax)
    integer :: cmax
    type(node_t), intent(in), target :: node
    type(node_t), pointer :: current
    cmax = quantum_numbers_get_max_color_value (node%qn)
    current => node%child_first
    do while (associated (current))
      cmax = max (cmax, node_get_max_color_value (current))
      current => current%next
    end do
  end function node_get_max_color_value
end function state_matrix_get_max_color_value

```

Building the quantum state

The procedure generates a branch associated to the input array of quantum numbers. If the branch exists already, it is used.

Optionally, we set the matrix-element index, a value (which may be added to the previous one), and increment one of the possible counters. We may also return the matrix element index of the current node.

```

<State matrices: state matrix: TBP>+≡
  procedure :: add_state => state_matrix_add_state

<State matrices: procedures>+≡
  subroutine state_matrix_add_state (state, qn, index, value, &
    sum_values, counter_index, ignore_sub_for_qn, me_index)
    class(state_matrix_t), intent(inout) :: state
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: index
    complex(default), intent(in), optional :: value
    logical, intent(in), optional :: sum_values
    integer, intent(in), optional :: counter_index
    logical, intent(in), optional :: ignore_sub_for_qn
    integer, intent(out), optional :: me_index
    logical :: set_index, get_index, add
    set_index = present (index)
    get_index = present (me_index)
    add = .false.; if (present (sum_values)) add = sum_values
    if (state%depth == 0) then
      state%depth = size (qn)
    else if (state%depth /= size (qn)) then
      call state%write ()
      call msg_bug ("State matrix: depth mismatch")
    end if
    if (size (qn) > 0) call node_make_branch (state%root, qn)
contains
    recursive subroutine node_make_branch (parent, qn)
      type(node_t), pointer :: parent
      type(quantum_numbers_t), dimension(:), intent(in) :: qn
      type(node_t), pointer :: child
      logical :: match
      match = .false.
      child => parent%child_first
      SCAN_CHILDREN: do while (associated (child))
        if (present (ignore_sub_for_qn)) then
          if (ignore_sub_for_qn) then
            match = quantum_numbers_eq_wo_sub (child%qn, qn(1))
          else
            match = child%qn == qn(1)
          end if
        else
          match = child%qn == qn(1)
        end if
        if (match) exit SCAN_CHILDREN
        child => child%next
      end do SCAN_CHILDREN
      if (.not. match) then

```

```

        call node_append_child (parent, child)
        child%qn = qn(1)
    end if
    select case (size (qn))
    case (1)
        if (.not. match) then
            state%n_matrix_elements = state%n_matrix_elements + 1
            child%me_index = state%n_matrix_elements
        end if
        if (set_index) then
            child%me_index = index
        end if
        if (get_index) then
            me_index = child%me_index
        end if
        if (present (counter_index)) then
            if (.not. allocated (child%me_count)) then
                allocate (child%me_count (state%n_counters))
                child%me_count = 0
            end if
            child%me_count(counter_index) = child%me_count(counter_index) + 1
        end if
        if (present (value)) then
            if (add) then
                child%me = child%me + value
            else
                child%me = value
            end if
        end if
    case (2:)
        call node_make_branch (child, qn(2:))
    end select
end subroutine node_make_branch
end subroutine state_matrix_add_state

```

Remove irrelevant flavor/color/helicity labels and the corresponding branchings. The masks indicate which particles are affected; the masks length should coincide with the depth of the trie (without the root node). Recursively scan the whole tree, starting from the leaf nodes and working up to the root node. If a mask entry is set for the current tree level, scan the children there. For each child within that level make a new empty branch where the masked quantum number is undefined. Then recursively combine all following children with matching quantum number into this new node and move on.

(State matrices: state matrix: TBP)+≡

```

    procedure :: collapse => state_matrix_collapse

```

(State matrices: procedures)+≡

```

    subroutine state_matrix_collapse (state, mask)
        class(state_matrix_t), intent(inout) :: state
        type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
        type(state_matrix_t) :: red_state
        if (state%is_defined ()) then
            call state%reduce (mask, red_state)

```

```

        call state%final ()
        state = red_state
    end if
end subroutine state_matrix_collapse

```

Transform the given state matrix into a reduced state matrix where some quantum numbers are removed, as indicated by the mask. The procedure creates a new state matrix, so the old one can be deleted after this if it is no longer used.

It is said that the matrix element ordering is lost afterwards. We allow to keep the original matrix element index in the new state matrix. If the matrix element indices are kept, we do not freeze the state matrix. After reordering the matrix element indices by `state_matrix_reorder_me`, the state matrix can be frozen.

```

<State matrices: state matrix: TBP>+≡
  procedure :: reduce => state_matrix_reduce

<State matrices: procedures>+≡
  subroutine state_matrix_reduce (state, mask, red_state, keep_me_index)
    class(state_matrix_t), intent(in), target :: state
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    type(state_matrix_t), intent(out) :: red_state
    logical, optional, intent(in) :: keep_me_index
    logical :: opt_keep_me_index
    type(state_iterator_t) :: it
    type(quantum_numbers_t), dimension(size(mask)) :: qn
    opt_keep_me_index = .false.
    if (present (keep_me_index)) opt_keep_me_index = keep_me_index
    call red_state%init ()
    call it%init (state)
    do while (it%is_valid ())
      qn = it%get_quantum_numbers ()
      call qn%undefine (mask)
      if (opt_keep_me_index) then
        call red_state%add_state (qn, index = it%get_me_index ())
      else
        call red_state%add_state (qn)
      end if
      call it%advance ()
    end do
    if (.not. opt_keep_me_index) then
      call red_state%freeze ()
    end if
  end subroutine state_matrix_reduce

```

Reorder the matrix elements – not the tree itself. The procedure is necessary in case the matrix element indices were kept when reducing over quantum numbers and one wants to reintroduce the previous order of the matrix elements.

```

<State matrices: state matrix: TBP>+≡
  procedure :: reorder_me => state_matrix_reorder_me

<State matrices: procedures>+≡
  subroutine state_matrix_reorder_me (state, ordered_state)
    class(state_matrix_t), intent(in), target :: state

```

```

type(state_matrix_t), intent(out) :: ordered_state
type(state_iterator_t) :: it
type(quantum_numbers_t), dimension(state%depth) :: qn
integer, dimension(:), allocatable :: me_index
integer :: i
call ordered_state%init ()
call get_me_index_sorted (state, me_index)
i = 1; call it%init (state)
do while (it%is_valid ())
    qn = it%get_quantum_numbers ()
    call ordered_state%add_state (qn, index = me_index(i))
    i = i + 1; call it%advance ()
end do
call ordered_state%freeze ()
contains
subroutine get_me_index_sorted (state, me_index)
    class(state_matrix_t), intent(in), target :: state
    integer, dimension(:), allocatable, intent(out) :: me_index
    type(state_iterator_t) :: it
    integer :: i, j
    integer, dimension(:), allocatable :: me_index_unsorted, me_index_sorted
    associate (n_matrix_elements => state%get_n_matrix_elements ())
        allocate (me_index(n_matrix_elements), source = 0)
        allocate (me_index_sorted(n_matrix_elements), source = 0)
        allocate (me_index_unsorted(n_matrix_elements), source = 0)
        i = 1; call it%init (state)
        do while (it%is_valid ())
            me_index_unsorted(i) = it%get_me_index ()
            i = i + 1
            call it%advance ()
        end do
        me_index_sorted = sort (me_index_unsorted)
        ! We do not care about efficiency at this point.
        UNSORTED: do i = 1, n_matrix_elements
            SORTED: do j = 1, n_matrix_elements
                if (me_index_unsorted(i) == me_index_sorted(j)) then
                    me_index(i) = j
                    cycle UNSORTED
                end if
            end do SORTED
        end do UNSORTED
    end associate
end subroutine get_me_index_sorted
end subroutine state_matrix_reorder_me

```

Sets all matrix elements whose flavor structure is a duplicate of another flavor structure to zero. We need this for the real finite to ignore duplicate flavor structures while keeping the indices identical to the singular real component. When comparing the flavor structures, we take into account permutations of final- state particles. To do this properly, we keep only the non-hard flavors and the initial-state flavors, i.e. the first two hard flavors fixed.

(State matrices: state matrix: TBP)+≡

```

procedure :: set_duplicate_flv_zero => state_matrix_set_duplicate_flv_zero

```

```

<State matrices: procedures>+≡
subroutine state_matrix_set_duplicate_flv_zero (state)
  class(state_matrix_t), intent(inout), target :: state
  type(quantum_numbers_t), dimension(state%depth) :: qn
  type(flavor_t) :: flv
  class(state_flv_content_t), allocatable :: state_flv
  logical, dimension(:), allocatable :: hard_mask, sort_mask, duplicate_mask
  integer :: i, j, n_in, n_flvs
  n_flvs = state%get_depth ()
  n_in = 2
  !!! TODO (PS-28-07-21) n_in should not be hard coded to work for decays
  !!! This assumes that the positions of the non-hard flavors are the same for all flavor struct
  qn = state%get_quantum_number(1)
  allocate (hard_mask(n_flvs))
  do i = 1, n_flvs
    flv = qn(i)%get_flavor()
    hard_mask(i) = flv%is_hard_process ()
  end do
  allocate (sort_mask(n_flvs))
  sort_mask = hard_mask
  j = 0
  do i = 1, n_flvs
    if (j == n_in) exit
    if (sort_mask(i)) then
      sort_mask(i) = .false.
      j = j + 1
    end if
  end do
  allocate (state_flv)
  call state_flv%fill (state, sort_mask)
  call state_flv%find_duplicates (duplicate_mask)
  do i = 1, state%get_n_matrix_elements ()
    if (duplicate_mask(i)) then
      call state%set_matrix_element_single(i, cmplx(zero, zero, default))
    end if
  end do
end subroutine state_matrix_set_duplicate_flv_zero

```

This subroutine sets up the matrix-element array. The leaf nodes acquire the index values that point to the appropriate matrix-element entry.

We recursively scan the trie. Once we arrive at a leaf node, the index is increased and associated to that node. Finally, we allocate the matrix-element array with the appropriate size.

If matrix element values are temporarily stored within the leaf nodes, we scan the state again and transfer them to the matrix-element array.

```

<State matrices: state matrix: TBP>+≡
procedure :: freeze => state_matrix_freeze

<State matrices: procedures>+≡
subroutine state_matrix_freeze (state)
  class(state_matrix_t), intent(inout), target :: state
  type(state_iterator_t) :: it
  if (associated (state%root)) then

```

```

        if (allocated (state%me)) deallocate (state%me)
        allocate (state%me (state%n_matrix_elements))
        state%me = 0
        call state%set_n_sub ()
    end if
    if (state%leaf_nodes_store_values) then
        call it%init (state)
        do while (it%is_valid ())
            state%me(it%get_me_index ()) = it%get_matrix_element ()
            call it%advance ()
        end do
        state%leaf_nodes_store_values = .false.
    end if
end subroutine state_matrix_freeze

```

Direct access to the value array

Several methods for setting a value directly are summarized in this generic:

```

<State matrices: state matrix: TBP>+≡
generic :: set_matrix_element => set_matrix_element_qn
generic :: set_matrix_element => set_matrix_element_all
generic :: set_matrix_element => set_matrix_element_array
generic :: set_matrix_element => set_matrix_element_single
generic :: set_matrix_element => set_matrix_element_clone
procedure :: set_matrix_element_qn => state_matrix_set_matrix_element_qn
procedure :: set_matrix_element_all => state_matrix_set_matrix_element_all
procedure :: set_matrix_element_array => &
    state_matrix_set_matrix_element_array
procedure :: set_matrix_element_single => &
    state_matrix_set_matrix_element_single
procedure :: set_matrix_element_clone => &
    state_matrix_set_matrix_element_clone

```

Set a value that corresponds to a quantum number array:

```

<State matrices: procedures>+≡
subroutine state_matrix_set_matrix_element_qn (state, qn, value)
    class(state_matrix_t), intent(inout), target :: state
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    complex(default), intent(in) :: value
    type(state_iterator_t) :: it
    if (.not. allocated (state%me)) then
        allocate (state%me (size(qn)))
    end if
    call it%init (state)
    call it%go_to_qn (qn)
    call it%set_matrix_element (value)
end subroutine state_matrix_set_matrix_element_qn

```

Set all matrix elements to a single value

```

<State matrices: procedures>+≡
subroutine state_matrix_set_matrix_element_all (state, value)
    class(state_matrix_t), intent(inout) :: state

```

```

        complex(default), intent(in) :: value
        if (.not. allocated (state%me)) then
            allocate (state%me (state%n_matrix_elements))
        end if
        state%me = value
    end subroutine state_matrix_set_matrix_element_all

```

Set the matrix-element array directly.

```

<State matrices: procedures>+≡
subroutine state_matrix_set_matrix_element_array (state, value, range)
    class(state_matrix_t), intent(inout) :: state
    complex(default), intent(in), dimension(:) :: value
    integer, intent(in), dimension(:), optional :: range
    if (present (range)) then
        state%me(range) = value
    else
        if (.not. allocated (state%me)) &
            allocate (state%me (size (value)))
        state%me(:) = value
    end if
end subroutine state_matrix_set_matrix_element_array

```

Set a matrix element at position i to value.

```

<State matrices: procedures>+≡
pure subroutine state_matrix_set_matrix_element_single (state, i, value)
    class(state_matrix_t), intent(inout) :: state
    integer, intent(in) :: i
    complex(default), intent(in) :: value
    if (.not. allocated (state%me)) then
        allocate (state%me (state%n_matrix_elements))
    end if
    state%me(i) = value
end subroutine state_matrix_set_matrix_element_single

```

Clone the matrix elements from another (matching) state matrix.

```

<State matrices: procedures>+≡
subroutine state_matrix_set_matrix_element_clone (state, state1)
    class(state_matrix_t), intent(inout) :: state
    type(state_matrix_t), intent(in) :: state1
    if (.not. allocated (state1%me)) return
    if (.not. allocated (state%me)) allocate (state%me (size (state1%me)))
    state%me = state1%me
end subroutine state_matrix_set_matrix_element_clone

```

Add a value to a matrix element

```

<State matrices: state matrix: TBP>+≡
procedure :: add_to_matrix_element => state_matrix_add_to_matrix_element

<State matrices: procedures>+≡
subroutine state_matrix_add_to_matrix_element (state, qn, value, match_only_flavor)
    class(state_matrix_t), intent(inout), target :: state
    type(quantum_numbers_t), dimension(:), intent(in) :: qn

```



```

complex(default), intent(in) :: value
logical, intent(in), optional :: match_only_flavor
type(state_iterator_t) :: it
call it%init (state)
call it%go_to_qn (qn, match_only_flavor)
if (it%is_valid ()) then
    call it%add_to_matrix_element (value)
else
    call msg_fatal ("Cannot add to matrix element - it%node not allocated")
end if
end subroutine state_matrix_add_to_matrix_element

```

12.1.3 State iterators

Accessing the quantum state from outside is best done using a specialized iterator, i.e., a pointer to a particular branch of the quantum state trie. Technically, the iterator contains a pointer to a leaf node, but via parent pointers it allows to access the whole branch where the leaf is attached. For quick access, we also keep the branch depth (which is assumed to be universal for a quantum state).

```

<State matrices: public>+≡
public :: state_iterator_t

<State matrices: types>+≡
type :: state_iterator_t
private
integer :: depth = 0
type(state_matrix_t), pointer :: state => null ()
type(node_t), pointer :: node => null ()
contains
<State matrices: state iterator: TBP>
end type state_iterator_t

```

The initializer: Point at the first branch. Note that this cannot be pure, thus not be elemental, because the iterator can be used to manipulate data in the state matrix.

```

<State matrices: state iterator: TBP>≡
procedure :: init => state_iterator_init

<State matrices: procedures>+≡
subroutine state_iterator_init (it, state)
class(state_iterator_t), intent(out) :: it
type(state_matrix_t), intent(in), target :: state
it%state => state
it%depth = state%depth
if (state%is_defined ()) then
    it%node => state%root
    do while (associated (it%node%child_first))
        it%node => it%node%child_first
    end do
else
    it%node => null ()
end if

```

```
end subroutine state_iterator_init
```

Go forward. Recursively programmed: if the next node does not exist, go back to the parent node and look at its successor (if present), etc.

There is a possible pitfall in the implementation: If the dummy pointer argument to the `find_next` routine is used directly, we still get the correct result for the iterator, but calling the recursion on `node%parent` means that we manipulate a parent pointer in the original state in addition to the iterator. Making a local copy of the pointer avoids this. Using pointer intent would be helpful, but we do not yet rely on this F2003 feature.

```
<State matrices: state iterator: TBP>+≡
  procedure :: advance => state_iterator_advance

<State matrices: procedures>+≡
  subroutine state_iterator_advance (it)
    class(state_iterator_t), intent(inout) :: it
    call find_next (it%node)
  contains
    recursive subroutine find_next (node_in)
      type(node_t), intent(in), target :: node_in
      type(node_t), pointer :: node
      node => node_in
      if (associated (node%next)) then
        node => node%next
        do while (associated (node%child_first))
          node => node%child_first
        end do
        it%node => node
      else if (associated (node%parent)) then
        call find_next (node%parent)
      else
        it%node => null ()
      end if
    end subroutine find_next
  end subroutine state_iterator_advance
```

If all has been scanned, the iterator is at an undefined state. Check for this:

```
<State matrices: state iterator: TBP>+≡
  procedure :: is_valid => state_iterator_is_valid

<State matrices: procedures>+≡
  function state_iterator_is_valid (it) result (defined)
    logical :: defined
    class(state_iterator_t), intent(in) :: it
    defined = associated (it%node)
  end function state_iterator_is_valid
```

Return the matrix-element index that corresponds to the current node

```
<State matrices: state iterator: TBP>+≡
  procedure :: get_me_index => state_iterator_get_me_index
```

```

<State matrices: procedures>+≡
function state_iterator_get_me_index (it) result (n)
  integer :: n
  class(state_iterator_t), intent(in) :: it
  n = it%node%me_index
end function state_iterator_get_me_index

```

Return the number of times this quantum-number state has been added (noting that it is physically inserted only the first time). Note that for each state, there is an array of counters.

```

<State matrices: state iterator: TBP>+≡
procedure :: get_me_count => state_iterator_get_me_count

```

```

<State matrices: procedures>+≡
function state_iterator_get_me_count (it) result (n)
  integer, dimension(:), allocatable :: n
  class(state_iterator_t), intent(in) :: it
  if (allocated (it%node%me_count)) then
    allocate (n (size (it%node%me_count)))
    n = it%node%me_count
  else
    allocate (n (0))
  end if
end function state_iterator_get_me_count

```

```

<State matrices: state iterator: TBP>+≡
procedure :: get_depth => state_iterator_get_depth

```

```

<State matrices: procedures>+≡
pure function state_iterator_get_depth (state_iterator) result (depth)
  integer :: depth
  class(state_iterator_t), intent(in) :: state_iterator
  depth = state_iterator%depth
end function state_iterator_get_depth

```

Proceed to the state associated with the quantum numbers qn.

```

<State matrices: state iterator: TBP>+≡
procedure :: go_to_qn => state_iterator_go_to_qn

```

```

<State matrices: procedures>+≡
subroutine state_iterator_go_to_qn (it, qn, match_only_flavor)
  class(state_iterator_t), intent(inout) :: it
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  logical, intent(in), optional :: match_only_flavor
  type(quantum_numbers_t), dimension(:), allocatable :: qn_hard, qn_tmp
  logical :: match_flg
  match_flg = .false.; if (present (match_only_flavor)) match_flg = .true.
  do while (it%is_valid ())
    if (match_flg) then
      qn_tmp = it%get_quantum_numbers ()
      qn_hard = pack (qn_tmp, qn_tmp%are_hard_process ())
      if (all (qn .fmatch. qn_hard)) then
        return
      end if
    end if
  end do
end subroutine state_iterator_go_to_qn

```

```

        else
            call it%advance ()
        end if
    else
        if (all (qn == it%get_quantum_numbers ())) then
            return
        else
            call it%advance ()
        end if
    end if
end do
end subroutine state_iterator_go_to_qn

```

Use the iterator to retrieve quantum-number information:

```

<State matrices: state iterator: TBP>+≡
generic :: get_quantum_numbers => get_qn_multi, get_qn_slice, &
    get_qn_range, get_qn_single
generic :: get_flavor => get_flv_multi, get_flv_slice, &
    get_flv_range, get_flv_single
generic :: get_color => get_col_multi, get_col_slice, &
    get_col_range, get_col_single
generic :: get_helicity => get_hel_multi, get_hel_slice, &
    get_hel_range, get_hel_single

```

```

<State matrices: state iterator: TBP>+≡
procedure :: get_qn_multi => state_iterator_get_qn_multi
procedure :: get_qn_slice => state_iterator_get_qn_slice
procedure :: get_qn_range => state_iterator_get_qn_range
procedure :: get_qn_single => state_iterator_get_qn_single
procedure :: get_flv_multi => state_iterator_get_flv_multi
procedure :: get_flv_slice => state_iterator_get_flv_slice
procedure :: get_flv_range => state_iterator_get_flv_range
procedure :: get_flv_single => state_iterator_get_flv_single
procedure :: get_col_multi => state_iterator_get_col_multi
procedure :: get_col_slice => state_iterator_get_col_slice
procedure :: get_col_range => state_iterator_get_col_range
procedure :: get_col_single => state_iterator_get_col_single
procedure :: get_hel_multi => state_iterator_get_hel_multi
procedure :: get_hel_slice => state_iterator_get_hel_slice
procedure :: get_hel_range => state_iterator_get_hel_range
procedure :: get_hel_single => state_iterator_get_hel_single

```

These versions return the whole quantum number array

```

<State matrices: procedures>+≡
function state_iterator_get_qn_multi (it) result (qn)
    class(state_iterator_t), intent(in) :: it
    type(quantum_numbers_t), dimension(it%depth) :: qn
    type(node_t), pointer :: node
    integer :: i
    node => it%node
    do i = it%depth, 1, -1
        qn(i) = node%qn
        node => node%parent
    end do

```

```

end function state_iterator_get_qn_multi

function state_iterator_get_flv_multi (it) result (flv)
  class(state_iterator_t), intent(in) :: it
  type(flavor_t), dimension(it%depth) :: flv
  flv = quantum_numbers_get_flavor &
    (it%get_quantum_numbers ())
end function state_iterator_get_flv_multi

function state_iterator_get_col_multi (it) result (col)
  class(state_iterator_t), intent(in) :: it
  type(color_t), dimension(it%depth) :: col
  col = quantum_numbers_get_color &
    (it%get_quantum_numbers ())
end function state_iterator_get_col_multi

function state_iterator_get_hel_multi (it) result (hel)
  class(state_iterator_t), intent(in) :: it
  type(helicity_t), dimension(it%depth) :: hel
  hel = quantum_numbers_get_helicity &
    (it%get_quantum_numbers ())
end function state_iterator_get_hel_multi

```

An array slice (derived from the above).

(State matrices: procedures)+≡

```

function state_iterator_get_qn_slice (it, index) result (qn)
  class(state_iterator_t), intent(in) :: it
  integer, dimension(:), intent(in) :: index
  type(quantum_numbers_t), dimension(size(index)) :: qn
  type(quantum_numbers_t), dimension(it%depth) :: qn_tmp
  qn_tmp = state_iterator_get_qn_multi (it)
  qn = qn_tmp(index)
end function state_iterator_get_qn_slice

function state_iterator_get_flv_slice (it, index) result (flv)
  class(state_iterator_t), intent(in) :: it
  integer, dimension(:), intent(in) :: index
  type(flavor_t), dimension(size(index)) :: flv
  flv = quantum_numbers_get_flavor &
    (it%get_quantum_numbers (index))
end function state_iterator_get_flv_slice

function state_iterator_get_col_slice (it, index) result (col)
  class(state_iterator_t), intent(in) :: it
  integer, dimension(:), intent(in) :: index
  type(color_t), dimension(size(index)) :: col
  col = quantum_numbers_get_color &
    (it%get_quantum_numbers (index))
end function state_iterator_get_col_slice

function state_iterator_get_hel_slice (it, index) result (hel)
  class(state_iterator_t), intent(in) :: it
  integer, dimension(:), intent(in) :: index
  type(helicity_t), dimension(size(index)) :: hel

```

```

        hel = quantum_numbers_get_helicity &
              (it%get_quantum_numbers (index))
    end function state_iterator_get_hel_slice

```

An array range (implemented directly).

(State matrices: procedures)+≡

```

function state_iterator_get_qn_range (it, k1, k2) result (qn)
    class(state_iterator_t), intent(in) :: it
    integer, intent(in) :: k1, k2
    type(quantum_numbers_t), dimension(k2-k1+1) :: qn
    type(node_t), pointer :: node
    integer :: i
    node => it%node
    SCAN: do i = it%depth, 1, -1
        if (k1 <= i .and. i <= k2) then
            qn(i-k1+1) = node%qn
        else
            node => node%parent
        end if
    end do SCAN
end function state_iterator_get_qn_range

function state_iterator_get_flv_range (it, k1, k2) result (flv)
    class(state_iterator_t), intent(in) :: it
    integer, intent(in) :: k1, k2
    type(flavor_t), dimension(k2-k1+1) :: flv
    flv = quantum_numbers_get_flavor &
          (it%get_quantum_numbers (k1, k2))
end function state_iterator_get_flv_range

function state_iterator_get_col_range (it, k1, k2) result (col)
    class(state_iterator_t), intent(in) :: it
    integer, intent(in) :: k1, k2
    type(color_t), dimension(k2-k1+1) :: col
    col = quantum_numbers_get_color &
          (it%get_quantum_numbers (k1, k2))
end function state_iterator_get_col_range

function state_iterator_get_hel_range (it, k1, k2) result (hel)
    class(state_iterator_t), intent(in) :: it
    integer, intent(in) :: k1, k2
    type(helicity_t), dimension(k2-k1+1) :: hel
    hel = quantum_numbers_get_helicity &
          (it%get_quantum_numbers (k1, k2))
end function state_iterator_get_hel_range

```

Just a specific single element

(State matrices: procedures)+≡

```

function state_iterator_get_qn_single (it, k) result (qn)
    class(state_iterator_t), intent(in) :: it
    integer, intent(in) :: k
    type(quantum_numbers_t) :: qn
    type(node_t), pointer :: node

```

```

integer :: i
node => it%node
SCAN: do i = it%depth, 1, -1
  if (i == k) then
    qn = node%qn
    exit SCAN
  else
    node => node%parent
  end if
end do SCAN
end function state_iterator_get_qn_single

function state_iterator_get_flv_single (it, k) result (flv)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(flavor_t) :: flv
  flv = quantum_numbers_get_flavor &
    (it%get_quantum_numbers (k))
end function state_iterator_get_flv_single

function state_iterator_get_col_single (it, k) result (col)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(color_t) :: col
  col = quantum_numbers_get_color &
    (it%get_quantum_numbers (k))
end function state_iterator_get_col_single

function state_iterator_get_hel_single (it, k) result (hel)
  class(state_iterator_t), intent(in) :: it
  integer, intent(in) :: k
  type(helicity_t) :: hel
  hel = quantum_numbers_get_helicity &
    (it%get_quantum_numbers (k))
end function state_iterator_get_hel_single

```

Assign a model pointer to the current flavor entries.

```

<State matrices: state iterator: TBP>+≡
  procedure :: set_model => state_iterator_set_model

<State matrices: procedures>+≡
  subroutine state_iterator_set_model (it, model)
    class(state_iterator_t), intent(inout) :: it
    class(model_data_t), intent(in), target :: model
    type(node_t), pointer :: node
    integer :: i
    node => it%node
    do i = it%depth, 1, -1
      call node%qn%set_model (model)
      node => node%parent
    end do
  end subroutine state_iterator_set_model

```

Modify the hard-interaction tag of the current flavor entries at a specific posi-

tion, in-place.

```

<State matrices: state iterator: TBP>+≡
  procedure :: retag_hard_process => state_iterator_retag_hard_process

<State matrices: procedures>+≡
  subroutine state_iterator_retag_hard_process (it, i, hard)
    class(state_iterator_t), intent(inout) :: it
    integer, intent(in) :: i
    logical, intent(in) :: hard
    type(node_t), pointer :: node
    integer :: j
    node => it%node
    do j = 1, it%depth-i
      node => node%parent
    end do
    call node%qn%tag_hard_process (hard)
  end subroutine state_iterator_retag_hard_process

```

Retrieve the matrix element value associated with the current node.

```

<State matrices: state iterator: TBP>+≡
  procedure :: get_matrix_element => state_iterator_get_matrix_element

<State matrices: procedures>+≡
  function state_iterator_get_matrix_element (it) result (me)
    complex(default) :: me
    class(state_iterator_t), intent(in) :: it
    if (it%state%leaf_nodes_store_values) then
      me = it%node%me
    else if (it%node%me_index /= 0) then
      me = it%state%me(it%node%me_index)
    else
      me = 0
    end if
  end function state_iterator_get_matrix_element

```

Set the matrix element value using the state iterator.

```

<State matrices: state iterator: TBP>+≡
  procedure :: set_matrix_element => state_iterator_set_matrix_element

<State matrices: procedures>+≡
  subroutine state_iterator_set_matrix_element (it, value)
    class(state_iterator_t), intent(inout) :: it
    complex(default), intent(in) :: value
    if (it%node%me_index /= 0) it%state%me(it%node%me_index) = value
  end subroutine state_iterator_set_matrix_element

<State matrices: state iterator: TBP>+≡
  procedure :: add_to_matrix_element => state_iterator_add_to_matrix_element

<State matrices: procedures>+≡
  subroutine state_iterator_add_to_matrix_element (it, value)
    class(state_iterator_t), intent(inout) :: it
    complex(default), intent(in) :: value
    if (it%node%me_index /= 0) &

```



```

        it%state%me(it%node%me_index) = it%state%me(it%node%me_index) + value
    end subroutine state_iterator_add_to_matrix_element

```

12.1.4 Operations on quantum states

Return a deep copy of a state matrix.

```

<State matrices: public>+≡
    public :: assignment(=)

<State matrices: interfaces>≡
    interface assignment(=)
        module procedure state_matrix_assign
    end interface

<State matrices: procedures>+≡
    subroutine state_matrix_assign (state_out, state_in)
        type(state_matrix_t), intent(out) :: state_out
        type(state_matrix_t), intent(in), target :: state_in
        type(state_iterator_t) :: it
        if (.not. state_in%is_defined ()) return
        call state_out%init ()
        call it%init (state_in)
        do while (it%is_valid ())
            call state_out%add_state (it%get_quantum_numbers (), &
                it%get_me_index ())
            call it%advance ()
        end do
        if (allocated (state_in%me)) then
            allocate (state_out%me (size (state_in%me)))
            state_out%me = state_in%me
        end if
        state_out%n_sub = state_in%n_sub
    end subroutine state_matrix_assign

```

Determine the indices of all diagonal matrix elements.

```

<State matrices: state matrix: TBP>+≡
    procedure :: get_diagonal_entries => state_matrix_get_diagonal_entries

<State matrices: procedures>+≡
    subroutine state_matrix_get_diagonal_entries (state, i)
        class(state_matrix_t), intent(in) :: state
        integer, dimension(:), allocatable, intent(out) :: i
        integer, dimension(state%n_matrix_elements) :: tmp
        integer :: n
        type(state_iterator_t) :: it
        type(quantum_numbers_t), dimension(:), allocatable :: qn
        n = 0
        call it%init (state)
        allocate (qn (it%depth))
        do while (it%is_valid ())
            qn = it%get_quantum_numbers ()
            if (all (qn%are_diagonal ())) then

```

```

        n = n + 1
        tmp(n) = it%get_me_index ()
    end if
    call it%advance ()
end do
allocate (i(n))
if (n > 0) i = tmp(:n)
end subroutine state_matrix_get_diagonal_entries

```

Normalize all matrix elements, i.e., multiply by a common factor. Assuming that the factor is nonzero, of course.

```

⟨State matrices: state matrix: TBP⟩+≡
    procedure :: renormalize => state_matrix_renormalize

⟨State matrices: procedures⟩+≡
    subroutine state_matrix_renormalize (state, factor)
        class(state_matrix_t), intent(inout) :: state
        complex(default), intent(in) :: factor
        state%me = state%me * factor
    end subroutine state_matrix_renormalize

```

Renormalize the state matrix by its trace, if nonzero. The renormalization is reflected in the state-matrix norm.

```

⟨State matrices: state matrix: TBP⟩+≡
    procedure :: normalize_by_trace => state_matrix_normalize_by_trace

⟨State matrices: procedures⟩+≡
    subroutine state_matrix_normalize_by_trace (state)
        class(state_matrix_t), intent(inout) :: state
        real(default) :: trace
        trace = state%trace ()
        if (trace /= 0) then
            state%me = state%me / trace
            state%norm = state%norm * trace
        end if
    end subroutine state_matrix_normalize_by_trace

```

Analogous, but renormalize by maximal (absolute) value.

```

⟨State matrices: state matrix: TBP⟩+≡
    procedure :: normalize_by_max => state_matrix_normalize_by_max

⟨State matrices: procedures⟩+≡
    subroutine state_matrix_normalize_by_max (state)
        class(state_matrix_t), intent(inout) :: state
        real(default) :: m
        m = maxval (abs (state%me))
        if (m /= 0) then
            state%me = state%me / m
            state%norm = state%norm * m
        end if
    end subroutine state_matrix_normalize_by_max

```

Explicitly set the norm of a state matrix.

```

<State matrices: state matrix: TBP>+≡
  procedure :: set_norm => state_matrix_set_norm

<State matrices: procedures>+≡
  subroutine state_matrix_set_norm (state, norm)
    class(state_matrix_t), intent(inout) :: state
    real(default), intent(in) :: norm
    state%norm = norm
  end subroutine state_matrix_set_norm

```

Return the sum of all matrix element values.

```

<State matrices: state matrix: TBP>+≡
  procedure :: sum => state_matrix_sum

<State matrices: procedures>+≡
  pure function state_matrix_sum (state) result (value)
    complex(default) :: value
    class(state_matrix_t), intent(in) :: state
    value = sum (state%me)
  end function state_matrix_sum

```

Return the trace of a state matrix, i.e., the sum over all diagonal values.

If `qn_in` is provided, only branches that match this quantum-numbers array in flavor and helicity are considered. (This mode is used for selecting a color state.)

```

<State matrices: state matrix: TBP>+≡
  procedure :: trace => state_matrix_trace

<State matrices: procedures>+≡
  function state_matrix_trace (state, qn_in) result (trace)
    complex(default) :: trace
    class(state_matrix_t), intent(in), target :: state
    type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    type(state_iterator_t) :: it
    allocate (qn (state%get_depth ()))
    trace = 0
    call it%init (state)
    do while (it%is_valid ())
      qn = it%get_quantum_numbers ()
      if (present (qn_in)) then
        if (.not. all (qn .fmatch. qn_in)) then
          call it%advance (); cycle
        end if
      end if
      if (all (qn%are_diagonal ())) then
        trace = trace + it%get_matrix_element ()
      end if
      call it%advance ()
    end do
  end function state_matrix_trace

```

Append new states which are color-contracted versions of the existing states. The matrix element index of each color contraction coincides with the index of its origin, so no new matrix elements are generated. After this operation, no `freeze` must be performed anymore.

```

<State matrices: state matrix: TBP>+≡
  procedure :: add_color_contractions => state_matrix_add_color_contractions

<State matrices: procedures>+≡
  subroutine state_matrix_add_color_contractions (state)
    class(state_matrix_t), intent(inout), target :: state
    type(state_iterator_t) :: it
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn_con
    integer, dimension(:), allocatable :: me_index
    integer :: depth, n_me, i, j
    depth = state%get_depth ()
    n_me = state%get_n_matrix_elements ()
    allocate (qn (depth, n_me))
    allocate (me_index (n_me))
    i = 0
    call it%init (state)
    do while (it%is_valid ())
      i = i + 1
      qn(:,i) = it%get_quantum_numbers ()
      me_index(i) = it%get_me_index ()
      call it%advance ()
    end do
    do i = 1, n_me
      call quantum_number_array_make_color_contractions (qn(:,i), qn_con)
      do j = 1, size (qn_con, 2)
        call state%add_state (qn_con(:,j), index = me_index(i))
      end do
    end do
  end subroutine state_matrix_add_color_contractions

```

This procedure merges two state matrices of equal depth. For each quantum number (flavor, color, helicity), we take the entry from the first argument where defined, otherwise the second one. (If both are defined, we get an off-diagonal matrix.) The resulting trie combines the information of the input tries in all possible ways. Note that values are ignored, all values in the result are zero.

```

<State matrices: public>+≡
  public :: merge_state_matrices

<State matrices: procedures>+≡
  subroutine merge_state_matrices (state1, state2, state3)
    type(state_matrix_t), intent(in), target :: state1, state2
    type(state_matrix_t), intent(out) :: state3
    type(state_iterator_t) :: it1, it2
    type(quantum_numbers_t), dimension(state1%depth) :: qn1, qn2
    if (state1%depth /= state2%depth) then
      call state1%write ()
      call state2%write ()
      call msg_bug ("State matrices merge impossible: incompatible depths")
    end if
  end subroutine merge_state_matrices

```

```

call state3%init ()
call it1%init (state1)
do while (it1%is_valid ())
  qn1 = it1%get_quantum_numbers ()
  call it2%init (state2)
  do while (it2%is_valid ())
    qn2 = it2%get_quantum_numbers ()
    call state3%add_state (qn1 .merge. qn2)
    call it2%advance ()
  end do
  call it1%advance ()
end do
call state3%freeze ()
end subroutine merge_state_matrices

```

Multiply matrix elements from two state matrices. Choose the elements as given by the integer index arrays, multiply them and store the sum of products in the indicated matrix element. The suffixes mean: c=conjugate first factor; f=include weighting factor.

Note that the `dot_product` intrinsic function conjugates its first complex argument. This is intended for the c suffix case, but must be reverted for the plain-product case.

We provide analogous subroutines for just summing over state matrix entries. The `evaluate_sum` variant includes the state-matrix norm in the evaluation, the `evaluate_me_sum` takes into account just the matrix elements proper.

(State matrices: state matrix: TBP)+≡

```

procedure :: evaluate_product => state_matrix_evaluate_product
procedure :: evaluate_product_cf => state_matrix_evaluate_product_cf
procedure :: evaluate_square_c => state_matrix_evaluate_square_c
procedure :: evaluate_sum => state_matrix_evaluate_sum
procedure :: evaluate_me_sum => state_matrix_evaluate_me_sum

```

(State matrices: procedures)+≡

```

pure subroutine state_matrix_evaluate_product &
  (state, i, state1, state2, index1, index2)
class(state_matrix_t), intent(inout) :: state
integer, intent(in) :: i
type(state_matrix_t), intent(in) :: state1, state2
integer, dimension(:), intent(in) :: index1, index2
state%me(i) = &
  dot_product (conjg (state1%me(index1)), state2%me(index2))
state%norm = state1%norm * state2%norm
end subroutine state_matrix_evaluate_product

pure subroutine state_matrix_evaluate_product_cf &
  (state, i, state1, state2, index1, index2, factor)
class(state_matrix_t), intent(inout) :: state
integer, intent(in) :: i
type(state_matrix_t), intent(in) :: state1, state2
integer, dimension(:), intent(in) :: index1, index2
complex(default), dimension(:), intent(in) :: factor
state%me(i) = &
  dot_product (state1%me(index1), factor * state2%me(index2))

```

```

state%norm = state1%norm * state2%norm
end subroutine state_matrix_evaluate_product_cf

pure subroutine state_matrix_evaluate_square_c (state, i, state1, index1)
class(state_matrix_t), intent(inout) :: state
integer, intent(in) :: i
type(state_matrix_t), intent(in) :: state1
integer, dimension(:), intent(in) :: index1
state%me(i) = &
    dot_product (state1%me(index1), state1%me(index1))
state%norm = abs (state1%norm) ** 2
end subroutine state_matrix_evaluate_square_c

pure subroutine state_matrix_evaluate_sum (state, i, state1, index1)
class(state_matrix_t), intent(inout) :: state
integer, intent(in) :: i
type(state_matrix_t), intent(in) :: state1
integer, dimension(:), intent(in) :: index1
state%me(i) = &
    sum (state1%me(index1)) * state1%norm
end subroutine state_matrix_evaluate_sum

pure subroutine state_matrix_evaluate_me_sum (state, i, state1, index1)
class(state_matrix_t), intent(inout) :: state
integer, intent(in) :: i
type(state_matrix_t), intent(in) :: state1
integer, dimension(:), intent(in) :: index1
state%me(i) = sum (state1%me(index1))
end subroutine state_matrix_evaluate_me_sum

```

Outer product (of states and matrix elements):

```

<State matrices: public>+≡
public :: outer_multiply

<State matrices: interfaces>+≡
interface outer_multiply
    module procedure outer_multiply_pair
    module procedure outer_multiply_array
end interface

```

This procedure constructs the outer product of two state matrices.

```

<State matrices: procedures>+≡
subroutine outer_multiply_pair (state1, state2, state3)
type(state_matrix_t), intent(in), target :: state1, state2
type(state_matrix_t), intent(out) :: state3
type(state_iterator_t) :: it1, it2
type(quantum_numbers_t), dimension(state1%depth) :: qn1
type(quantum_numbers_t), dimension(state2%depth) :: qn2
type(quantum_numbers_t), dimension(state1%depth+state2%depth) :: qn3
complex(default) :: val1, val2
call state3%init (store_values = .true.)
call it1%init (state1)
do while (it1%is_valid ())

```

```

      qn1 = it1%get_quantum_numbers ()
      val1 = it1%get_matrix_element ()
      call it2%init (state2)
      do while (it2%is_valid ())
        qn2 = it2%get_quantum_numbers ()
        val2 = it2%get_matrix_element ()
        qn3(:state1%depth) = qn1
        qn3(state1%depth+1:) = qn2
        call state3%add_state (qn3, value=val1 * val2)
        call it2%advance ()
      end do
      call it1%advance ()
    end do
    call state3%freeze ()
  end subroutine outer_multiply_pair

```

This executes the above routine iteratively for an arbitrary number of state matrices.

(State matrices: procedures)+≡

```

subroutine outer_multiply_array (state_in, state_out)
  type(state_matrix_t), dimension(:), intent(in), target :: state_in
  type(state_matrix_t), intent(out) :: state_out
  type(state_matrix_t), dimension(:), allocatable, target :: state_tmp
  integer :: i, n
  n = size (state_in)
  select case (n)
    case (0)
      call state_out%init ()
    case (1)
      state_out = state_in(1)
    case (2)
      call outer_multiply_pair (state_in(1), state_in(2), state_out)
    case default
      allocate (state_tmp (n-2))
      call outer_multiply_pair (state_in(1), state_in(2), state_tmp(1))
      do i = 2, n - 2
        call outer_multiply_pair (state_tmp(i-1), state_in(i+1), state_tmp(i))
      end do
      call outer_multiply_pair (state_tmp(n-2), state_in(n), state_out)
      do i = 1, size(state_tmp)
        call state_tmp(i)%final ()
      end do
    end select
end subroutine outer_multiply_array

```

12.1.5 Factorization

In physical events, the state matrix is factorized into single-particle state matrices. This is essentially a measurement.

In a simulation, we select one particular branch of the state matrix with a probability that is determined by the matrix elements at the leaves. (This makes sense only if the state matrix represents a squared amplitude.) The selection is

based on a (random) value x between 0 and one that is provided as the third argument.

For flavor and color, we select a unique value for each particle. For polarization, we have three options (modes). Option 1 is to drop helicity information altogether and sum over all diagonal helicities. Option 2 is to select a unique diagonal helicity in the same way as flavor and color. Option 3 is, for each particle, to trace over all remaining helicities in order to obtain an array of independent single-particle helicity matrices.

Only branches that match the given quantum-number array `qn_in`, if present, are considered. For this array, color is ignored.

If the optional `correlated_state` is provided, it is assigned the correlated density matrix for the selected flavor-color branch, so multi-particle spin correlations remain available even if they are dropped in the single-particle density matrices. This should be done by the caller for the choice `FM_CORRELATED_HELICITY`, which otherwise is handled as `FM_IGNORE_HELICITY`.

The algorithm is as follows: First, we determine the normalization by summing over all diagonal matrix elements. In a second scan, we select one of the diagonal matrix elements by a cumulative comparison with the normalized random number. In the corresponding quantum number array, we undefine the helicity entries. Then, we scan the third time. For each branch that matches the selected quantum number array (i.e., definite flavor and color, arbitrary helicity), we determine its contribution to any of the single-particle state matrices. The matrix-element value is added if all other quantum numbers are diagonal, while the helicity of the chosen particle may be arbitrary; this helicity determines the branch in the single-particle state.

As a result, flavor and color quantum numbers are selected with the correct probability. Within this subset of states, each single-particle state matrix results from tracing over all other particles. Note that the single-particle state matrices are not normalized.

The flag `ok` is set to false if the matrix element sum is zero, so factorization is not possible. This can happen if an event did not pass cuts.

```

<State matrices: parameters>≡
  integer, parameter, public :: FM_IGNORE_HELICITY = 1
  integer, parameter, public :: FM_SELECT_HELICITY = 2
  integer, parameter, public :: FM_FACTOR_HELICITY = 3
  integer, parameter, public :: FM_CORRELATED_HELICITY = 4

<State matrices: state matrix: TBP>+≡
  procedure :: factorize => state_matrix_factorize

<State matrices: procedures>+≡
  subroutine state_matrix_factorize &
    (state, mode, x, ok, single_state, correlated_state, qn_in)
    class(state_matrix_t), intent(in), target :: state
    integer, intent(in) :: mode
    real(default), intent(in) :: x
    logical, intent(out) :: ok
    type(state_matrix_t), &
      dimension(:), allocatable, intent(out) :: single_state
    type(state_matrix_t), intent(out), optional :: correlated_state
    type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in

```



```

type(state_iterator_t) :: it
real(default) :: s, xt
complex(default) :: value
integer :: i, depth
type(quantum_numbers_t), dimension(:), allocatable :: qn, qn1
type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
logical, dimension(:), allocatable :: diagonal
logical, dimension(:, :), allocatable :: mask
ok = .true.
if (x /= 0) then
    xt = x * abs (state%trace (qn_in))
else
    xt = 0
end if
s = 0
depth = state%get_depth ()
allocate (qn (depth), qn1 (depth), diagonal (depth))
call it%init (state)
do while (it%is_valid ())
    qn = it%get_quantum_numbers ()
    if (present (qn_in)) then
        if (.not. all (qn .fmatch. qn_in)) then
            call it%advance (); cycle
        end if
    end if
    if (all (qn%are_diagonal ())) then
        value = abs (it%get_matrix_element ())
        s = s + value
        if (s > xt) exit
    end if
    call it%advance ()
end do
if (.not. it%is_valid ()) then
    if (s == 0) ok = .false.
    call it%init (state)
end if
allocate (single_state (depth))
do i = 1, depth
    call single_state(i)%init (store_values = .true.)
end do
if (present (correlated_state)) &
    call correlated_state%init (store_values = .true.)
qn = it%get_quantum_numbers ()
select case (mode)
case (FM_SELECT_HELICITY) ! single branch selected; shortcut
    do i = 1, depth
        call single_state(i)%add_state ([qn(i)], value=value)
    end do
    if (.not. present (correlated_state)) then
        do i = 1, size(single_state)
            call single_state(i)%freeze ()
        end do
        return
    end if

```

```

end select
allocate (qn_mask (depth))
call qn_mask%init (.false., .false., .false., .true.)
call qn%undefine (qn_mask)
select case (mode)
case (FM_FACTOR_HELICITY)
  allocate (mask (depth, depth))
  mask = .false.
  forall (i = 1:depth) mask(i,i) = .true.
end select
call it%init (state)
do while (it%is_valid ())
  qn1 = it%get_quantum_numbers ()
  if (all (qn .match. qn1)) then
    diagonal = qn1%are_diagonal ()
    value = it%get_matrix_element ()
    select case (mode)
    case (FM_IGNORE_HELICITY, FM_CORRELATED_HELICITY)
      !!! trace over diagonal states that match qn
      if (all (diagonal)) then
        do i = 1, depth
          call single_state(i)%add_state &
            ([qn(i)], value=value, sum_values=.true.)
        end do
      end if
    case (FM_FACTOR_HELICITY) !!! trace over all other particles
      do i = 1, depth
        if (all (diagonal .or. mask(:,i))) then
          call single_state(i)%add_state &
            ([qn1(i)], value=value, sum_values=.true.)
        end if
      end do
    end select
    if (present (correlated_state)) &
      call correlated_state%add_state (qn1, value=value)
  end if
  call it%advance ()
end do
do i = 1, depth
  call single_state(i)%freeze ()
end do
if (present (correlated_state)) &
  call correlated_state%freeze ()
end subroutine state_matrix_factorize

```

Auxiliary functions

(State matrices: state matrix: TBP)+≡

```

procedure :: get_polarization_density_matrix &
=> state_matrix_get_polarization_density_matrix

```

(State matrices: procedures)+≡

```

function state_matrix_get_polarization_density_matrix (state) result (pol_matrix)

```

```

real(default), dimension(:,:), allocatable :: pol_matrix
class(state_matrix_t), intent(in) :: state
type(node_t), pointer :: current => null ()
!!! What's the generic way to allocate the matrix?
allocate (pol_matrix (4,4)); pol_matrix = 0
if (associated (state%root%child_first)) then
  current => state%root%child_first
  do while (associated (current))
    call current%qn%write ()
    current => current%next
  end do
else
  call msg_fatal ("Polarization state not allocated!")
end if
end function state_matrix_get_polarization_density_matrix

```

Quantum-number matching

This feature allows us to check whether a given string of PDG values matches, in any ordering, any of the flavor combinations that the state matrix provides. We will also request the permutation of the successful match.

This type provides an account of the state's flavor content. We store all flavor combinations, as `pdg` values, in an array, assuming that the length is uniform.

We check only the entries selected by `mask_match`. Among those, only the entries selected by `mask_sort` are sorted and thus matched without respecting array element order. The entries that correspond to a true value in the associated `mask` are sorted. The mapping from the original state to the sorted state is given by the index array `map`.

```

<State matrices: public>+≡
  public :: state_flv_content_t

<State matrices: types>+≡
  type :: state_flv_content_t
    private
    integer, dimension(:,:), allocatable :: pdg
    integer, dimension(:,:), allocatable :: map
    logical, dimension(:), allocatable :: mask
  contains
    <State matrices: state flv content: TBP>
  end type state_flv_content_t

```

Output (debugging aid).

```

<State matrices: state flv content: TBP>≡
  procedure :: write => state_flv_content_write

<State matrices: procedures>+≡
  subroutine state_flv_content_write (state_flv, unit)
    class(state_flv_content_t), intent(in), target :: state_flv
    integer, intent(in), optional :: unit
    integer :: u, n, d, i, j
    u = given_output_unit (unit)

```

```

d = size (state_flv%pdg, 1)
n = size (state_flv%pdg, 2)
do i = 1, n
  write (u, "(2x,'PDG =')", advance="no")
  do j = 1, d
    write (u, "(1x,I0)", advance="no") state_flv%pdg(j,i)
  end do
  write (u, "(' :: map = (')", advance="no")
  do j = 1, d
    write (u, "(1x,I0)", advance="no") state_flv%map(j,i)
  end do
  write (u, "(' )')")
end do
end subroutine state_flv_content_write

```

Initialize with table length and mask. Each row of the `map` array, of length d , is initialized with $(0, 1, \dots, d)$.

```

<State matrices: state flv content: TBP>+≡
  procedure :: init => state_flv_content_init

<State matrices: procedures>+≡
  subroutine state_flv_content_init (state_flv, n, mask)
    class(state_flv_content_t), intent(out) :: state_flv
    integer, intent(in) :: n
    logical, dimension(:), intent(in) :: mask
    integer :: d, i
    d = size (mask)
    allocate (state_flv%pdg (d, n), source = 0)
    allocate (state_flv%map (d, n), source = spread ([i, i = 1, d], 2, n))
    allocate (state_flv%mask (d), source = mask)
  end subroutine state_flv_content_init

```

Manually fill the entries, one flavor set and mapping at a time.

```

<State matrices: state flv content: TBP>+≡
  procedure :: set_entry => state_flv_content_set_entry

<State matrices: procedures>+≡
  subroutine state_flv_content_set_entry (state_flv, i, pdg, map)
    class(state_flv_content_t), intent(inout) :: state_flv
    integer, intent(in) :: i
    integer, dimension(:), intent(in) :: pdg, map
    state_flv%pdg(:,i) = pdg
    where (map /= 0)
      state_flv%map(:,i) = map
    end where
  end subroutine state_flv_content_set_entry

```

Given a state matrix, determine the flavor content. That is, scan the state matrix and extract flavor only, build a new state matrix from that.

```

<State matrices: state flv content: TBP>+≡
  procedure :: fill => state_flv_content_fill

```

```

<State matrices: procedures>+≡
subroutine state_flv_content_fill &
  (state_flv, state_full, mask)
  class(state_flv_content_t), intent(out) :: state_flv
  type(state_matrix_t), intent(in), target :: state_full
  logical, dimension(:), intent(in) :: mask
  type(state_matrix_t), target :: state_tmp
  type(state_iterator_t) :: it
  type(flavor_t), dimension(:), allocatable :: flv
  integer, dimension(:), allocatable :: pdg, pdg_subset
  integer, dimension(:), allocatable :: idx, map_subset, idx_subset, map
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  integer :: n, d, c, i
  call state_tmp%init ()
  d = state_full%get_depth ()
  allocate (flv (d), qn (d), pdg (d), idx (d), map (d))
  idx = [(i, i = 1, d)]
  c = count (mask)
  allocate (pdg_subset (c), map_subset (c), idx_subset (c))
  call it%init (state_full)
  do while (it%is_valid ())
    flv = it%get_flavor ()
    call qn%init (flv)
    call state_tmp%add_state (qn)
    call it%advance ()
  end do
  n = state_tmp%get_n_leaves ()
  call state_flv%init (n, mask)
  i = 0
  call it%init (state_tmp)
  do while (it%is_valid ())
    i = i + 1
    flv = it%get_flavor ()
    pdg = flv%get_pdg ()
    idx_subset = pack (idx, mask)
    pdg_subset = pack (pdg, mask)
    map_subset = order_abs (pdg_subset)
    map = unpack (idx_subset (map_subset), mask, idx)
    call state_flv%set_entry (i, &
      unpack (pdg_subset(map_subset), mask, pdg), &
      order (map))
    call it%advance ()
  end do
  call state_tmp%final ()
end subroutine state_flv_content_fill

```

Match a given flavor string against the flavor content. We sort the input string and check whether it matches any of the stored strings. If yes, return the mapping.

Only PDG entries under the preset mask are sorted before matching. The other entries must match exactly (i.e., without reordering). A zero entry matches anything. In any case, the length of the PDG string must be equal to the length d of the individual flavor-state entries.

```

<State matrices: state flv content: TBP>+≡
  procedure :: match => state_flv_content_match

<State matrices: procedures>+≡
  subroutine state_flv_content_match (state_flv, pdg, success, map)
    class(state_flv_content_t), intent(in) :: state_flv
    integer, dimension(:), intent(in) :: pdg
    logical, intent(out) :: success
    integer, dimension(:), intent(out) :: map
    integer, dimension(:), allocatable :: pdg_subset, pdg_sorted, map1, map2
    integer, dimension(:), allocatable :: idx, map_subset, idx_subset
    integer :: i, n, c, d
    c = count (state_flv%mask)
    d = size (state_flv%pdg, 1)
    n = size (state_flv%pdg, 2)
    allocate (idx (d), source = [(i, i = 1, d)])
    allocate (idx_subset (c), pdg_subset (c), map_subset (c))
    allocate (pdg_sorted (d), map1 (d), map2 (d))
    idx_subset = pack (idx, state_flv%mask)
    pdg_subset = pack (pdg, state_flv%mask)
    map_subset = order_abs (pdg_subset)
    pdg_sorted = unpack (pdg_subset(map_subset), state_flv%mask, pdg)
    success = .false.
    do i = 1, n
      if (all (pdg_sorted == state_flv%pdg(:,i) &
        .or. pdg_sorted == 0)) then
        success = .true.
        exit
      end if
    end do
    if (success) then
      map1 = state_flv%map(:,i)
      map2 = unpack (idx_subset(map_subset), state_flv%mask, idx)
      map = map2(map1)
      where (pdg == 0) map = 0
    end if
  end subroutine state_flv_content_match

```

Check if a given PDG code occurs anywhere in the table.

```

<State matrices: state flv content: TBP>+≡
  procedure :: contains => state_flv_content_contains

<State matrices: procedures>+≡
  function state_flv_content_contains (state_flv, pdg) result (success)
    class(state_flv_content_t), intent(in) :: state_flv
    integer, intent(in) :: pdg
    logical :: success
    success = any (state_flv%pdg == pdg)
  end function state_flv_content_contains

<State matrices: procedures>+≡
  elemental function pacify_complex (c_in) result (c_pac)
    complex(default), intent(in) :: c_in
    complex(default) :: c_pac

```

```

c_pac = c_in
if (real(c_pac) == -real(c_pac)) then
  c_pac = &
    cmplx (0._default, aimag(c_pac), kind=default)
end if
if (aimag(c_pac) == -aimag(c_pac)) then
  c_pac = &
    cmplx (real(c_pac), 0._default, kind=default)
end if
end function pacify_complex

```

Looks for flavor structures that only differ by a permutation of the masked flavors. The result is returned in form of a mask which is `.true.` at the positions of a duplicate flavor structure from the second encounter on. This routine implements the naive approach: We go through all flavor structures and compare each one with each preceding one. This works but is $\mathcal{O}(n^2)$ in the number of flavor structures. Using a table to remember which flavor structure has already been encountered, it would be possible to find the duplicates in $\mathcal{O}(n)$.

```

<State matrices: state flv content: TBP>+≡
  procedure :: find_duplicates => state_flv_content_find_duplicates

<State matrices: procedures>+≡
  subroutine state_flv_content_find_duplicates (state_flv, duplicate_mask)
    class(state_flv_content_t), intent(in) :: state_flv
    logical, dimension(:), allocatable, intent(out) :: duplicate_mask
    integer, dimension(:), allocatable :: flvst
    integer :: i1, i2, n_flvsts
    logical :: found_once
    n_flvsts = size (state_flv%pdg, 2)
    allocate (duplicate_mask (n_flvsts))
    duplicate_mask = .false.
    do i1 = 1, n_flvsts
      found_once = .false.
      flvst = state_flv%pdg(:,i1)
      do i2 = 1, i1
        if (all(flvst == state_flv%pdg(:,i2))) then
          if (found_once) then
            duplicate_mask(i1) = .true.
            exit
          else
            found_once = .true.
          end if
        end if
      end do
    end do
  end subroutine state_flv_content_find_duplicates

```

12.1.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<state_matrices_ut.f90>≡
  <File header>

```

```

module state_matrices_ut
  use unit_tests
  use state_matrices_util

  <Standard module head>

  <State matrices: public test>

  contains

  <State matrices: test driver>

end module state_matrices_ut
<state_matrices_util.f90>≡
  <File header>

  module state_matrices_util

    <Use kinds>
    use io_units
    use format_defs, only: FMT_19
    use flavors
    use colors
    use helicities
    use quantum_numbers

    use state_matrices

    <Standard module head>

    <State matrices: test declarations>

    contains

    <State matrices: tests>

  end module state_matrices_util
API: driver for the unit tests below.
<State matrices: public test>≡
  public :: state_matrix_test
<State matrices: test driver>≡
  subroutine state_matrix_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <State matrices: execute tests>
  end subroutine state_matrix_test

```

Create two quantum states of equal depth and merge them.

```

<State matrices: execute tests>≡
  call test (state_matrix_1, "state_matrix_1", &
    "check merge of quantum states of equal depth", &

```



```

        u, results)

<State matrices: test declarations>≡
    public :: state_matrix_1

<State matrices: tests>≡
    subroutine state_matrix_1 (u)
        integer, intent(in) :: u
        type(state_matrix_t) :: state1, state2, state3
        type(flavor_t), dimension(3) :: flv
        type(color_t), dimension(3) :: col
        type(quantum_numbers_t), dimension(3) :: qn

        write (u, "(A)")  "* Test output: state_matrix_1"
        write (u, "(A)")  "*   Purpose: create and merge two quantum states"
        write (u, "(A)")

        write (u, "(A)")  "*   Initialization"
        write (u, "(A)")

        write (u, "(A)")  "*   State matrix 1"
        write (u, "(A)")

        call state1%init ()
        call flv%init ([1, 2, 11])
        call qn%init (flv, helicity ([ 1, 1, 1]))
        call state1%add_state (qn)
        call qn%init (flv, helicity ([ 1, 1, 1], [-1, 1, -1]))
        call state1%add_state (qn)
        call state1%freeze ()
        call state1%write (u)

        write (u, "(A)")
        write (u, "(A)")  "*   State matrix 2"
        write (u, "(A)")

        call state2%init ()
        call col(1)%init ([501])
        call col(2)%init ([-501])
        call col(3)%init ([0])
        call qn%init (col, helicity ([-1, -1, 0]))
        call state2%add_state (qn)
        call col(3)%init ([99])
        call qn%init (col, helicity ([-1, -1, 0]))
        call state2%add_state (qn)
        call state2%freeze ()
        call state2%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Merge the state matrices"
        write (u, "(A)")

        call merge_state_matrices (state1, state2, state3)
        call state3%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Collapse the state matrix"
write (u, "(A)")

call state3%collapse (quantum_numbers_mask (.false., .false., &
      [.true.,.false.,.false.]))
call state3%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call state1%final ()
call state2%final ()
call state3%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: state_matrix_1"
write (u, "(A)")

end subroutine state_matrix_1

```

Create a correlated three-particle state matrix and factorize it.

```

<State matrices: execute tests>+≡
call test (state_matrix_2, "state_matrix_2", &
      "check factorizing 3-particle state matrix", &
      u, results)

<State matrices: test declarations>+≡
public :: state_matrix_2

<State matrices: tests>+≡
subroutine state_matrix_2 (u)
  integer, intent(in) :: u
  type(state_matrix_t) :: state
  type(state_matrix_t), dimension(:), allocatable :: single_state
  type(state_matrix_t) :: correlated_state
  integer :: f, h11, h12, h21, h22, i, mode
  type(flavor_t), dimension(2) :: flv
  type(color_t), dimension(2) :: col
  type(helicity_t), dimension(2) :: hel
  type(quantum_numbers_t), dimension(2) :: qn
  logical :: ok

  write (u, "(A)")
  write (u, "(A)")  "* Test output: state_matrix_2"
  write (u, "(A)")  "* Purpose: factorize correlated 3-particle state"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call state%init ()
  do f = 1, 2
    do h11 = -1, 1, 2

```

```

do h12 = -1, 1, 2
  do h21 = -1, 1, 2
    do h22 = -1, 1, 2
      call flv%init ([f, -f])
      call col(1)%init ([1])
      call col(2)%init ([-1])
      call hel%init ([h11,h12], [h21, h22])
      call qn%init (flv, col, hel)
      call state%add_state (qn)
    end do
  end do
end do
end do
end do
call state%freeze ()
call state%write (u)

write (u, "(A)")
write (u, "(A,'('," // FMT_19 // ",',''," // FMT_19 // ",')')") &
  "Trace = ", state%trace ()
write (u, "(A)")

do mode = 1, 3
  write (u, "(A)")
  write (u, "(A,I1)")  "Mode = ", mode
  call state%factorize &
    (mode, 0.15_default, ok, single_state, correlated_state)
  do i = 1, size (single_state)
    write (u, "(A)")
    call single_state(i)%write (u)
    write (u, "(A,'('," // FMT_19 // ",',''," // FMT_19 // ",')')") &
      "Trace = ", single_state(i)%trace ()
  end do
  write (u, "(A)")
  call correlated_state%write (u)
  write (u, "(A,'('," // FMT_19 // ",',''," // FMT_19 // ",')')") &
    "Trace = ", correlated_state%trace ()
  do i = 1, size(single_state)
    call single_state(i)%final ()
  end do
  call correlated_state%final ()
end do

write (u, "(A)")
write (u, "(A)")  "Cleanup"

call state%final ()

write (u, "(A)")
write (u, "(A)")  "Test output end: state_matrix_2"

end subroutine state_matrix_2

```

Create a colored state matrix and add color contractions.

```

<State matrices: execute tests>+≡
    call test (state_matrix_3, "state_matrix_3", &
        "check factorizing 3-particle state matrix", &
        u, results)

<State matrices: test declarations>+≡
    public :: state_matrix_3

<State matrices: tests>+≡
    subroutine state_matrix_3 (u)
        use physics_defs, only: HADRON_REMNANT_TRIPLET, HADRON_REMNANT_OCTET
        integer, intent(in) :: u
        type(state_matrix_t) :: state
        type(flavor_t), dimension(4) :: flv
        type(color_t), dimension(4) :: col
        type(quantum_numbers_t), dimension(4) :: qn

        write (u, "(A)")  "* Test output: state_matrix_3"
        write (u, "(A)")  "* Purpose: add color connections to colored state"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call state%init ()
        call flv%init ([ 1, -HADRON_REMNANT_TRIPLET, -1, HADRON_REMNANT_TRIPLET ])
        call col(1)%init ([17])
        call col(2)%init ([-17])
        call col(3)%init ([-19])
        call col(4)%init ([19])
        call qn%init (flv, col)
        call state%add_state (qn)
        call flv%init ([ 1, -HADRON_REMNANT_TRIPLET, 21, HADRON_REMNANT_OCTET ])
        call col(1)%init ([17])
        call col(2)%init ([-17])
        call col(3)%init ([3, -5])
        call col(4)%init ([5, -3])
        call qn%init (flv, col)
        call state%add_state (qn)
        call state%freeze ()

        write (u, "(A)")  "* State:"
        write (u, "(A)")

        call state%write (u)
        call state%add_color_contractions ()

        write (u, "(A)")  "* State with contractions:"
        write (u, "(A)")

        call state%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

```

```

call state%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: state_matrx_3"

end subroutine state_matrix_3

```

Create a correlated three-particle state matrix, write it to file and read again.

```

<State matrices: execute tests>+≡
call test (state_matrix_4, "state_matrix_4", &
  "check raw I/O", &
  u, results)

<State matrices: test declarations>+≡
public :: state_matrix_4

<State matrices: tests>+≡
subroutine state_matrix_4 (u)
  integer, intent(in) :: u
  type(state_matrix_t), allocatable :: state
  integer :: f, h11, h12, h21, h22, i
  type(flavor_t), dimension(2) :: flv
  type(color_t), dimension(2) :: col
  type(helicity_t), dimension(2) :: hel
  type(quantum_numbers_t), dimension(2) :: qn
  integer :: unit, iostat

  write (u, "(A)")
  write (u, "(A)")  "* Test output: state_matrix_4"
  write (u, "(A)")  "* Purpose: raw I/O for correlated 3-particle state"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  allocate (state)

  call state%init ()
  do f = 1, 2
    do h11 = -1, 1, 2
      do h12 = -1, 1, 2
        do h21 = -1, 1, 2
          do h22 = -1, 1, 2
            call flv%init ([f, -f])
            call col(1)%init ([1])
            call col(2)%init ([-1])
            call hel%init ([h11, h12], [h21, h22])
            call qn%init (flv, col, hel)
            call state%add_state (qn)
          end do
        end do
      end do
    end do
  end do
  call state%freeze ()

```

```

call state%set_norm (3._default)
do i = 1, state%get_n_leaves ()
    call state%set_matrix_element (i, cmplx (2 * i, 2 * i + 1, default))
end do

call state%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write to file and read again "
write (u, "(A)")

unit = free_unit ()
open (unit, action="readwrite", form="unformatted", status="scratch")
call state%write_raw (unit)
call state%final ()
deallocate (state)

allocate(state)
rewind (unit)
call state%read_raw (unit, iostat=iostat)
close (unit)

call state%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call state%final ()
deallocate (state)

write (u, "(A)")
write (u, "(A)")  "* Test output end: state_matrix_4"

end subroutine state_matrix_4

```

Create a flavor-content object for a given state matrix and match it against trial flavor (i.e., PDG) strings.

```

<State matrices: execute tests>+≡
    call test (state_matrix_5, "state_matrix_5", &
        "check flavor content", &
        u, results)

<State matrices: test declarations>+≡
    public :: state_matrix_5

<State matrices: tests>+≡
    subroutine state_matrix_5 (u)
        integer, intent(in) :: u
        type(state_matrix_t), allocatable, target :: state
        type(state_iterator_t) :: it
        type(state_flv_content_t), allocatable :: state_flv
        type(flavor_t), dimension(4) :: flv1, flv2, flv3, flv4
        type(color_t), dimension(4) :: col1, col2
        type(helicity_t), dimension(4) :: hel1, hel2, hel3

```

```

type(quantum_numbers_t), dimension(4) :: qn
logical, dimension(4) :: mask

write (u, "(A)")  "* Test output: state_matrix_5"
write (u, "(A)")  "* Purpose: check flavor-content state"
write (u, "(A)")

write (u, "(A)")  "* Set up arbitrary state matrix"
write (u, "(A)")

call flv1%init ([1, 4, 2, 7])
call flv2%init ([1, 3,-3, 8])
call flv3%init ([5, 6, 3, 7])
call flv4%init ([6, 3, 5, 8])
call hel1%init ([0, 1, -1, 0])
call hel2%init ([0, 1, 1, 1])
call hel3%init ([1, 0, 0, 0])
call col1(1)%init ([0])
call col1(2)%init ([0])
call col1(3)%init ([0])
call col1(4)%init ([0])
call col2(1)%init ([5, -6])
call col2(2)%init ([0])
call col2(3)%init ([6, -5])
call col2(4)%init ([0])

allocate (state)
call state%init ()
call qn%init (flv1, col1, hel1)
call state%add_state (qn)
call qn%init (flv1, col1, hel2)
call state%add_state (qn)
call qn%init (flv3, col1, hel3)
call state%add_state (qn)
call qn%init (flv4, col1, hel3)
call state%add_state (qn)
call qn%init (flv1, col2, hel3)
call state%add_state (qn)
call qn%init (flv2, col2, hel2)
call state%add_state (qn)
call qn%init (flv2, col2, hel1)
call state%add_state (qn)
call qn%init (flv2, col1, hel1)
call state%add_state (qn)
call qn%init (flv3, col1, hel1)
call state%add_state (qn)
call qn%init (flv3, col2, hel3)
call state%add_state (qn)
call qn%init (flv1, col1, hel1)
call state%add_state (qn)

write (u, "(A)")  "* Quantum number content"
write (u, "(A)")

```

```

call it%init (state)
do while (it%is_valid ())
    call quantum_numbers_write (it%get_quantum_numbers (), u)
    write (u, *)
    call it%advance ()
end do

write (u, "(A)")
write (u, "(A)")  "* Extract the flavor content"
write (u, "(A)")

mask = [.true., .true., .true., .false.]

allocate (state_flv)
call state_flv%fill (state, mask)
call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Match trial sets"
write (u, "(A)")

call check ([1, 2, 3, 0])
call check ([1, 4, 2, 0])
call check ([4, 2, 1, 0])
call check ([1, 3, -3, 0])
call check ([1, -3, 3, 0])
call check ([6, 3, 5, 0])

write (u, "(A)")
write (u, "(A)")  "* Determine the flavor content with mask"
write (u, "(A)")

mask = [.false., .true., .true., .false.]

call state_flv%fill (state, mask)
call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Match trial sets"
write (u, "(A)")

call check ([1, 2, 3, 0])
call check ([1, 4, 2, 0])
call check ([4, 2, 1, 0])
call check ([1, 3, -3, 0])
call check ([1, -3, 3, 0])
call check ([6, 3, 5, 0])

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

deallocate (state_flv)

call state%final ()

```



```

deallocate (state)

write (u, "(A)")
write (u, "(A)")  "* Test output end: state_matrix_5"

contains

subroutine check (pdg)
  integer, dimension(4), intent(in) :: pdg
  integer, dimension(4) :: map
  logical :: success
  call state_flv%match (pdg, success, map)
  write (u, "(2x,4(1x,I0),':',1x,L1)", advance="no")  pdg, success
  if (success) then
    write (u, "(2x,'map = (' ,4(1x,I0),' )')")  map
  else
    write (u, *)
  end if
end subroutine check

end subroutine state_matrix_5

```

Create a state matrix with full flavor, color and helicity information. Afterwards, reduce such that it is only differential in flavor and initial-state helicities. This is used when preparing states for beam- polarized computations with external matrix element providers.

```

<State matrices: execute tests>+≡
  call test (state_matrix_6, "state_matrix_6", &
    "check state matrix reduction", &
    u, results)

<State matrices: test declarations>+≡
  public :: state_matrix_6

<State matrices: tests>+≡
  subroutine state_matrix_6 (u)
    integer, intent(in) :: u
    type(state_matrix_t), allocatable :: state_orig, state_reduced
    type(flavor_t), dimension(4) :: flv
    type(helicity_t), dimension(4) :: hel
    type(color_t), dimension(4) :: col
    type(quantum_numbers_t), dimension(4) :: qn
    type(quantum_numbers_mask_t), dimension(4) :: qn_mask
    integer :: h1, h2, h3 , h4
    integer :: n_states = 0

    write (u, "(A)")  "* Test output: state_matrix_6"
    write (u, "(A)")  "* Purpose: Check state matrix reduction"
    write (u, "(A)")

    write (u, "(A)")  "* Set up helicity-diagonal state matrix"
    write (u, "(A)")

    allocate (state_orig)

```

```

call state_orig%init ()

call flv%init ([11, -11, 1, -1])
call col(3)%init ([1])
call col(4)%init ([-1])
do h1 = -1, 1, 2
  do h2 = -1, 1, 2
    do h3 = -1, 1, 2
      do h4 = -1, 1, 2
        n_states = n_states + 1
        call hel%init ([h1, h2, h3, h4], [h1, h2, h3, h4])
        call qn%init (flv, col, hel)
        call state_orig%add_state (qn)
      end do
    end do
  end do
end do
call state_orig%freeze ()

write (u, "(A)") "* Original state: "
write (u, "(A)")
call state_orig%write (u)

write (u, "(A)")
write (u, "(A)") "* Setup quantum mask: "

call qn_mask%init ([.false., .false., .false., .false.], &
                  [.true., .true., .true., .true.], &
                  [.false., .false., .true., .true.])
call quantum_numbers_mask_write (qn_mask, u)
write (u, "(A)")
write (u, "(A)") "* Reducing the state matrix using above mask"
write (u, "(A)")
allocate (state_reduced)
call state_orig%reduce (qn_mask, state_reduced)

write (u, "(A)") "* Reduced state matrix: "
call state_reduced%write (u)

write (u, "(A)") "* Test output end: state_matrix_6"
end subroutine state_matrix_6

```

Create a state matrix with full flavor, color and helicity information. Afterwards, reduce such that it is only differential in flavor and initial-state helicities, and keeping old indices. Afterwards reorder the reduced state matrix in accordance to the original state matrix.

```

<State matrices: execute tests>+≡
  call test (state_matrix_7, "state_matrix_7", &
            "check ordered state matrix reduction", &
            u, results)

<State matrices: test declarations>+≡
  public :: state_matrix_7

```

<State matrices: tests>+≡

```

subroutine state_matrix_7 (u)
  integer, intent(in) :: u
  type(state_matrix_t), allocatable :: state_orig, state_reduced, &
    state_ordered
  type(flavor_t), dimension(4) :: flv
  type(helicity_t), dimension(4) :: hel
  type(color_t), dimension(4) :: col
  type(quantum_numbers_t), dimension(4) :: qn
  type(quantum_numbers_mask_t), dimension(4) :: qn_mask
  integer :: h1, h2, h3 , h4
  integer :: n_states = 0

  write (u, "(A)") "* Test output: state_matrix_7"
  write (u, "(A)") "* Purpose: Check ordered state matrix reduction"
  write (u, "(A)")

  write (u, "(A)") "* Set up helicity-diagonal state matrix"
  write (u, "(A)")

  allocate (state_orig)
  call state_orig%init ()

  call flv%init ([11, -11, 1, -1])
  call col(3)%init ([1])
  call col(4)%init ([-1])
  do h1 = -1, 1, 2
    do h2 = -1, 1, 2
      do h3 = -1, 1, 2
        do h4 = -1, 1, 2
          n_states = n_states + 1
          call hel%init ([h1, h2, h3, h4], [h1, h2, h3, h4])
          call qn%init (flv, col, hel)
          call state_orig%add_state (qn)
        end do
      end do
    end do
  end do
  call state_orig%freeze ()

  write (u, "(A)") "* Original state: "
  write (u, "(A)")
  call state_orig%write (u)

  write (u, "(A)")
  write (u, "(A)") "* Setup quantum mask: "

  call qn_mask%init ([.false., .false., .false., .false.], &
    [.true., .true., .true., .true.], &
    [.false., .false., .true., .true.])
  call quantum_numbers_mask_write (qn_mask, u)
  write (u, "(A)")
  write (u, "(A)") "* Reducing the state matrix using above mask and keeping the old indices:"
  write (u, "(A)")

```

```

allocate (state_reduced)
call state_orig%reduce (qn_mask, state_reduced, keep_me_index = .true.)

write (u, "(A)") "* Reduced state matrix with kept indices: "
call state_reduced%write (u)

write (u, "(A)")
write (u, "(A)") "* Reordering reduced state matrix:"
write (u, "(A)")
allocate (state_ordered)
call state_reduced%reorder_me (state_ordered)

write (u, "(A)") "* Reduced and ordered state matrix:"
call state_ordered%write (u)

write (u, "(A)") "* Test output end: state_matrix_6"
end subroutine state_matrix_7

```

12.2 Interactions

This module defines the `interaction_t` type. It is an extension of the `state_matrix_t` type.

The state matrix is a representation of a multi-particle density matrix. It implements all possible flavor, color, and quantum-number assignments of the entries in a generic density matrix, and it can hold a complex matrix element for each entry. (Note that this matrix can hold non-diagonal entries in color and helicity space.) The `interaction_t` object associates this with a list of momenta, such that the whole object represents a multi-particle state.

The `interaction_t` holds information about which particles are incoming, virtual (i.e., kept for the records), or outgoing. Each particle can be associated to a source within another interaction. This allows us to automatically fill those interaction momenta which have been computed or defined elsewhere. It also contains internal parent-child relations and flags for (virtual) particles which are to be treated as resonances.

A quantum-number mask array summarizes, for each particle within the interaction, the treatment of flavor, color, or helicity (expose or ignore). A list of locks states which particles are bound to have an identical quantum-number mask. This is useful when the mask is changed at one place.

```

<interactions.f90>≡
<File header>

module interactions

<Use kinds>
  use io_units
  use diagnostics
  use sorting
  use lorentz
  use flavors
  use colors

```

```

    use helicities
    use quantum_numbers
    use state_matrices

```

⟨Standard module head⟩

⟨Interactions: public⟩

⟨Interactions: types⟩

⟨Interactions: interfaces⟩

contains

⟨Interactions: procedures⟩

```

end module interactions

```

Given an ordered list of quantum numbers (without any subtraction index) map this list to a state matrix, such that each list index corresponds to an index of a set of quantum numbers in the state matrix, hence, the matrix element.

The (unphysical) subtraction index is not a genuine quantum number and as such handled specially.

⟨Interactions: public⟩≡

```

    public :: qn_index_map_t

```

⟨Interactions: types⟩≡

```

    type :: qn_index_map_t
    private
    type(quantum_numbers_t), dimension(:, :), allocatable :: qn_flv
    type(quantum_numbers_t), dimension(:, :), allocatable :: qn_hel
    logical :: flip_hel = .false.
    integer :: n_flv = 0, n_hel = 0, n_sub = 0
    integer, dimension(:, :, :), allocatable :: index
    integer, dimension(:, :, :), allocatable :: sf_index_born, sf_index_real
    contains
    ⟨Interactions: qn index map: TBP⟩
end type qn_index_map_t

```

Construct a mapping from interaction to an array of (sorted) quantum numbers.

We strip all non-elementary particles (like beam) from the quantum numbers which we retrieve from the interaction.

We consider helicity matrix elements only, when `qn_hel` is allocated. Else the helicity index is handled trivially as 1.

For the rescaling of the structure functions in the real subtraction and DGLAP components we need a mapping (initialized by `qn_index_map_init_sf`) from the real and born flavor structure indices to the structure function chain interaction matrix element with the correct initial state quantum numbers. This is stored in `sf_index_born` and `sf_index_real`. The array `index` is only needed for the initialisation of the Born and real index arrays and is therefore deallocated again.

⟨Interactions: qn index map: TBP⟩≡

```

    generic :: init => init_trivial, &

```

```

        init_involved, &
        init_sf
procedure, private :: init_trivial => qn_index_map_init_trivial
procedure, private :: init_involved => qn_index_map_init_involved
procedure, private :: init_sf => qn_index_map_init_sf

<Interactions: procedures>≡
subroutine qn_index_map_init_trivial (self, int)
  class(qn_index_map_t), intent(out) :: self
  class(interaction_t), intent(in) :: int
  integer :: qn
  self%n_flv = int%get_n_matrix_elements ()
  self%n_hel = 1
  self%n_sub = 0
  allocate (self%index(self%n_flv, self%n_hel, 0:self%n_sub), source = 0)
  do qn = 1, self%n_flv
    self%index(qn, 1, 0) = qn
  end do
end subroutine qn_index_map_init_trivial

subroutine qn_index_map_init_involved (self, int, qn_flv, n_sub, qn_hel)
  class(qn_index_map_t), intent(out) :: self
  type(interaction_t), intent(in) :: int
  type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
  integer, intent(in) :: n_sub
  type(quantum_numbers_t), dimension(:, :), intent(in), optional :: qn_hel
  type(quantum_numbers_t), dimension(:, :), allocatable :: qn, qn_int
  integer :: i, i_flv, i_hel, i_sub
  self%qn_flv = qn_flv
  self%n_flv = size (qn_flv, dim=2)
  self%n_sub = n_sub
  if (present (qn_hel)) then
    if (size (qn_flv, dim=1) /= size (qn_hel, dim=1)) then
      call msg_bug ("[qn_index_map_init] number of particles does not match.")
    end if
    self%qn_hel = qn_hel
    self%n_hel = size (qn_hel, dim=2)
  else
    self%n_hel = 1
  end if
  allocate (self%index (self%n_flv, self%n_hel, 0:self%n_sub), source=0)
  associate (n_me => int%get_n_matrix_elements ())
    do i = 1, n_me
      qn_int = int%get_quantum_numbers (i, by_me_index = .true.)
      qn = pack (qn_int, qn_int%are_hard_process ())
      i_flv = find_flv_index (self, qn)
      i_hel = 1; if (allocated (self%qn_hel)) &
        i_hel = find_hel_index (self, qn)
      i_sub = find_sub_index (self, qn)
      self%index(i_flv, i_hel, i_sub) = i
    end do
  end associate
contains
  integer function find_flv_index (self, qn) result (i_flv)
    type(qn_index_map_t), intent(in) :: self

```

```

type(quantum_numbers_t), dimension(:), intent(in) :: qn
integer :: j
i_flv = 0
do j = 1, self%n_flv
  if (.not. all (qn .fmatch. self%qn_flv(:, j))) cycle
  i_flv = j
  exit
end do
if (i_flv < 1) then
  call msg_message ("QN:")
  call quantum_numbers_write (qn)
  call msg_message ("")
  call msg_message ("QN_FLV:")
  do j = 1, self%n_flv
    call quantum_numbers_write (self%qn_flv(:, j))
    call msg_message ("")
  end do
  call msg_bug ("[find_flv_index] could not find flv in qn_flv.")
end if
end function find_flv_index

integer function find_hel_index (self, qn) result (i_hel)
type(qn_index_map_t), intent(in) :: self
type(quantum_numbers_t), dimension(:), intent(in) :: qn
integer :: j
i_hel = 0
do j = 1, self%n_hel
  if (.not. all (qn .hmatch. self%qn_hel(:, j))) cycle
  i_hel = j
  exit
end do
if (i_hel < 1) then
  call msg_message ("QN:")
  call quantum_numbers_write (qn)
  call msg_message ("")
  call msg_message ("QN_HEL:")
  do j = 1, self%n_hel
    call quantum_numbers_write (self%qn_hel(:, j))
    call msg_message ("")
  end do
  call msg_bug ("[find_hel_index] could not find hel in qn_hel.")
end if
end function find_hel_index

integer function find_sub_index (self, qn) result (i_sub)
type(qn_index_map_t), intent(in) :: self
type(quantum_numbers_t), dimension(:), intent(in) :: qn
integer :: s
i_sub = -1
do s = 0, self%n_sub
  if ((all (pack(qn%get_sub (), qn%get_sub () > 0) == s)) &
    .or. (all (qn%get_sub () == 0) .and. s == 0)) then
    i_sub = s
    exit
  end if
end do

```

```

        end if
    end do
    if (i_sub < 0) then
        call msg_message ("QN:")
        call quantum_numbers_write (qn)
        call msg_bug ("[find_sub_index] could not find sub in qn.")
    end if
end function find_sub_index
end subroutine qn_index_map_init_involved

subroutine qn_index_map_init_sf (self, int, qn_flv, n_flv_born, n_flv_real)
class(qn_index_map_t), intent(out) :: self
type(interaction_t), intent(in) :: int
integer, intent(in) :: n_flv_born, n_flv_real
type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
type(quantum_numbers_t), dimension(:, :), allocatable :: qn_int
type(quantum_numbers_t), dimension(:), allocatable :: qn_int_tmp
integer :: i, i_sub, n_flv, n_hard
n_flv = int%get_n_matrix_elements ()
qn_int_tmp = int%get_quantum_numbers (1, by_me_index = .true.)
n_hard = count (qn_int_tmp%are_hard_process ())
allocate (qn_int(n_hard, n_flv))
do i = 1, n_flv
    qn_int_tmp = int%get_quantum_numbers (i, by_me_index = .true.)
    qn_int(:, i) = pack (qn_int_tmp, qn_int_tmp%are_hard_process ())
end do
call self%init (int, qn_int, int%get_n_sub ())
allocate (self%sf_index_born(n_flv_born, 0:self%n_sub))
allocate (self%sf_index_real(n_flv_real, 0:self%n_sub))
do i_sub = 0, self%n_sub
    do i = 1, n_flv_born
        self%sf_index_born(i, i_sub) = self%get_index_by_qn (qn_flv(:, i), i_sub)
    end do
    do i = 1, n_flv_real
        self%sf_index_real(i, i_sub) = &
            self%get_index_by_qn (qn_flv(:, n_flv_born + i), i_sub)
    end do
end do
deallocate (self%index)
end subroutine qn_index_map_init_sf

```

Write the index map to unit.

(Interactions: qn index map: TBP)+≡

```
procedure :: write => qn_index_map_write
```

(Interactions: procedures)+≡

```

subroutine qn_index_map_write (self, unit)
class(qn_index_map_t), intent(in) :: self
integer, intent(in), optional :: unit
integer :: u, i_flv, i_hel, i_sub
u = given_output_unit (unit); if (u < 0) return
write (u, *) "flip_hel: ", self%flip_hel
do i_flv = 1, self%n_flv
    if (allocated (self%qn_flv)) &

```



```

        call quantum_numbers_write (self%qn_flv(:, i_flv))
write (u, *)
do i_hel = 1, self%n_hel
    if (allocated (self%qn_hel)) then
        call quantum_numbers_write (self%qn_hel(:, i_hel))
        write (u, *)
    end if
do i_sub = 0, self%n_sub
    write (u, *) &
        "(" , i_flv, ",", i_hel, ",", i_sub, ")" => ", self%index(i_flv, i_hel, i_sub)
end do
end do
end do
end subroutine qn_index_map_write

```

Set helicity convention. If flip, then we flip the helicities of anti-particles and we remap the indices accordingly.

(Interactions: qn index map: TBP)+≡

```

    procedure :: set_helicity_flip => qn_index_map_set_helicity_flip

```

(Interactions: procedures)+≡

```

subroutine qn_index_map_set_helicity_flip (self, yorn)
    class(qn_index_map_t), intent(inout) :: self
    logical, intent(in) :: yorn
    integer :: i, i_flv, i_hel, i_hel_new
    type(quantum_numbers_t), dimension(:, :), allocatable :: qn_hel_flip
    integer, dimension(:, :, :), allocatable :: index
    if (.not. allocated (self%qn_hel)) then
        call msg_bug ("[qn_index_map_set_helicity_flip] &
            &cannot flip not-given helicity.")
    end if
    allocate (index (self%n_flv, self%n_hel, 0:self%n_sub), &
        source=self%index)
    self%flip_hel = yorn
    if (self%flip_hel) then
do i_flv = 1, self%n_flv
    qn_hel_flip = self%qn_hel
do i_hel = 1, self%n_hel
    do i = 1, size (self%qn_flv, dim=1)
        if (is_anti_particle (self%qn_flv(i, i_flv))) then
            call qn_hel_flip(i, i_hel)%flip_helicity ()
        end if
    end do
end do
do i_hel = 1, self%n_hel
    i_hel_new = find_hel_index (qn_hel_flip, self%qn_hel(:, i_hel))
    self%index(i_flv, i_hel_new, :) = index(i_flv, i_hel, :)
end do
end do
end if
contains
    logical function is_anti_particle (qn) result (yorn)
        type(quantum_numbers_t), intent(in) :: qn
        type(flavor_t) :: flv

```

```

        flv = qn%get_flavor ()
        yorn = flv%get_pdg () < 0
    end function is_anti_particle

    integer function find_hel_index (qn_sort, qn) result (i_hel)
        type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_sort
        type(quantum_numbers_t), dimension(:, :), intent(in) :: qn
        integer :: j
        do j = 1, size(qn_sort, dim=2)
            if (.not. all (qn .hmatch. qn_sort(:, j))) cycle
            i_hel = j
            exit
        end do
    end function find_hel_index
end subroutine qn_index_map_set_helicity_flip

```

Map from the previously given quantum number and subtraction index (latter ranging from 0 to n_sub) to the (interaction) matrix element.

<Interactions: qn index map: TBP>+≡

```

    procedure :: get_index => qn_index_map_get_index

```

<Interactions: procedures>+≡

```

    integer function qn_index_map_get_index (self, i_flv, i_hel, i_sub) result (index)
        class(qn_index_map_t), intent(in) :: self
        integer, intent(in) :: i_flv
        integer, intent(in), optional :: i_hel
        integer, intent(in), optional :: i_sub
        integer :: i_sub_opt, i_hel_opt
        i_sub_opt = 0; if (present (i_sub)) &
            i_sub_opt = i_sub
        i_hel_opt = 1; if (present (i_hel)) &
            i_hel_opt = i_hel
        index = 0
        if (.not. allocated (self%index)) then
            call msg_bug ("[qn_index_map_get_index] The index map is not allocated.")
        end if
        index = self%index(i_flv, i_hel_opt, i_sub_opt)
        if (index <= 0) then
            call self%write ()
            call msg_bug ("[qn_index_map_get_index] The index for the given quantum numbers could not b
        end if
    end function qn_index_map_get_index

```

Get n_flv.

<Interactions: qn index map: TBP>+≡

```

    procedure :: get_n_flv => qn_index_map_get_n_flv

```

<Interactions: procedures>+≡

```

    integer function qn_index_map_get_n_flv (self) result (n_flv)
        class(qn_index_map_t), intent(in) :: self
        n_flv = self%n_flv
    end function qn_index_map_get_n_flv

```

Get `n_hel`.

```

<Interactions: qn index map: TBP>+≡
  procedure :: get_n_hel => qn_index_map_get_n_hel

<Interactions: procedures>+≡
  integer function qn_index_map_get_n_hel (self) result (n_hel)
    class(qn_index_map_t), intent(in) :: self
    n_hel = self%n_hel
  end function qn_index_map_get_n_hel

```

Get `n_sub`.

```

<Interactions: qn index map: TBP>+≡
  procedure :: get_n_sub => qn_index_map_get_n_sub

<Interactions: procedures>+≡
  integer function qn_index_map_get_n_sub (self) result (n_sub)
    class(qn_index_map_t), intent(in) :: self
    n_sub = self%n_sub
  end function qn_index_map_get_n_sub

```

Gets the index for the matrix element corresponding to a set of quantum numbers. So far, it ignores helicity (and color) indices.

```

<Interactions: qn index map: TBP>+≡
  procedure :: get_index_by_qn => qn_index_map_get_index_by_qn

<Interactions: procedures>+≡
  integer function qn_index_map_get_index_by_qn (self, qn, i_sub) result (index)
    class(qn_index_map_t), intent(in) :: self
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: i_sub
    integer :: i_qn
    if (size(qn) /= size(self%qn_flv, dim = 1)) &
      call msg_bug ("[qn_index_map_get_index_by_qn] number of particles does not match.")
    do i_qn = 1, self%n_flv
      if (all (qn .fmatch. self%qn_flv(:, i_qn))) then
        index = self%get_index (i_qn, i_sub = i_sub)
        return
      end if
    end do
    call self%write ()
    call msg_bug ("[qn_index_map_get_index_by_qn] The index for the given quantum &
      & numbers could not be retrieved.")
  end function qn_index_map_get_index_by_qn

```

```

<Interactions: qn index map: TBP>+≡
  procedure :: get_sf_index_born => qn_index_map_get_sf_index_born

<Interactions: procedures>+≡
  integer function qn_index_map_get_sf_index_born (self, i_born, i_sub) result (index)
    class(qn_index_map_t), intent(in) :: self
    integer, intent(in) :: i_born, i_sub
    index = self%sf_index_born(i_born, i_sub)
  end function qn_index_map_get_sf_index_born

```

```

<Interactions: qn index map: TBP>+≡
  procedure :: get_sf_index_real => qn_index_map_get_sf_index_real

<Interactions: procedures>+≡
  integer function qn_index_map_get_sf_index_real (self, i_real, i_sub) result (index)
    class(qn_index_map_t), intent(in) :: self
    integer, intent(in) :: i_real, i_sub
    index = self%sf_index_real(i_real, i_sub)
  end function qn_index_map_get_sf_index_real

```

12.2.1 External interaction links

Each particle in an interaction can have a link to a corresponding particle in another interaction. This allows to fetch the momenta of incoming or virtual particles from the interaction where they are defined. The link object consists of a pointer to the interaction and an index.

```

<Interactions: types>+≡
  type :: external_link_t
  private
    type(interaction_t), pointer :: int => null ()
    integer :: i
  end type external_link_t

```

Set an external link.

```

<Interactions: procedures>+≡
  subroutine external_link_set (link, int, i)
    type(external_link_t), intent(out) :: link
    type(interaction_t), target, intent(in) :: int
    integer, intent(in) :: i
    if (i /= 0) then
      link%int => int
      link%i = i
    end if
  end subroutine external_link_set

```

Reassign an external link to a new interaction (which should be an image of the original target).

```

<Interactions: procedures>+≡
  subroutine external_link_reassign (link, int_src, int_target)
    type(external_link_t), intent(inout) :: link
    type(interaction_t), intent(in) :: int_src
    type(interaction_t), intent(in), target :: int_target
    if (associated (link%int)) then
      if (link%int%tag == int_src%tag) link%int => int_target
    end if
  end subroutine external_link_reassign

```

Return true if the link is set

```

<Interactions: procedures>+≡
  function external_link_is_set (link) result (flag)
    logical :: flag

```

```

        type(external_link_t), intent(in) :: link
        flag = associated (link%int)
    end function external_link_is_set

```

Return the interaction pointer.

```

<Interactions: public>+≡
    public :: external_link_get_ptr
<Interactions: procedures>+≡
    function external_link_get_ptr (link) result (int)
        type(interaction_t), pointer :: int
        type(external_link_t), intent(in) :: link
        int => link%int
    end function external_link_get_ptr

```

Return the index within that interaction

```

<Interactions: public>+≡
    public :: external_link_get_index
<Interactions: procedures>+≡
    function external_link_get_index (link) result (i)
        integer :: i
        type(external_link_t), intent(in) :: link
        i = link%i
    end function external_link_get_index

```

Return a pointer to the momentum of the corresponding particle. If there is no association, return a null pointer.

```

<Interactions: procedures>+≡
    function external_link_get_momentum_ptr (link) result (p)
        type(vector4_t), pointer :: p
        type(external_link_t), intent(in) :: link
        if (associated (link%int)) then
            p => link%int%p(link%i)
        else
            p => null ()
        end if
    end function external_link_get_momentum_ptr

```

12.2.2 Internal relations

In addition to the external links, particles within the interaction have parent-child relations. Here, more than one link is possible, and we set up an array.

```

<Interactions: types>+≡
    type :: internal_link_list_t
        private
        integer :: length = 0
        integer, dimension(:), allocatable :: link
    contains
        <Interactions: internal link list: TBP>
    end type internal_link_list_t

```

Output, non-advancing.

```

<Interactions: internal link list: TBP>≡
  procedure :: write => internal_link_list_write

<Interactions: procedures>+≡
  subroutine internal_link_list_write (object, unit)
    class(internal_link_list_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    do i = 1, object%length
      write (u, "(1x,I0)", advance="no") object%link(i)
    end do
  end subroutine internal_link_list_write

```

Append an item. Start with an array size of 2 and double the size if necessary.

Make sure that the indices are stored in ascending order. To this end, shift the existing entries right, starting from the end, as long as they are larger than the new entry.

```

<Interactions: internal link list: TBP>+≡
  procedure :: append => internal_link_list_append

<Interactions: procedures>+≡
  subroutine internal_link_list_append (link_list, link)
    class(internal_link_list_t), intent(inout) :: link_list
    integer, intent(in) :: link
    integer :: l, j
    integer, dimension(:), allocatable :: tmp
    l = link_list%length
    if (allocated (link_list%link)) then
      if (l == size (link_list%link)) then
        allocate (tmp (2 * l))
        tmp(:l) = link_list%link
        call move_alloc (from = tmp, to = link_list%link)
      end if
    else
      allocate (link_list%link (2))
    end if
    link_list%link(l+1) = link
    SHIFT_LINK_IN_PLACE: do j = l, 1, -1
      if (link >= link_list%link(j)) then
        exit SHIFT_LINK_IN_PLACE
      else
        link_list%link(j+1) = link_list%link(j)
        link_list%link(j) = link
      end if
    end do SHIFT_LINK_IN_PLACE
    link_list%length = l + 1
  end subroutine internal_link_list_append

```

Return true if the link list is nonempty:

```

<Interactions: internal link list: TBP>+≡
  procedure :: has_entries => internal_link_list_has_entries

```

```

<Interactions: procedures>+≡
  function internal_link_list_has_entries (link_list) result (flag)
    class(internal_link_list_t), intent(in) :: link_list
    logical :: flag
    flag = link_list%length > 0
  end function internal_link_list_has_entries

```

Return the list length

```

<Interactions: internal link list: TBP>+≡
  procedure :: get_length => internal_link_list_get_length

<Interactions: procedures>+≡
  function internal_link_list_get_length (link_list) result (length)
    class(internal_link_list_t), intent(in) :: link_list
    integer :: length
    length = link_list%length
  end function internal_link_list_get_length

```

Return an entry.

```

<Interactions: internal link list: TBP>+≡
  procedure :: get_link => internal_link_list_get_link

<Interactions: procedures>+≡
  function internal_link_list_get_link (link_list, i) result (link)
    class(internal_link_list_t), intent(in) :: link_list
    integer, intent(in) :: i
    integer :: link
    if (i <= link_list%length) then
      link = link_list%link(i)
    else
      call msg_bug ("Internal link list: out of bounds")
    end if
  end function internal_link_list_get_link

```

12.2.3 The interaction type

An interaction is an entangled system of particles. Thus, the interaction object consists of two parts: the subevent, and the quantum state which technically is a trie. The subnode levels beyond the trie root node are in correspondence to the subevent, so both should be traversed in parallel.

The subevent is implemented as an allocatable array of four-momenta. The first `n_in` particles are incoming, `n_vir` particles in-between can be kept for bookkeeping, and the last `n_out` particles are outgoing.

Distinct interactions are linked by their particles: for each particle, we have the possibility of links to corresponding particles in other interactions. Furthermore, for bookkeeping purposes we have a self-link array `relations` where the parent-child relations are kept, and a flag array `resonant` which is set for an intermediate resonance.

Each momentum is associated with masks for flavor, color, and helicity. If a mask entry is set, the associated quantum number is to be ignored for that particle. If any mask has changed, the flag `update` is set.

We can have particle pairs locked together. If this is the case, the corresponding mask entries are bound to be equal. This is useful for particles that go through the interaction.

The interaction tag serves bookkeeping purposes. In particular, it identifies links in printout.

```

<Interactions: public>+≡
    public :: interaction_t

<Interactions: types>+≡
    type :: interaction_t
        private
        integer :: tag = 0
        type(state_matrix_t) :: state_matrix
        integer :: n_in = 0
        integer :: n_vir = 0
        integer :: n_out = 0
        integer :: n_tot = 0
        logical, dimension(:), allocatable :: p_is_known
        type(vector4_t), dimension(:), allocatable :: p
        type(external_link_t), dimension(:), allocatable :: source
        type(internal_link_list_t), dimension(:), allocatable :: parents
        type(internal_link_list_t), dimension(:), allocatable :: children
        logical, dimension(:), allocatable :: resonant
        type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
        integer, dimension(:), allocatable :: hel_lock
        logical :: update_state_matrix = .false.
        logical :: update_values = .false.
        type(qn_index_map_t) :: qn_index
    contains
    <Interactions: interaction: TBP>
    end type interaction_t

```

Initialize the particle array with a fixed size. The first `n_in` particles are incoming, the rest outgoing. Masks are optional. There is also an optional tag. The interaction still needs fixing the values, but that is to be done after all branches have been added.

Interaction tags are assigned consecutively, using a `saved` variable local to this procedure. If desired, we can provide a seed for the interaction tags. Such a seed should be positive. The default seed is one. `tag=0` indicates an empty interaction.

If `set_relations` is set and true, we establish parent-child relations for all incoming and outgoing particles. Virtual particles are skipped; this option is normally used only for interactions without virtual particles.

```

<Interactions: interaction: TBP>≡
    procedure :: basic_init => interaction_init

<Interactions: procedures>+≡
    subroutine interaction_init &
        (int, n_in, n_vir, n_out, &
         tag, resonant, mask, hel_lock, set_relations, store_values)
    class(interaction_t), intent(out) :: int
    integer, intent(in) :: n_in, n_vir, n_out
    integer, intent(in), optional :: tag

```



```

logical, dimension(:), intent(in), optional :: resonant
type(quantum_numbers_mask_t), dimension(:), intent(in), optional :: mask
integer, dimension(:), intent(in), optional :: hel_lock
logical, intent(in), optional :: set_relations, store_values
logical :: set_rel
integer :: i, j
set_rel = .false.; if (present (set_relations)) set_rel = set_relations
call interaction_set_tag (int, tag)
call int%state_matrix%init (store_values)
int%n_in = n_in
int%n_vir = n_vir
int%n_out = n_out
int%n_tot = n_in + n_vir + n_out
allocate (int%p_is_known (int%n_tot))
int%p_is_known = .false.
allocate (int%p (int%n_tot))
allocate (int%source (int%n_tot))
allocate (int%parents (int%n_tot))
allocate (int%children (int%n_tot))
allocate (int%resonant (int%n_tot))
if (present (resonant)) then
    int%resonant = resonant
else
    int%resonant = .false.
end if
allocate (int%mask (int%n_tot))
allocate (int%hel_lock (int%n_tot))
if (present (mask)) then
    int%mask = mask
end if
if (present (hel_lock)) then
    int%hel_lock = hel_lock
else
    int%hel_lock = 0
end if
int%update_state_matrix = .false.
int%update_values = .true.
if (set_rel) then
    do i = 1, n_in
        do j = 1, n_out
            call int%relate (i, n_in + j)
        end do
    end do
end if
end subroutine interaction_init

```

(Interactions: interaction: TBP)+≡

```

generic :: init_qn_index => init_qn_index_trivial, &
                                     init_qn_index_involved, &
                                     init_qn_index_sf
procedure :: init_qn_index_trivial => interaction_init_qn_index_trivial
procedure :: init_qn_index_involved => interaction_init_qn_index_involved
procedure :: init_qn_index_sf => interaction_init_qn_index_sf

```

<Interactions: procedures>+≡

```

subroutine interaction_init_qn_index_trivial (int)
  class(interaction_t), intent(inout) :: int
  call int%qn_index%init (int)
end subroutine interaction_init_qn_index_trivial

subroutine interaction_init_qn_index_involved (int, qn_flv, n_sub, qn_hel)
  class(interaction_t), intent(inout) :: int
  type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
  integer, intent(in) :: n_sub
  type(quantum_numbers_t), dimension(:, :), intent(in), optional :: qn_hel
  call int%qn_index%init (int, qn_flv, n_sub, qn_hel)
end subroutine interaction_init_qn_index_involved

subroutine interaction_init_qn_index_sf (int, qn_flv, n_flv_born, n_flv_real)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: n_flv_born, n_flv_real
  type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_flv
  call int%qn_index%init (int, qn_flv, n_flv_born, n_flv_real)
end subroutine interaction_init_qn_index_sf

```

<Interactions: interaction: TBP>+≡

```

procedure :: set_qn_index_helicity_flip => interaction_set_qn_index_helicity_flip

```

<Interactions: procedures>+≡

```

subroutine interaction_set_qn_index_helicity_flip (int, yorn)
  class(interaction_t), intent(inout) :: int
  logical, intent(in) :: yorn
  call int%qn_index%set_helicity_flip (yorn)
end subroutine interaction_set_qn_index_helicity_flip

```

<Interactions: interaction: TBP>+≡

```

procedure :: get_qn_index => interaction_get_qn_index
procedure :: get_sf_qn_index_born => interaction_get_sf_qn_index_born
procedure :: get_sf_qn_index_real => interaction_get_sf_qn_index_real

```

<Interactions: procedures>+≡

```

integer function interaction_get_qn_index (int, i_flv, i_hel, i_sub) result (index)
  class(interaction_t), intent(in) :: int
  integer, intent(in) :: i_flv
  integer, intent(in), optional :: i_hel
  integer, intent(in), optional :: i_sub
  index = int%qn_index%get_index (i_flv, i_hel, i_sub)
end function interaction_get_qn_index

integer function interaction_get_sf_qn_index_born (int, i_born, i_sub) result (index)
  class(interaction_t), intent(in) :: int
  integer, intent(in) :: i_born, i_sub
  index = int%qn_index%get_sf_index_born (i_born, i_sub)
end function interaction_get_sf_qn_index_born

integer function interaction_get_sf_qn_index_real (int, i_real, i_sub) result (index)
  class(interaction_t), intent(in) :: int
  integer, intent(in) :: i_real, i_sub

```

```

        index = int%qn_index%get_sf_index_real (i_real, i_sub)
    end function interaction_get_sf_qn_index_real

```

<Interactions: interaction: TBP>+≡

```

    procedure :: get_qn_index_n_flv => interaction_get_qn_index_n_flv
    procedure :: get_qn_index_n_hel => interaction_get_qn_index_n_hel
    procedure :: get_qn_index_n_sub => interaction_get_qn_index_n_sub

```

<Interactions: procedures>+≡

```

    integer function interaction_get_qn_index_n_flv (int) result (index)
        class(interaction_t), intent(in) :: int
        index = int%qn_index%get_n_flv ()
    end function interaction_get_qn_index_n_flv

```

```

    integer function interaction_get_qn_index_n_hel (int) result (index)
        class(interaction_t), intent(in) :: int
        index = int%qn_index%get_n_hel ()
    end function interaction_get_qn_index_n_hel

```

```

    integer function interaction_get_qn_index_n_sub (int) result (index)
        class(interaction_t), intent(in) :: int
        index = int%qn_index%get_n_sub ()
    end function interaction_get_qn_index_n_sub

```

Set or create a unique tag for the interaction. Without interaction, reset the tag counter.

<Interactions: procedures>+≡

```

    subroutine interaction_set_tag (int, tag)
        type(interaction_t), intent(inout), optional :: int
        integer, intent(in), optional :: tag
        integer, save :: stored_tag = 1
        if (present (int)) then
            if (present (tag)) then
                int%tag = tag
            else
                int%tag = stored_tag
                stored_tag = stored_tag + 1
            end if
        else if (present (tag)) then
            stored_tag = tag
        else
            stored_tag = 1
        end if
    end subroutine interaction_set_tag

```

The public interface for the previous procedure only covers the reset functionality.

<Interactions: public>+≡

```

    public :: reset_interaction_counter

```

<Interactions: procedures>+≡

```

    subroutine reset_interaction_counter (tag)
        integer, intent(in), optional :: tag

```

```

        call interaction_set_tag (tag=tag)
    end subroutine reset_interaction_counter

```

Finalizer: The state-matrix object contains pointers.

```

<Interactions: interaction: TBP>+≡
    procedure :: final => interaction_final

<Interactions: procedures>+≡
    subroutine interaction_final (object)
        class(interaction_t), intent(inout) :: object
        call object%state_matrix%final ()
    end subroutine interaction_final

```

Output. The **verbose** option refers to the state matrix output.

```

<Interactions: interaction: TBP>+≡
    procedure :: basic_write => interaction_write

<Interactions: procedures>+≡
    subroutine interaction_write &
        (int, unit, verbose, show_momentum_sum, show_mass, show_state, &
         col_verbose, testflag)
        class(interaction_t), intent(in) :: int
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: show_state, col_verbose, testflag
        integer :: u
        integer :: i, index_link
        type(interaction_t), pointer :: int_link
        logical :: show_st
        u = given_output_unit (unit); if (u < 0) return
        show_st = .true.; if (present (show_state)) show_st = show_state
        if (int%tag /= 0) then
            write (u, "(1x,A,I0)") "Interaction: ", int%tag
            do i = 1, int%n_tot
                if (i == 1 .and. int%n_in > 0) then
                    write (u, "(1x,A)") "Incoming:"
                else if (i == int%n_in + 1 .and. int%n_vir > 0) then
                    write (u, "(1x,A)") "Virtual:"
                else if (i == int%n_in + int%n_vir + 1 .and. int%n_out > 0) then
                    write (u, "(1x,A)") "Outgoing:"
                end if
                write (u, "(1x,A,1x,I0)", advance="no") "Particle", i
                if (allocated (int%resonant)) then
                    if (int%resonant(i)) then
                        write (u, "(A)") "[r]"
                    else
                        write (u, *)
                    end if
                else
                    write (u, *)
                end if
            end do
            if (allocated (int%p)) then
                if (int%p_is_known(i)) then
                    call vector4_write (int%p(i), u, show_mass, testflag)
                end if
            end if
        end if
    end subroutine interaction_write

```

```

        else
            write (u, "(A)") " [momentum undefined]"
        end if
    else
        write (u, "(A)") " [momentum not allocated]"
    end if
    if (allocated (int%mask)) then
        write (u, "(1x,A)", advance="no") "mask [fch] = "
        call int%mask(i)%write (u)
        write (u, *)
    end if
    if (int%parents(i)%has_entries () &
        .or. int%children(i)%has_entries ()) then
        write (u, "(1x,A)", advance="no") "internal links:"
        call int%parents(i)%write (u)
        if (int%parents(i)%has_entries ()) &
            write (u, "(1x,A)", advance="no") "=>"
        write (u, "(1x,A)", advance="no") "X"
        if (int%children(i)%has_entries ()) &
            write (u, "(1x,A)", advance="no") "=>"
        call int%children(i)%write (u)
        write (u, *)
    end if
    if (allocated (int%hel_lock)) then
        if (int%hel_lock(i) /= 0) then
            write (u, "(1x,A,1x,I0)") "helicity lock:", int%hel_lock(i)
        end if
    end if
    if (external_link_is_set (int%source(i))) then
        write (u, "(1x,A)", advance="no") "source:"
        int_link => external_link_get_ptr (int%source(i))
        index_link = external_link_get_index (int%source(i))
        write (u, "(1x,'(,I0,)',I0)", advance="no") &
            int_link%tag, index_link
        write (u, *)
    end if
end do
if (present (show_momentum_sum)) then
    if (allocated (int%p) .and. show_momentum_sum) then
        write (u, "(1x,A)") "Incoming particles (sum):"
        call vector4_write &
            (sum (int%p(1 : int%n_in)), u, show_mass = show_mass)
        write (u, "(1x,A)") "Outgoing particles (sum):"
        call vector4_write &
            (sum (int%p(int%n_in + int%n_vir + 1 : )), &
                u, show_mass = show_mass)
        write (u, *)
    end if
end if
if (show_st) then
    call int%write_state_matrix (write_value_list = verbose, &
        verbose = verbose, unit = unit, col_verbose = col_verbose, &
        testflag = testflag)
end if

```

```

    else
        write (u, "(1x,A)") "Interaction: [empty]"
    end if
end subroutine interaction_write

```

<Interactions: interaction: TBP>+≡

```

    procedure :: write_state_matrix => interaction_write_state_matrix

```

<Interactions: procedures>+≡

```

    subroutine interaction_write_state_matrix (int, unit, write_value_list, &
        verbose, col_verbose, testflag)
        class(interaction_t), intent(in) :: int
        logical, intent(in), optional :: write_value_list, verbose, col_verbose
        logical, intent(in), optional :: testflag
        integer, intent(in), optional :: unit
        call int%state_matrix%write (write_value_list = verbose, &
            verbose = verbose, unit = unit, col_verbose = col_verbose, &
            testflag = testflag)
    end subroutine interaction_write_state_matrix

```

Reduce the `state_matrix` over the quantum mask. During the reduce procedure the iterator does not conserve the order of the matrix element respective their quantum numbers. Setting the `keep_order` results in a reorder state matrix with reintroduced matrix element indices.

<Interactions: interaction: TBP>+≡

```

    procedure :: reduce_state_matrix => interaction_reduce_state_matrix

```

<Interactions: procedures>+≡

```

    subroutine interaction_reduce_state_matrix (int, qn_mask, keep_order)
        class(interaction_t), intent(inout) :: int
        type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask
        logical, optional, intent(in) :: keep_order
        type(state_matrix_t) :: state
        logical :: opt_keep_order
        opt_keep_order = .false.
        if (present (keep_order)) opt_keep_order = keep_order
        call int%state_matrix%reduce (qn_mask, state, keep_me_index = keep_order)
        int%state_matrix = state
        if (opt_keep_order) then
            call int%state_matrix%reorder_me (state)
            int%state_matrix = state
        end if
    end subroutine interaction_reduce_state_matrix

```

Assignment: We implement this as a deep copy. This applies, in particular, to the state-matrix and internal-link components. Furthermore, the new interaction acquires a new tag.

<Interactions: public>+≡

```

    public :: assignment(=)

```

<Interactions: interfaces>≡

```

    interface assignment(=)
        module procedure interaction_assign
    end interface

```

```
end interface
```

(*Interactions: procedures*)+=

```
subroutine interaction_assign (int_out, int_in)
  type(interaction_t), intent(out) :: int_out
  type(interaction_t), intent(in), target :: int_in
  call interaction_set_tag (int_out)
  int_out%state_matrix = int_in%state_matrix
  int_out%n_in = int_in%n_in
  int_out%n_out = int_in%n_out
  int_out%n_vir = int_in%n_vir
  int_out%n_tot = int_in%n_tot
  if (allocated (int_in%p_is_known)) then
    allocate (int_out%p_is_known (size (int_in%p_is_known)))
    int_out%p_is_known = int_in%p_is_known
  end if
  if (allocated (int_in%p)) then
    allocate (int_out%p (size (int_in%p)))
    int_out%p = int_in%p
  end if
  if (allocated (int_in%source)) then
    allocate (int_out%source (size (int_in%source)))
    int_out%source = int_in%source
  end if
  if (allocated (int_in%parents)) then
    allocate (int_out%parents (size (int_in%parents)))
    int_out%parents = int_in%parents
  end if
  if (allocated (int_in%children)) then
    allocate (int_out%children (size (int_in%children)))
    int_out%children = int_in%children
  end if
  if (allocated (int_in%resonant)) then
    allocate (int_out%resonant (size (int_in%resonant)))
    int_out%resonant = int_in%resonant
  end if
  if (allocated (int_in%mask)) then
    allocate (int_out%mask (size (int_in%mask)))
    int_out%mask = int_in%mask
  end if
  if (allocated (int_in%hel_lock)) then
    allocate (int_out%hel_lock (size (int_in%hel_lock)))
    int_out%hel_lock = int_in%hel_lock
  end if
  int_out%update_state_matrix = int_in%update_state_matrix
  int_out%update_values = int_in%update_values
end subroutine interaction_assign
```

12.2.4 Methods inherited from the state matrix member

Until F2003 is standard, we cannot implement inheritance directly. Therefore, we need wrappers for “inherited” methods.

Make a new branch in the state matrix if it does not yet exist. This is not just a wrapper but it introduces the interaction mask: where a quantum number is masked, it is not transferred but set undefined. After this, the value array has to be updated.

```

<Interactions: interaction: TBP>+≡
  procedure :: add_state => interaction_add_state

<Interactions: procedures>+≡
  subroutine interaction_add_state &
    (int, qn, index, value, sum_values, counter_index, ignore_sub_for_qn, me_index)
    class(interaction_t), intent(inout) :: int
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    integer, intent(in), optional :: index
    complex(default), intent(in), optional :: value
    logical, intent(in), optional :: sum_values
    integer, intent(in), optional :: counter_index
    logical, intent(in), optional :: ignore_sub_for_qn
    integer, intent(out), optional :: me_index
    type(quantum_numbers_t), dimension(size(qn)) :: qn_tmp
    qn_tmp = qn
    call qn_tmp%undefine (int%mask)
    call int%state_matrix%add_state (qn_tmp, index, value, sum_values, &
      counter_index, ignore_sub_for_qn, me_index)
    int%update_values = .true.
  end subroutine interaction_add_state

<Interactions: interaction: TBP>+≡
  procedure :: set_duplicate_flv_zero => interaction_set_duplicate_flv_zero

<Interactions: procedures>+≡
  subroutine interaction_set_duplicate_flv_zero (int)
    class(interaction_t), intent(inout) :: int
    call int%state_matrix%set_duplicate_flv_zero ()
  end subroutine interaction_set_duplicate_flv_zero

```

Freeze the quantum state: First collapse the quantum state, i.e., remove quantum numbers if any mask has changed, then fix the array of value pointers.

```

<Interactions: interaction: TBP>+≡
  procedure :: freeze => interaction_freeze

<Interactions: procedures>+≡
  subroutine interaction_freeze (int)
    class(interaction_t), intent(inout) :: int
    if (int%update_state_matrix) then
      call int%state_matrix%collapse (int%mask)
      int%update_state_matrix = .false.
      int%update_values = .true.
    end if
    if (int%update_values) then
      call int%state_matrix%freeze ()
      int%update_values = .false.
    end if
  end subroutine interaction_freeze

```


Return true if the state matrix is empty.

```

<Interactions: interaction: TBP>+≡
  procedure :: is_empty => interaction_is_empty

<Interactions: procedures>+≡
  pure function interaction_is_empty (int) result (flag)
    logical :: flag
    class(interaction_t), intent(in) :: int
    flag = int%state_matrix%is_empty ()
  end function interaction_is_empty

```

Get the number of values stored in the state matrix:

```

<Interactions: interaction: TBP>+≡
  procedure :: get_n_matrix_elements => &
    interaction_get_n_matrix_elements

<Interactions: procedures>+≡
  pure function interaction_get_n_matrix_elements (int) result (n)
    integer :: n
    class(interaction_t), intent(in) :: int
    n = int%state_matrix%get_n_matrix_elements ()
  end function interaction_get_n_matrix_elements

```

```

<Interactions: interaction: TBP>+≡
  procedure :: get_state_depth => interaction_get_state_depth

```

```

<Interactions: procedures>+≡
  function interaction_get_state_depth (int) result (n)
    integer :: n
    class(interaction_t), intent(in) :: int
    n = int%state_matrix%get_depth ()
  end function interaction_get_state_depth

```

```

<Interactions: interaction: TBP>+≡
  procedure :: get_n_in_helicities => interaction_get_n_in_helicities

```

```

<Interactions: procedures>+≡
  function interaction_get_n_in_helicities (int) result (n_hel)
    integer :: n_hel
    class(interaction_t), intent(in) :: int
    type(interaction_t) :: int_copy
    type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    integer :: i
    allocate (qn_mask (int%n_tot))
    do i = 1, int%n_tot
      if (i <= int%n_in) then
        call qn_mask(i)%init (.true., .true., .false.)
      else
        call qn_mask(i)%init (.true., .true., .true.)
      end if
    end do
    int_copy = int
    call int_copy%set_mask (qn_mask)
  end function interaction_get_n_in_helicities

```

```

call int_copy%freeze ()
allocate (qn (int_copy%state_matrix%get_n_matrix_elements (), &
            int_copy%state_matrix%get_depth ()))
qn = int_copy%get_quantum_numbers ()
n_hel = 0
do i = 1, size (qn, dim=1)
    if (all (qn(:, i)%get_subtraction_index () == 0)) n_hel = n_hel + 1
end do
call int_copy%final ()
deallocate (qn_mask)
deallocate (qn)
end function interaction_get_n_in_helicities

```

Get the size of the me-array of the associated state matrix for debugging purposes

```

<Interactions: interaction: TBP>+≡
    procedure :: get_me_size => interaction_get_me_size

<Interactions: procedures>+≡
    pure function interaction_get_me_size (int) result (n)
        integer :: n
        class(interaction_t), intent(in) :: int
        n = int%state_matrix%get_me_size ()
    end function interaction_get_me_size

```

Get the norm of the state matrix (if the norm has been taken out, otherwise this would be unity).

```

<Interactions: interaction: TBP>+≡
    procedure :: get_norm => interaction_get_norm

<Interactions: procedures>+≡
    pure function interaction_get_norm (int) result (norm)
        real(default) :: norm
        class(interaction_t), intent(in) :: int
        norm = int%state_matrix%get_norm ()
    end function interaction_get_norm

```

```

<Interactions: interaction: TBP>+≡
    procedure :: get_n_sub => interaction_get_n_sub

<Interactions: procedures>+≡
    function interaction_get_n_sub (int) result (n_sub)
        integer :: n_sub
        class(interaction_t), intent(in) :: int
        n_sub = int%state_matrix%get_n_sub ()
    end function interaction_get_n_sub

```

Get the quantum number array that corresponds to a given index.

```

<Interactions: interaction: TBP>+≡
    generic :: get_quantum_numbers => get_quantum_numbers_single, &
        get_quantum_numbers_all, &
        get_quantum_numbers_all_qn_mask

    procedure :: get_quantum_numbers_single => &
        interaction_get_quantum_numbers_single

```

```

procedure :: get_quantum_numbers_all => &
    interaction_get_quantum_numbers_all
procedure :: get_quantum_numbers_all_qn_mask => &
    interaction_get_quantum_numbers_all_qn_mask

<Interactions: procedures>+≡
function interaction_get_quantum_numbers_single (int, i, by_me_index) result (qn)
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    class(interaction_t), intent(in), target :: int
    integer, intent(in) :: i
    logical, intent(in), optional :: by_me_index
    allocate (qn (int%state_matrix%get_depth ()))
    qn = int%state_matrix%get_quantum_number (i, by_me_index)
end function interaction_get_quantum_numbers_single

function interaction_get_quantum_numbers_all (int) result (qn)
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    class(interaction_t), intent(in), target :: int
    integer :: i
    <Interactions: get quantum numbers all>
<Interactions: get quantum numbers all>≡
    allocate (qn (int%state_matrix%get_depth(), &
        int%state_matrix%get_n_matrix_elements ()))
    do i = 1, int%state_matrix%get_n_matrix_elements ()
        qn (:, i) = int%state_matrix%get_quantum_number (i)
    end do

<Interactions: procedures>+≡
end function interaction_get_quantum_numbers_all

function interaction_get_quantum_numbers_all_qn_mask (int, qn_mask) &
    result (qn)
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    class(interaction_t), intent(in) :: int
    type(quantum_numbers_mask_t), intent(in) :: qn_mask
    integer :: n_redundant, n_all, n_me
    integer :: i
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn_all
    <Interactions: get quantum numbers all qn mask>
<Interactions: get quantum numbers all qn mask>≡
    call int%state_matrix%get_quantum_numbers (qn_all)
    n_redundant = count (qn_all%are_redundant (qn_mask))
    n_all = size (qn_all)
    !!! Number of matrix elements = survivors / n_particles
    n_me = (n_all - n_redundant) / int%state_matrix%get_depth ()
    allocate (qn (int%state_matrix%get_depth(), n_me))
    do i = 1, n_me
        if (.not. any (qn_all(i, :)%are_redundant (qn_mask))) &
            qn (:, i) = qn_all (i, :)
    end do

<Interactions: procedures>+≡
end function interaction_get_quantum_numbers_all_qn_mask

```

```

<Interactions: interaction: TBP>+≡
  procedure :: get_quantum_numbers_all_sub => interaction_get_quantum_numbers_all_sub

<Interactions: procedures>+≡
  subroutine interaction_get_quantum_numbers_all_sub (int, qn)
    class(interaction_t), intent(in) :: int
    type(quantum_numbers_t), dimension(:,:), allocatable, intent(out) :: qn
    integer :: i
  <Interactions: get quantum numbers all>
  end subroutine interaction_get_quantum_numbers_all_sub

<Interactions: interaction: TBP>+≡
  procedure :: get_flavors => interaction_get_flavors

<Interactions: procedures>+≡
  subroutine interaction_get_flavors (int, only_elementary, qn_mask, flv)
    class(interaction_t), intent(in), target :: int
    logical, intent(in) :: only_elementary
    type(quantum_numbers_mask_t), intent(in), dimension(:), optional :: qn_mask
    integer, intent(out), dimension(:,:), allocatable :: flv
    call int%state_matrix%get_flavors (only_elementary, qn_mask, flv)
  end subroutine interaction_get_flavors

<Interactions: interaction: TBP>+≡
  procedure :: get_quantum_numbers_mask => interaction_get_quantum_numbers_mask

<Interactions: procedures>+≡
  subroutine interaction_get_quantum_numbers_mask (int, qn_mask, qn)
    class(interaction_t), intent(in) :: int
    type(quantum_numbers_mask_t), intent(in) :: qn_mask
    type(quantum_numbers_t), dimension(:,:), allocatable, intent(out) :: qn
    integer :: n_redundant, n_all, n_me
    integer :: i
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn_all
  <Interactions: get quantum numbers all qn mask>
  end subroutine interaction_get_quantum_numbers_mask

```

Get the matrix element that corresponds to a set of quantum numbers, a given index, or return the whole array.

```

<Interactions: interaction: TBP>+≡
  generic :: get_matrix_element => get_matrix_element_single
  generic :: get_matrix_element => get_matrix_element_array
  procedure :: get_matrix_element_single => &
    interaction_get_matrix_element_single
  procedure :: get_matrix_element_array => &
    interaction_get_matrix_element_array

<Interactions: procedures>+≡
  elemental function interaction_get_matrix_element_single (int, i) result (me)
    complex(default) :: me
    class(interaction_t), intent(in) :: int
    integer, intent(in) :: i
    me = int%state_matrix%get_matrix_element (i)
  end function interaction_get_matrix_element_single

```

<Interactions: procedures>+≡

```
function interaction_get_matrix_element_array (int) result (me)
  complex(default), dimension(:), allocatable :: me
  class(interaction_t), intent(in) :: int
  allocate (me (int%get_n_matrix_elements ()))
  me = int%state_matrix%get_matrix_element ( )
end function interaction_get_matrix_element_array
```

Set the complex value(s) stored in the quantum state.

<Interactions: interaction: TBP>+≡

```
generic :: set_matrix_element => interaction_set_matrix_element_qn, &
  interaction_set_matrix_element_all, &
  interaction_set_matrix_element_array, &
  interaction_set_matrix_element_single, &
  interaction_set_matrix_element_clone
procedure :: interaction_set_matrix_element_qn
procedure :: interaction_set_matrix_element_all
procedure :: interaction_set_matrix_element_array
procedure :: interaction_set_matrix_element_single
procedure :: interaction_set_matrix_element_clone
```

Indirect access via the quantum number array:

<Interactions: procedures>+≡

```
subroutine interaction_set_matrix_element_qn (int, qn, val)
  class(interaction_t), intent(inout) :: int
  type(quantum_numbers_t), dimension(:), intent(in) :: qn
  complex(default), intent(in) :: val
  call int%state_matrix%set_matrix_element (qn, val)
end subroutine interaction_set_matrix_element_qn
```

Set all entries of the matrix-element array to a given value.

<Interactions: procedures>+≡

```
subroutine interaction_set_matrix_element_all (int, value)
  class(interaction_t), intent(inout) :: int
  complex(default), intent(in) :: value
  call int%state_matrix%set_matrix_element (value)
end subroutine interaction_set_matrix_element_all
```

Set the matrix-element array directly.

<Interactions: procedures>+≡

```
subroutine interaction_set_matrix_element_array (int, value, range)
  class(interaction_t), intent(inout) :: int
  complex(default), intent(in), dimension(:) :: value
  integer, intent(in), dimension(:), optional :: range
  call int%state_matrix%set_matrix_element (value, range)
end subroutine interaction_set_matrix_element_array

pure subroutine interaction_set_matrix_element_single (int, i, value)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  complex(default), intent(in) :: value
  call int%state_matrix%set_matrix_element (i, value)
end subroutine interaction_set_matrix_element_single
```

Clone from another (matching) interaction.

```

<Interactions: procedures>+≡
  subroutine interaction_set_matrix_element_clone (int, int1)
    class(interaction_t), intent(inout) :: int
    class(interaction_t), intent(in) :: int1
    call int%state_matrix%set_matrix_element (int1%state_matrix)
  end subroutine interaction_set_matrix_element_clone

```

```

<Interactions: interaction: TBP>+≡
  procedure :: set_only_matrix_element => interaction_set_only_matrix_element

```

```

<Interactions: procedures>+≡
  subroutine interaction_set_only_matrix_element (int, i, value)
    class(interaction_t), intent(inout) :: int
    integer, intent(in) :: i
    complex(default), intent(in) :: value
    call int%set_matrix_element (cmplx (0, 0, default))
    call int%set_matrix_element (i, value)
  end subroutine interaction_set_only_matrix_element

```

```

<Interactions: interaction: TBP>+≡
  procedure :: add_to_matrix_element => interaction_add_to_matrix_element

```

```

<Interactions: procedures>+≡
  subroutine interaction_add_to_matrix_element (int, qn, value, match_only_flavor)
    class(interaction_t), intent(inout) :: int
    type(quantum_numbers_t), dimension(:), intent(in) :: qn
    complex(default), intent(in) :: value
    logical, intent(in), optional :: match_only_flavor
    call int%state_matrix%add_to_matrix_element (qn, value, match_only_flavor)
  end subroutine interaction_add_to_matrix_element

```

Get the indices of any diagonal matrix elements.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_diagonal_entries => interaction_get_diagonal_entries

```

```

<Interactions: procedures>+≡
  subroutine interaction_get_diagonal_entries (int, i)
    class(interaction_t), intent(in) :: int
    integer, dimension(:), allocatable, intent(out) :: i
    call int%state_matrix%get_diagonal_entries (i)
  end subroutine interaction_get_diagonal_entries

```

Renormalize the state matrix by its trace, if nonzero. The renormalization is reflected in the state-matrix norm.

```

<Interactions: interaction: TBP>+≡
  procedure :: normalize_by_trace => interaction_normalize_by_trace

```

```

<Interactions: procedures>+≡
  subroutine interaction_normalize_by_trace (int)
    class(interaction_t), intent(inout) :: int
    call int%state_matrix%normalize_by_trace ()
  end subroutine interaction_normalize_by_trace

```

Analogous, but renormalize by maximal (absolute) value.

```

<Interactions: interaction: TBP>+≡
  procedure :: normalize_by_max => interaction_normalize_by_max

<Interactions: procedures>+≡
  subroutine interaction_normalize_by_max (int)
    class(interaction_t), intent(inout) :: int
    call int%state_matrix%normalize_by_max ()
  end subroutine interaction_normalize_by_max

```

Explicitly set the norm value (of the state matrix).

```

<Interactions: interaction: TBP>+≡
  procedure :: set_norm => interaction_set_norm

<Interactions: procedures>+≡
  subroutine interaction_set_norm (int, norm)
    class(interaction_t), intent(inout) :: int
    real(default), intent(in) :: norm
    call int%state_matrix%set_norm (norm)
  end subroutine interaction_set_norm

```

```

<Interactions: interaction: TBP>+≡
  procedure :: set_state_matrix => interaction_set_state_matrix

<Interactions: procedures>+≡
  subroutine interaction_set_state_matrix (int, state)
    class(interaction_t), intent(inout) :: int
    type(state_matrix_t), intent(in) :: state
    int%state_matrix = state
  end subroutine interaction_set_state_matrix

```

Return the maximum absolute value of color indices.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_max_color_value => &
    interaction_get_max_color_value

<Interactions: procedures>+≡
  function interaction_get_max_color_value (int) result (cmax)
    class(interaction_t), intent(in) :: int
    integer :: cmax
    cmax = int%state_matrix%get_max_color_value ()
  end function interaction_get_max_color_value

```

Factorize the state matrix into single-particle state matrices, the branch selection depending on a (random) value between 0 and 1; optionally also return a correlated state matrix.

```

<Interactions: interaction: TBP>+≡
  procedure :: factorize => interaction_factorize

```

```

<Interactions: procedures>+=
  subroutine interaction_factorize &
    (int, mode, x, ok, single_state, correlated_state, qn_in)
    class(interaction_t), intent(in), target :: int
    integer, intent(in) :: mode
    real(default), intent(in) :: x
    logical, intent(out) :: ok
    type(state_matrix_t), &
      dimension(:), allocatable, intent(out) :: single_state
    type(state_matrix_t), intent(out), optional :: correlated_state
    type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_in
    call int%state_matrix%factorize &
      (mode, x, ok, single_state, correlated_state, qn_in)
  end subroutine interaction_factorize

```

Sum all matrix element values

```

<Interactions: interaction: TBP>+=
  procedure :: sum => interaction_sum

<Interactions: procedures>+=
  function interaction_sum (int) result (value)
    class(interaction_t), intent(in) :: int
    complex(default) :: value
    value = int%state_matrix%sum ()
  end function interaction_sum

```

Append new states which are color-contracted versions of the existing states. The matrix element index of each color contraction coincides with the index of its origin, so no new matrix elements are generated. After this operation, no `freeze` must be performed anymore.

```

<Interactions: interaction: TBP>+=
  procedure :: add_color_contractions => &
    interaction_add_color_contractions

<Interactions: procedures>+=
  subroutine interaction_add_color_contractions (int)
    class(interaction_t), intent(inout) :: int
    call int%state_matrix%add_color_contractions ()
  end subroutine interaction_add_color_contractions

```

Multiply matrix elements from two interactions. Choose the elements as given by the integer index arrays, multiply them and store the sum of products in the indicated matrix element. The suffixes mean: c=conjugate first factor; f=include weighting factor.

```

<Interactions: interaction: TBP>+=
  procedure :: evaluate_product => interaction_evaluate_product
  procedure :: evaluate_product_cf => interaction_evaluate_product_cf
  procedure :: evaluate_square_c => interaction_evaluate_square_c
  procedure :: evaluate_sum => interaction_evaluate_sum
  procedure :: evaluate_me_sum => interaction_evaluate_me_sum

```


(Interactions: procedures)+≡

```

pure subroutine interaction_evaluate_product &
  (int, i, int1, int2, index1, index2)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(in) :: int1, int2
  integer, dimension(:), intent(in) :: index1, index2
  call int%state_matrix%evaluate_product &
    (i, int1%state_matrix, int2%state_matrix, &
     index1, index2)
end subroutine interaction_evaluate_product

pure subroutine interaction_evaluate_product_cf &
  (int, i, int1, int2, index1, index2, factor)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(in) :: int1, int2
  integer, dimension(:), intent(in) :: index1, index2
  complex(default), dimension(:), intent(in) :: factor
  call int%state_matrix%evaluate_product_cf &
    (i, int1%state_matrix, int2%state_matrix, &
     index1, index2, factor)
end subroutine interaction_evaluate_product_cf

pure subroutine interaction_evaluate_square_c (int, i, int1, index1)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(in) :: int1
  integer, dimension(:), intent(in) :: index1
  call int%state_matrix%evaluate_square_c (i, int1%state_matrix, index1)
end subroutine interaction_evaluate_square_c

pure subroutine interaction_evaluate_sum (int, i, int1, index1)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(in) :: int1
  integer, dimension(:), intent(in) :: index1
  call int%state_matrix%evaluate_sum (i, int1%state_matrix, index1)
end subroutine interaction_evaluate_sum

pure subroutine interaction_evaluate_me_sum (int, i, int1, index1)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(in) :: int1
  integer, dimension(:), intent(in) :: index1
  call int%state_matrix%evaluate_me_sum (i, int1%state_matrix, index1)
end subroutine interaction_evaluate_me_sum

```

Tag quantum numbers of the state matrix as part of the hard process, according to the indices specified in *tag*. If no *tag* is given, all quantum numbers are tagged as part of the hard process.

(Interactions: interaction: TBP)+≡

```

procedure :: tag_hard_process => interaction_tag_hard_process

```

```

<Interactions: procedures>+≡
subroutine interaction_tag_hard_process (int, tag)
  class(interaction_t), intent(inout) :: int
  integer, dimension(:), intent(in), optional :: tag
  type(state_matrix_t) :: state
  call int%state_matrix%tag_hard_process (state, tag)
  call int%state_matrix%final ()
  int%state_matrix = state
end subroutine interaction_tag_hard_process

```

Modify hard-interaction flags at the specified particle-position, in-place.

```

<Interactions: interaction: TBP>+≡
  procedure :: retag_hard_process => interaction_retag_hard_process

<Interactions: procedures>+≡
subroutine interaction_retag_hard_process (int, i, hard)
  class(interaction_t), intent(inout), target :: int
  integer, intent(in) :: i
  logical, intent(in) :: hard
  type(state_iterator_t) :: it
  call it%init (int%get_state_matrix_ptr ())
  do while (it%is_valid ())
    call it%retag_hard_process (i, hard)
    call it%advance ()
  end do
end subroutine interaction_retag_hard_process

```

12.2.5 Accessing contents

Return the integer tag.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_tag => interaction_get_tag

<Interactions: procedures>+≡
function interaction_get_tag (int) result (tag)
  class(interaction_t), intent(in) :: int
  integer :: tag
  tag = int%tag
end function interaction_get_tag

```

Return the number of particles.

```

<Interactions: interaction: TBP>+≡
  procedure :: get_n_tot => interaction_get_n_tot
  procedure :: get_n_in => interaction_get_n_in
  procedure :: get_n_vir => interaction_get_n_vir
  procedure :: get_n_out => interaction_get_n_out

<Interactions: procedures>+≡
pure function interaction_get_n_tot (object) result (n_tot)
  class(interaction_t), intent(in) :: object
  integer :: n_tot
  n_tot = object%n_tot

```

```

end function interaction_get_n_tot

pure function interaction_get_n_in (object) result (n_in)
  class(interaction_t), intent(in) :: object
  integer :: n_in
  n_in = object%n_in
end function interaction_get_n_in

pure function interaction_get_n_vir (object) result (n_vir)
  class(interaction_t), intent(in) :: object
  integer :: n_vir
  n_vir = object%n_vir
end function interaction_get_n_vir

pure function interaction_get_n_out (object) result (n_out)
  class(interaction_t), intent(in) :: object
  integer :: n_out
  n_out = object%n_out
end function interaction_get_n_out

```

Return a momentum index. The flags specify whether to keep/drop incoming, virtual, or outgoing momenta. Check for illegal values.

(Interactions: procedures)+≡

```

function idx (int, i, outgoing)
  integer :: idx
  type(interaction_t), intent(in) :: int
  integer, intent(in) :: i
  logical, intent(in), optional :: outgoing
  logical :: in, vir, out
  if (present (outgoing)) then
    in = .not. outgoing
    vir = .false.
    out = outgoing
  else
    in = .true.
    vir = .true.
    out = .true.
  end if
  idx = 0
  if (in) then
    if (vir) then
      if (out) then
        if (i <= int%n_tot) idx = i
      else
        if (i <= int%n_in + int%n_vir) idx = i
      end if
    else if (out) then
      if (i <= int%n_in) then
        idx = i
      else if (i <= int%n_in + int%n_out) then
        idx = int%n_vir + i
      end if
    else

```

```

        if (i <= int%n_in) idx = i
    end if
    else if (vir) then
        if (out) then
            if (i <= int%n_vir + int%n_out) idx = int%n_in + i
        else
            if (i <= int%n_vir) idx = int%n_in + i
        end if
    else if (out) then
        if (i <= int%n_out) idx = int%n_in + int%n_vir + i
    end if
    if (idx == 0) then
        call int%basic_write ()
        print *, i, in, vir, out
        call msg_bug (" Momentum index is out of range for this interaction")
    end if
end function idx

```

Return all or just a specific four-momentum.

(Interactions: interaction: TBP)+≡

```

generic :: get_momenta => get_momenta_all, get_momenta_idx
procedure :: get_momentum => interaction_get_momentum
procedure :: get_momenta_all => interaction_get_momenta_all
procedure :: get_momenta_idx => interaction_get_momenta_idx

```

(Interactions: procedures)+≡

```

function interaction_get_momenta_all (int, outgoing) result (p)
    class(interaction_t), intent(in) :: int
    type(vector4_t), dimension(:), allocatable :: p
    logical, intent(in), optional :: outgoing
    integer :: i
    if (present (outgoing)) then
        if (outgoing) then
            allocate (p (int%n_out))
        else
            allocate (p (int%n_in))
        end if
    else
        allocate (p (int%n_tot))
    end if
    do i = 1, size (p)
        p(i) = int%p(idx (int, i, outgoing))
    end do
end function interaction_get_momenta_all

function interaction_get_momenta_idx (int, jj) result (p)
    class(interaction_t), intent(in) :: int
    type(vector4_t), dimension(:), allocatable :: p
    integer, dimension(:), intent(in) :: jj
    allocate (p (size (jj)))
    p = int%p(jj)
end function interaction_get_momenta_idx

function interaction_get_momentum (int, i, outgoing) result (p)

```

```

class(interaction_t), intent(in) :: int
type(vector4_t) :: p
integer, intent(in) :: i
logical, intent(in), optional :: outgoing
p = int%p(idx (int, i, outgoing))
end function interaction_get_momentum

```

Return a shallow copy of the state matrix:

```

<Interactions: interaction: TBP>+≡
  procedure :: get_state_matrix_ptr => &
    interaction_get_state_matrix_ptr

<Interactions: procedures>+≡
  function interaction_get_state_matrix_ptr (int) result (state)
    class(interaction_t), intent(in), target :: int
    type(state_matrix_t), pointer :: state
    state => int%state_matrix
  end function interaction_get_state_matrix_ptr

```

Return the array of resonance flags

```

<Interactions: interaction: TBP>+≡
  procedure :: get_resonance_flags => interaction_get_resonance_flags

<Interactions: procedures>+≡
  function interaction_get_resonance_flags (int) result (resonant)
    class(interaction_t), intent(in) :: int
    logical, dimension(size(int%resonant)) :: resonant
    resonant = int%resonant
  end function interaction_get_resonance_flags

```

Return the quantum-numbers mask (or part of it)

```

<Interactions: interaction: TBP>+≡
  generic :: get_mask => get_mask_all, get_mask_slice
  procedure :: get_mask_all => interaction_get_mask_all
  procedure :: get_mask_slice => interaction_get_mask_slice

<Interactions: procedures>+≡
  function interaction_get_mask_all (int) result (mask)
    class(interaction_t), intent(in) :: int
    type(quantum_numbers_mask_t), dimension(size(int%mask)) :: mask
    mask = int%mask
  end function interaction_get_mask_all

  function interaction_get_mask_slice (int, index) result (mask)
    class(interaction_t), intent(in) :: int
    integer, dimension(:), intent(in) :: index
    type(quantum_numbers_mask_t), dimension(size(index)) :: mask
    mask = int%mask(index)
  end function interaction_get_mask_slice

```

Compute the invariant mass squared of the incoming particles (if any, otherwise outgoing).

```

<Interactions: public>+≡
  public :: interaction_get_s

```

```

<Interactions: procedures>+≡
function interaction_get_s (int) result (s)
  real(default) :: s
  type(interaction_t), intent(in) :: int
  if (int%n_in /= 0) then
    s = sum (int%p(:int%n_in)) ** 2
  else
    s = sum (int%p(int%n_vir + 1 : )) ** 2
  end if
end function interaction_get_s

```

Compute the Lorentz transformation that transforms the incoming particles from the center-of-mass frame to the lab frame where they are given. If the c.m. mass squared is negative or zero, return the identity.

```

<Interactions: public>+≡
public :: interaction_get_cm_transformation

<Interactions: procedures>+≡
function interaction_get_cm_transformation (int) result (lt)
  type(lorentz_transformation_t) :: lt
  type(interaction_t), intent(in) :: int
  type(vector4_t) :: p_cm
  real(default) :: s
  if (int%n_in /= 0) then
    p_cm = sum (int%p(:int%n_in))
  else
    p_cm = sum (int%p(int%n_vir+1:))
  end if
  s = p_cm ** 2
  if (s > 0) then
    lt = boost (p_cm, sqrt (s))
  else
    lt = identity
  end if
end function interaction_get_cm_transformation

```

Return flavor, momentum, and position of the first outgoing unstable particle present in the interaction. Note that we need not iterate through the state matrix; if there is an unstable particle, it will be present in all state-matrix entries.

```

<Interactions: public>+≡
public :: interaction_get_unstable_particle

<Interactions: procedures>+≡
subroutine interaction_get_unstable_particle (int, flv, p, i)
  type(interaction_t), intent(in), target :: int
  type(flavor_t), intent(out) :: flv
  type(vector4_t), intent(out) :: p
  integer, intent(out) :: i
  type(state_iterator_t) :: it
  type(flavor_t), dimension(int%n_tot) :: flv_array
  call it%init (int%state_matrix)
  flv_array = it%get_flavor ()

```

```

do i = int%n_in + int%n_vir + 1, int%n_tot
  if (.not. flv_array(i)%is_stable ()) then
    flv = flv_array(i)
    p = int%p(i)
    return
  end if
end do
end subroutine interaction_get_unstable_particle

```

Return the complete set of *outgoing* flavors, assuming that the flavor quantum number is not suppressed.

```

<Interactions: public>+≡
  public :: interaction_get_flv_out

<Interactions: procedures>+≡
  subroutine interaction_get_flv_out (int, flv)
    type(interaction_t), intent(in), target :: int
    type(flavor_t), dimension(:,:), allocatable, intent(out) :: flv
    type(state_iterator_t) :: it
    type(flavor_t), dimension(:), allocatable :: flv_state
    integer :: n_in, n_vir, n_out, n_tot, n_state, i
    n_in = int%get_n_in ()
    n_vir = int%get_n_vir ()
    n_out = int%get_n_out ()
    n_tot = int%get_n_tot ()
    n_state = int%get_n_matrix_elements ()
    allocate (flv (n_out, n_state))
    allocate (flv_state (n_tot))
    i = 1
    call it%init (int%get_state_matrix_ptr ())
    do while (it%is_valid ())
      flv_state = it%get_flavor ()
      flv(:,i) = flv_state(n_in + n_vir + 1 : )
      i = i + 1
      call it%advance ()
    end do
  end subroutine interaction_get_flv_out

```

Determine the flavor content of the interaction. We analyze the state matrix for this, and we select the outgoing particles of the hard process only for the required mask, which indicates the particles that can appear in any order in a matching event record.

We have to assume that any radiated particles (beam remnants) appear at the beginning of the particles marked as outgoing.

```

<Interactions: public>+≡
  public :: interaction_get_flv_content

<Interactions: procedures>+≡
  subroutine interaction_get_flv_content (int, state_flv, n_out_hard)
    type(interaction_t), intent(in), target :: int
    type(state_flv_content_t), intent(out) :: state_flv
    integer, intent(in) :: n_out_hard
    logical, dimension(:), allocatable :: mask

```

```

integer :: n_tot
n_tot = int%get_n_tot ()
allocate (mask (n_tot), source = .false.)
mask(n_tot-n_out_hard + 1 : ) = .true.
call state_flv%fill (int%get_state_matrix_ptr (), mask)
end subroutine interaction_get_flv_content

```

12.2.6 Modifying contents

Set the quantum numbers mask.

```

<Interactions: interaction: TBP>+≡
  procedure :: set_mask => interaction_set_mask

<Interactions: procedures>+≡
  subroutine interaction_set_mask (int, mask)
    class(interaction_t), intent(inout) :: int
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    if (size (int%mask) /= size (mask)) &
      call msg_fatal ("Attempting to set mask with unfitting size!")
    int%mask = mask
    int%update_state_matrix = .true.
  end subroutine interaction_set_mask

```

Merge a particular mask entry, respecting a possible helicity lock for this entry. We apply an OR relation, which means that quantum numbers are summed over if either of the two masks requires it.

```

<Interactions: procedures>+≡
  subroutine interaction_merge_mask_entry (int, i, mask)
    type(interaction_t), intent(inout) :: int
    integer, intent(in) :: i
    type(quantum_numbers_mask_t), intent(in) :: mask
    type(quantum_numbers_mask_t) :: mask_tmp
    integer :: ii
    ii = idx (int, i)
    if (int%mask(ii) .neqv. mask) then
      int%mask(ii) = int%mask(ii) .or. mask
      if (int%hel_lock(ii) /= 0) then
        call mask_tmp%assign (mask, helicity=.true.)
        int%mask(int%hel_lock(ii)) = int%mask(int%hel_lock(ii)) .or. mask_tmp
      end if
    end if
    int%update_state_matrix = .true.
  end subroutine interaction_merge_mask_entry

```

Fill the momenta array, do not care about the quantum numbers of particles.

```

<Interactions: interaction: TBP>+≡
  procedure :: reset_momenta => interaction_reset_momenta
  procedure :: set_momenta => interaction_set_momenta
  procedure :: set_momentum => interaction_set_momentum

```



```

<Interactions: procedures>+≡
subroutine interaction_reset_momenta (int)
  class(interaction_t), intent(inout) :: int
  int%p = vector4_null
  int%p_is_known = .true.
end subroutine interaction_reset_momenta

subroutine interaction_set_momenta (int, p, outgoing)
  class(interaction_t), intent(inout) :: int
  type(vector4_t), dimension(:), intent(in) :: p
  logical, intent(in), optional :: outgoing
  integer :: i, index
  do i = 1, size (p)
    index = idx (int, i, outgoing)
    int%p(index) = p(i)
    int%p_is_known(index) = .true.
  end do
end subroutine interaction_set_momenta

subroutine interaction_set_momentum (int, p, i, outgoing)
  class(interaction_t), intent(inout) :: int
  type(vector4_t), intent(in) :: p
  integer, intent(in) :: i
  logical, intent(in), optional :: outgoing
  integer :: index
  index = idx (int, i, outgoing)
  int%p(index) = p
  int%p_is_known(index) = .true.
end subroutine interaction_set_momentum

```

This more sophisticated version of setting values is used for structure functions, in particular if nontrivial flavor, color, and helicity may be present: set values selectively for the given flavors. If there is more than one flavor, scan the interaction and check for a matching flavor at the specified particle location. If it matches, insert the value that corresponds to this flavor.

```

<Interactions: public>+≡
public :: interaction_set_flavored_values

<Interactions: procedures>+≡
subroutine interaction_set_flavored_values (int, value, flv_in, pos)
  type(interaction_t), intent(inout) :: int
  complex(default), dimension(:), intent(in) :: value
  type(flavor_t), dimension(:), intent(in) :: flv_in
  integer, intent(in) :: pos
  type(state_iterator_t) :: it
  type(flavor_t) :: flv
  integer :: i
  if (size (value) == 1) then
    call int%set_matrix_element (value(1))
  else
    call it%init (int%state_matrix)
    do while (it%is_valid ())
      flv = it%get_flavor (pos)
      SCAN_FLV: do i = 1, size (value)

```

```

        if (flv == flv_in(i)) then
            call it%set_matrix_element (value(i))
            exit SCAN_FLV
        end if
    end do SCAN_FLV
    call it%advance ()
end do
end if
end subroutine interaction_set_flavored_values

```

12.2.7 Handling Linked interactions

Store relations between corresponding particles within one interaction. The first particle is the parent, the second one the child. Links are established in both directions.

These relations have no effect on the propagation of momenta etc., they are rather used for mother-daughter relations in event output.

```

<Interactions: interaction: TBP>+≡
    procedure :: relate => interaction_relate

<Interactions: procedures>+≡
    subroutine interaction_relate (int, i1, i2)
        class(interaction_t), intent(inout), target :: int
        integer, intent(in) :: i1, i2
        if (i1 /= 0 .and. i2 /= 0) then
            call int%children(i1)%append (i2)
            call int%parents(i2)%append (i1)
        end if
    end subroutine interaction_relate

```

Transfer internal parent-child relations defined within interaction `int1` to a new interaction `int` where the particle indices are mapped to. Some particles in `int1` may have no image in `int`. In that case, a child entry maps to zero, and we skip this relation.

Also transfer resonance flags.

```

<Interactions: interaction: TBP>+≡
    procedure :: transfer_relations => interaction_transfer_relations

<Interactions: procedures>+≡
    subroutine interaction_transfer_relations (int1, int2, map)
        class(interaction_t), intent(in) :: int1
        class(interaction_t), intent(inout), target :: int2
        integer, dimension(:), intent(in) :: map
        integer :: i, j, k
        do i = 1, size (map)
            do j = 1, int1%parents(i)%get_length ()
                k = int1%parents(i)%get_link (j)
                call int2%relate (map(k), map(i))
            end do
            if (map(i) /= 0) then
                int2%resonant(map(i)) = int1%resonant(i)
            end if
        end do
    end subroutine interaction_transfer_relations

```

```

end do
end subroutine interaction_transfer_relations

```

Make up internal parent-child relations for the particle(s) that are connected to a new interaction `int`.

If `resonant` is defined and true, the connections are marked as resonant in the result interaction. Also, the children of the resonant connections are untagged if they were tagged with hard-interaction flags previously.

```

<Interactions: interaction: TBP>+=
  procedure :: relate_connections => interaction_relate_connections

<Interactions: procedures>+=
  subroutine interaction_relate_connections &
    (int, int_in, connection_index, &
     map, map_connections, resonant)
    class(interaction_t), intent(inout), target :: int
    class(interaction_t), intent(in) :: int_in
    integer, dimension(:), intent(in) :: connection_index
    integer, dimension(:), intent(in) :: map, map_connections
    logical, intent(in), optional :: resonant
    logical :: reson
    integer :: i, j, i2, k2
    reson = .false.; if (present (resonant)) reson = resonant
    do i = 1, size (map_connections)
      k2 = connection_index(i)
      do j = 1, int_in%children(k2)%get_length ()
        i2 = int_in%children(k2)%get_link (j)
        call int%relate (map_connections(i), map(i2))
        if (reson) call int%retag_hard_process (map(i2), .false.)
      end do
      int%resonant(map_connections(i)) = reson
    end do
  end subroutine interaction_relate_connections

```

Return the number of source/target links of the internal connections of particle `i`.

```

<Interactions: public>+=
  public :: interaction_get_n_children
  public :: interaction_get_n_parents

<Interactions: procedures>+=
  function interaction_get_n_children (int, i) result (n)
    integer :: n
    type(interaction_t), intent(in) :: int
    integer, intent(in) :: i
    n = int%children(i)%get_length ()
  end function interaction_get_n_children

  function interaction_get_n_parents (int, i) result (n)
    integer :: n
    type(interaction_t), intent(in) :: int
    integer, intent(in) :: i
    n = int%parents(i)%get_length ()
  end function interaction_get_n_parents

```

```
end function interaction_get_n_parents
```

Return the source/target links of the internal connections of particle *i* as an array.

<Interactions: public>+≡

```
public :: interaction_get_children
public :: interaction_get_parents
```

<Interactions: procedures>+≡

```
function interaction_get_children (int, i) result (idx)
  integer, dimension(:), allocatable :: idx
  type(interaction_t), intent(in) :: int
  integer, intent(in) :: i
  integer :: k, l
  l = int%children(i)%get_length ()
  allocate (idx (l))
  do k = 1, l
    idx(k) = int%children(i)%get_link (k)
  end do
end function interaction_get_children
```

```
function interaction_get_parents (int, i) result (idx)
  integer, dimension(:), allocatable :: idx
  type(interaction_t), intent(in) :: int
  integer, intent(in) :: i
  integer :: k, l
  l = int%parents(i)%get_length ()
  allocate (idx (l))
  do k = 1, l
    idx(k) = int%parents(i)%get_link (k)
  end do
end function interaction_get_parents
```

Add a source link from an interaction to a corresponding particle within another interaction. These links affect the propagation of particles: the two linked particles are considered as the same particle, outgoing and incoming.

<Interactions: interaction: TBP>+≡

```
procedure :: set_source_link => interaction_set_source_link
```

<Interactions: procedures>+≡

```
subroutine interaction_set_source_link (int, i, int1, i1)
  class(interaction_t), intent(inout) :: int
  integer, intent(in) :: i
  class(interaction_t), intent(in), target :: int1
  integer, intent(in) :: i1
  if (i /= 0) call external_link_set (int%source(i), int1, i1)
end subroutine interaction_set_source_link
```

Reassign links to a new interaction (which is an image of the current interaction).

<Interactions: public>+≡

```
public :: interaction_reassign_links
```

```

<Interactions: procedures>+≡
subroutine interaction_reassign_links (int, int_src, int_target)
  type(interaction_t), intent(inout) :: int
  type(interaction_t), intent(in) :: int_src
  type(interaction_t), intent(in), target :: int_target
  integer :: i
  if (allocated (int%source)) then
    do i = 1, size (int%source)
      call external_link_reassign (int%source(i), int_src, int_target)
    end do
  end if
end subroutine interaction_reassign_links

```

Since links are one-directional, if we want to follow them backwards we have to scan all possibilities. This procedure returns the index of the particle within `int` which points to the particle `i1` within interaction `int1`. If unsuccessful, return zero.

```

<Interactions: public>+≡
public :: interaction_find_link

<Interactions: procedures>+≡
function interaction_find_link (int, int1, i1) result (i)
  integer :: i
  type(interaction_t), intent(in) :: int, int1
  integer, intent(in) :: i1
  type(interaction_t), pointer :: int_tmp
  do i = 1, int%n_tot
    int_tmp => external_link_get_ptr (int%source(i))
    if (int_tmp%tag == int1%tag) then
      if (external_link_get_index (int%source(i)) == i1) return
    end if
  end do
  i = 0
end function interaction_find_link

```

The inverse: return interaction pointer and index for the ultimate source of `i` within `int`.

```

<Interactions: interaction: TBP>+≡
procedure :: find_source => interaction_find_source

<Interactions: procedures>+≡
subroutine interaction_find_source (int, i, int1, i1)
  class(interaction_t), intent(in) :: int
  integer, intent(in) :: i
  type(interaction_t), intent(out), pointer :: int1
  integer, intent(out) :: i1
  type(external_link_t) :: link
  link = interaction_get_ultimate_source (int, i)
  int1 => external_link_get_ptr (link)
  i1 = external_link_get_index (link)
end subroutine interaction_find_source

```

Follow source links recursively to return the ultimate source of a particle.

(Interactions: procedures)+≡

```
function interaction_get_ultimate_source (int, i) result (link)
  type(external_link_t) :: link
  type(interaction_t), intent(in) :: int
  integer, intent(in) :: i
  type(interaction_t), pointer :: int_src
  integer :: i_src
  link = int%source(i)
  if (external_link_is_set (link)) then
    do
      int_src => external_link_get_ptr (link)
      i_src = external_link_get_index (link)
      if (external_link_is_set (int_src%source(i_src))) then
        link = int_src%source(i_src)
      else
        exit
      end if
    end do
  end if
end function interaction_get_ultimate_source
```

Update mask entries by merging them with corresponding masks in interactions linked to the current one. The mask determines quantum numbers which are summed over.

Note that both the mask of the current interaction and the mask of the linked interaction are updated (side effect!). This ensures that both agree for the linked particle.

(Interactions: public)+≡

```
public :: interaction_exchange_mask
```

(Interactions: procedures)+≡

```
subroutine interaction_exchange_mask (int)
  type(interaction_t), intent(inout) :: int
  integer :: i, index_link
  type(interaction_t), pointer :: int_link
  do i = 1, int%n_tot
    if (external_link_is_set (int%source(i))) then
      int_link => external_link_get_ptr (int%source(i))
      index_link = external_link_get_index (int%source(i))
      call interaction_merge_mask_entry &
        (int, i, int_link%mask(index_link))
      call interaction_merge_mask_entry &
        (int_link, index_link, int%mask(i))
    end if
  end do
  call int%freeze ()
end subroutine interaction_exchange_mask
```

Copy momenta from interactions linked to the current one.

(Interactions: interaction: TBP)+≡

```
procedure :: receive_momenta => interaction_receive_momenta
```

```

<Interactions: procedures>+≡
subroutine interaction_receive_momenta (int)
  class(interaction_t), intent(inout) :: int
  integer :: i, index_link
  type(interaction_t), pointer :: int_link
  do i = 1, int%n_tot
    if (external_link_is_set (int%source(i))) then
      int_link => external_link_get_ptr (int%source(i))
      index_link = external_link_get_index (int%source(i))
      call int%set_momentum (int_link%p(index_link), i)
    end if
  end do
end subroutine interaction_receive_momenta

```

The inverse operation: Copy momenta back to the interactions linked to the current one.

```

<Interactions: public>+≡
public :: interaction_send_momenta

<Interactions: procedures>+≡
subroutine interaction_send_momenta (int)
  type(interaction_t), intent(in) :: int
  integer :: i, index_link
  type(interaction_t), pointer :: int_link
  do i = 1, int%n_tot
    if (external_link_is_set (int%source(i))) then
      int_link => external_link_get_ptr (int%source(i))
      index_link = external_link_get_index (int%source(i))
      call int_link%set_momentum (int%p(i), index_link)
    end if
  end do
end subroutine interaction_send_momenta

```

For numerical comparisons: pacify all momenta in an interaction.

```

<Interactions: public>+≡
public :: interaction_pacify_momenta

<Interactions: procedures>+≡
subroutine interaction_pacify_momenta (int, acc)
  type(interaction_t), intent(inout) :: int
  real(default), intent(in) :: acc
  integer :: i
  do i = 1, int%n_tot
    call pacify (int%p(i), acc)
  end do
end subroutine interaction_pacify_momenta

```

For each subtraction entry starting from SUB = 0, we duplicate the original state matrix entries as is.

```

<Interactions: interaction: TBP>+≡
procedure :: declare_subtraction => interaction_declare_subtraction

```

```

<Interactions: procedures>+≡
subroutine interaction_declare_subtraction (int, n_sub)
  class(interaction_t), intent(inout), target :: int
  integer, intent(in) :: n_sub
  integer :: i_sub
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  type(state_matrix_t) :: state_matrix
  call state_matrix%init (store_values = .true.)
  allocate (qn (int%get_state_depth ()))
  do i_sub = 0, n_sub
    call it%init (int%state_matrix)
    do while (it%is_valid ())
      qn = it%get_quantum_numbers ()
      call qn%set_subtraction_index (i_sub)
      call state_matrix%add_state (qn, value = it%get_matrix_element ())
      call it%advance ()
    end do
  end do
  call state_matrix%freeze ()
  call state_matrix%set_n_sub ()
  call int%state_matrix%final ()
  int%state_matrix = state_matrix
end subroutine interaction_declare_subtraction

```

12.2.8 Recovering connections

When creating an evaluator for two interactions, we have to know by which particles they are connected. The connection indices can be determined if we have two linked interactions. We assume that `int1` is the source and `int2` the target, so the connections of interest are stored within `int2`. A connection is found if either the source is `int1`, or the (ultimate) source of a particle within `int2` coincides with the (ultimate) source of a particle within `int1`. The result is an array of index pairs.

To make things simple, we scan the interaction twice, once for counting hits, then allocate the array, then scan again and store the connections.

The connections are scanned for `int2`, which has sources in `int1`. It may happen that the order of connections is interchanged (crossed). We require the indices in `int1` to be sorted, so we reorder both index arrays correspondingly before returning them. (After this, the indices in `int2` may be out of order.)

```

<Interactions: public>+≡
public :: find_connections

<Interactions: procedures>+≡
subroutine find_connections (int1, int2, n, connection_index)
  class(interaction_t), intent(in) :: int1, int2
  integer, intent(out) :: n
  integer, dimension(:,:), intent(out), allocatable :: connection_index
  integer, dimension(:,:), allocatable :: conn_index_tmp
  integer, dimension(:), allocatable :: ordering
  integer :: i, j, k
  type(external_link_t) :: link1, link2

```



```

type(interaction_t), pointer :: int_link1, int_link2
n = 0
do i = 1, size (int2%source)
  link2 = interaction_get_ultimate_source (int2, i)
  if (external_link_is_set (link2)) then
    int_link2 => external_link_get_ptr (link2)
    if (int_link2%tag == int1%tag) then
      n = n + 1
    else
      k = external_link_get_index (link2)
      do j = 1, size (int1%source)
        link1 = interaction_get_ultimate_source (int1, j)
        if (external_link_is_set (link1)) then
          int_link1 => external_link_get_ptr (link1)
          if (int_link1%tag == int_link2%tag) then
            if (external_link_get_index (link1) == k) &
              n = n + 1
          end if
        end if
      end do
    end if
  end if
end do
allocate (conn_index_tmp (n, 2))
n = 0
do i = 1, size (int2%source)
  link2 = interaction_get_ultimate_source (int2, i)
  if (external_link_is_set (link2)) then
    int_link2 => external_link_get_ptr (link2)
    if (int_link2%tag == int1%tag) then
      n = n + 1
      conn_index_tmp(n,1) = external_link_get_index (int2%source(i))
      conn_index_tmp(n,2) = i
    else
      k = external_link_get_index (link2)
      do j = 1, size (int1%source)
        link1 = interaction_get_ultimate_source (int1, j)
        if (external_link_is_set (link1)) then
          int_link1 => external_link_get_ptr (link1)
          if (int_link1%tag == int_link2%tag) then
            if (external_link_get_index (link1) == k) then
              n = n + 1
              conn_index_tmp(n,1) = j
              conn_index_tmp(n,2) = i
            end if
          end if
        end if
      end do
    end if
  end if
end do
allocate (connection_index (n, 2))
if (n > 1) then
  allocate (ordering (n))

```

```

        ordering = order (conn_index_tmp(:,1))
        connection_index = conn_index_tmp(ordering,:)
    else
        connection_index = conn_index_tmp
    end if
end subroutine find_connections

```

12.2.9 Unit tests

Test module, followed by the corresponding implementation module.

<interactions_ut.f90>≡
<File header>

```

module interactions_ut
  use unit_tests
  use interactions_uti

```

<Standard module head>

<Interactions: public test>

contains

<Interactions: test driver>

```

end module interactions_ut

```

<interactions_uti.f90>≡
<File header>

```

module interactions_uti

```

<Use kinds>

```

  use lorentz
  use flavors
  use colors
  use helicities
  use quantum_numbers
  use state_matrices

```

```

  use interactions

```

<Standard module head>

<Interactions: test declarations>

contains

<Interactions: tests>

```

end module interactions_uti

```

API: driver for the unit tests below.

```

<Interactions: public test>≡
    public :: interaction_test

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

```

Generate an interaction of a polarized virtual photon and a colored quark which may be either up or down. Remove the quark polarization. Generate another interaction for the quark radiating a photon and link this to the first interaction. The radiation ignores polarization; transfer this information to the first interaction to simplify it. Then, transfer the momentum to the radiating quark and perform a splitting.

```

<Interactions: execute tests>≡
    call test (interaction_1, "interaction_1", &
        "check interaction setup", &
        u, results)

<Interactions: test declarations>≡
    public :: interaction_1

<Interactions: tests>≡
    subroutine interaction_1 (u)
        integer, intent(in) :: u
        type(interaction_t), target :: int, rad
        type(vector4_t), dimension(3) :: p
        type(quantum_numbers_mask_t), dimension(3) :: mask
        p(2) = vector4_moving (500._default, 500._default, 1)
        p(3) = vector4_moving (500._default, -500._default, 1)
        p(1) = p(2) + p(3)

        write (u, "(A)")  "** Test output: interaction"
        write (u, "(A)")  "** Purpose: check routines for interactions"
        write (u, "(A)")

        call int%basic_init (1, 0, 2, set_relations=.true., &
            store_values = .true. )
        call int_set (int, 1, -1, 1, 1, &
            cmplx (0.3_default, 0.1_default, kind=default))
        call int_set (int, 1, -1, -1, 1, &
            cmplx (0.5_default, -0.7_default, kind=default))
        call int_set (int, 1, 1, 1, 1, &
            cmplx (0.1_default, 0._default, kind=default))
        call int_set (int, -1, 1, -1, 2, &
            cmplx (0.4_default, -0.1_default, kind=default))
        call int_set (int, 1, 1, 1, 2, &
            cmplx (0.2_default, 0._default, kind=default))
        call int%freeze ()
        call int%set_momenta (p)
        mask = quantum_numbers_mask (.false., .false., [.true., .true., .true.])
    end subroutine interaction_1

```

```

call rad%basic_init (1, 0, 2, &
    mask=mask, set_relations=.true., store_values = .true.)
call rad_set (1)
call rad_set (2)
call rad%set_source_link (1, int, 2)
call interaction_exchange_mask (rad)
call rad%receive_momenta ()
p(1) = rad%get_momentum (1)
p(2) = 0.4_default * p(1)
p(3) = p(1) - p(2)
call rad%set_momenta (p(2:3), outgoing=.true.)
call int%freeze ()
call rad%freeze ()
call rad%set_matrix_element &
    (cmplx (0._default, 0._default, kind=default))
call int%basic_write (u)
write (u, "(A)")
call rad%basic_write (u)
write (u, "(A)")
write (u, "(A)")  "* Cleanup"
call int%final ()
call rad%final ()
write (u, "(A)")
write (u, "(A)")  "* Test interaction_1: successful."
contains
subroutine int_set (int, h1, h2, hq, q, val)
    type(interaction_t), target, intent(inout) :: int
    integer, intent(in) :: h1, h2, hq, q
    type(flavor_t), dimension(3) :: flv
    type(color_t), dimension(3) :: col
    type(helicity_t), dimension(3) :: hel
    type(quantum_numbers_t), dimension(3) :: qn
    complex(default), intent(in) :: val
    call flv%init ([21, q, -q])
    call col(2)%init_col_acl (5, 0)
    call col(3)%init_col_acl (0, 5)
    call hel%init ([h1, hq, -hq], [h2, hq, -hq])
    call qn%init (flv, col, hel)
    call int%add_state (qn)
    call int%set_matrix_element (val)
end subroutine int_set
subroutine rad_set (q)
    integer, intent(in) :: q
    type(flavor_t), dimension(3) :: flv
    type(quantum_numbers_t), dimension(3) :: qn
    call flv%init ([ q, q, 21 ])
    call qn%init (flv)
    call rad%add_state (qn)
end subroutine rad_set
end subroutine interaction_1

```

12.3 Matrix element evaluation

The `evaluator_t` type is an extension of the `interaction_t` type. It represents either a density matrix as the square of a transition matrix element, or the product of two density matrices. Usually, some quantum numbers are summed over in the result.

The `interaction_t` subobject represents a multi-particle interaction with incoming, virtual, and outgoing particles and the associated (not necessarily diagonal) density matrix of quantum state. When the evaluator is initialized, this interaction is constructed from the input interaction(s).

In addition, the initialization process sets up a multiplication table. For each matrix element of the result, it states which matrix elements are to be taken from the input interaction(s), multiplied (optionally, with an additional weight factor) and summed over.

Eventually, to a processes we associate a chain of evaluators which are to be evaluated sequentially. The physical event and its matrix element value(s) can be extracted from the last evaluator in such a chain.

Evaluators are constructed only once (as long as this is possible) during an initialization step. Then, for each event, momenta are computed and transferred among evaluators using the links within the interaction subobject. The multiplication tables enable fast evaluation of the result without looking at quantum numbers anymore.

```

<evaluators.f90>≡
  <File header>

  module evaluators

    <Use kinds>
    <Use strings>
    use io_units
    use format_defs, only: FMT_19
    use physics_defs, only: n_beams_rescaled
    use diagnostics
    use lorentz
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices
    use interactions

    <Standard module head>

    <Evaluators: public>

    <Evaluators: parameters>

    <Evaluators: types>

    <Evaluators: interfaces>

    contains

```

<Evaluators: procedures>

end module evaluators

12.3.1 Array of pairings

The evaluator contains an array of `pairing_array` objects. This makes up the multiplication table.

Each pairing array contains two lists of matrix element indices and a list of numerical factors. The matrix element indices correspond to the input interactions. The corresponding matrix elements are to be multiplied and optionally multiplied by a factor. The results are summed over to yield one specific matrix element of the result evaluator.

<Evaluators: types>≡

```
type :: pairing_array_t
  integer, dimension(:), allocatable :: i1, i2
  complex(default), dimension(:), allocatable :: factor
end type pairing_array_t
```

<Evaluators: procedures>≡

```
elemental subroutine pairing_array_init (pa, n, has_i2, has_factor)
  type(pairing_array_t), intent(out) :: pa
  integer, intent(in) :: n
  logical, intent(in) :: has_i2, has_factor
  allocate (pa%i1 (n))
  if (has_i2) allocate (pa%i2 (n))
  if (has_factor) allocate (pa%factor (n))
end subroutine pairing_array_init
```

<Evaluators: public>≡

```
public :: pairing_array_write
```

<Evaluators: procedures>+≡

```
subroutine pairing_array_write (pa, unit)
  type(pairing_array_t), intent(in) :: pa
  integer, intent(in), optional :: unit
  integer :: i, u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(A)", advance = "no") "["
  if (allocated (pa%i1)) then
    write (u, "(I0,A)", advance = "no") pa%i1, ","
  else
    write (u, "(A)", advance = "no") "x,"
  end if
  if (allocated (pa%i2)) then
    write (u, "(I0,A)", advance = "no") pa%i2, ","
  else
    write (u, "(A)", advance = "no") "x,"
  end if
  write (u, "(A)", advance = "no") "]"
  if (allocated (pa%factor)) then
```

```

        write (u, "(A,F5.4,A,F5.4,A)" );(, &
            real(pa%factor), ",", aimag(pa%factor), ")]"
    else
        write (u, "(A)" ) ""
    end if
end subroutine pairing_array_write

```

12.3.2 The evaluator type

Possible variants of evaluators:

```

⟨Evaluators: parameters⟩≡
    integer, parameter :: &
        EVAL_UNDEFINED = 0, &
        EVAL_PRODUCT = 1, &
        EVAL_SQUARED_FLOWS = 2, &
        EVAL_SQUARE_WITH_COLOR_FACTORS = 3, &
        EVAL_COLOR_CONTRACTION = 4, &
        EVAL_IDENTITY = 5, &
        EVAL_QN_SUM = 6

```

The evaluator type contains the result interaction and an array of pairing lists, one for each matrix element in the result interaction.

```

⟨Evaluators: public⟩+≡
    public :: evaluator_t

⟨Evaluators: types⟩+≡
    type, extends (interaction_t) :: evaluator_t
    private
        integer :: type = EVAL_UNDEFINED
        class(interaction_t), pointer :: int_in1 => null ()
        class(interaction_t), pointer :: int_in2 => null ()
        type(pairing_array_t), dimension(:), allocatable :: pairing_array
    contains
        ⟨Evaluators: evaluator: TBP⟩
    end type evaluator_t

```

Output.

```

⟨Evaluators: evaluator: TBP⟩≡
    procedure :: write => evaluator_write

⟨Evaluators: procedures⟩+≡
    subroutine evaluator_write (eval, unit, &
        verbose, show_momentum_sum, show_mass, show_state, show_table, &
        col_verbose, testflag)
        class(evaluator_t), intent(in) :: eval
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: show_state, show_table, col_verbose
        logical, intent(in), optional :: testflag
        logical :: conjugate, square, show_tab
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        show_tab = .true.; if (present (show_table)) show_tab = .false.
    end subroutine evaluator_write

```

```

call eval%basic_write &
    (unit, verbose, show_momentum_sum, show_mass, &
     show_state, col_verbose, testflag)
if (show_tab) then
    write (u, "(1x,A)") "Matrix-element multiplication"
    write (u, "(2x,A)", advance="no") "Input interaction 1:"
    if (associated (eval%int_in1)) then
        write (u, "(1x,I0)") eval%int_in1%get_tag ()
    else
        write (u, "(A)") " [undefined]"
    end if
    write (u, "(2x,A)", advance="no") "Input interaction 2:"
    if (associated (eval%int_in2)) then
        write (u, "(1x,I0)") eval%int_in2%get_tag ()
    else
        write (u, "(A)") " [undefined]"
    end if
    select case (eval%type)
    case (EVAL_SQUARED_FLOWS, EVAL_SQUARE_WITH_COLOR_FACTORS)
        conjugate = .true.
        square = .true.
    case (EVAL_IDENTITY)
        write (u, "(1x,A)") "Identity evaluator, pairing array unused"
        return
    case default
        conjugate = .false.
        square = .false.
    end select
    call eval%write_pairing_array (conjugate, square, u)
end if
end subroutine evaluator_write

```

(Evaluators: evaluator: TBP)+≡

```

procedure :: write_pairing_array => evaluator_write_pairing_array

```

(Evaluators: procedures)+≡

```

subroutine evaluator_write_pairing_array (eval, conjugate, square, unit)
    class(evaluator_t), intent(in) :: eval
    logical, intent(in) :: conjugate, square
    integer, intent(in), optional :: unit
    integer :: u, i, j
    u = given_output_unit (unit); if (u < 0) return
    if (allocated (eval%pairing_array)) then
        do i = 1, size (eval%pairing_array)
            write (u, "(2x,A,I0,A)") "ME(", i, ") = "
            do j = 1, size (eval%pairing_array(i)%i1)
                write (u, "(4x,A)", advance="no") "+"
                if (allocated (eval%pairing_array(i)%i2)) then
                    write (u, "(1x,A,I0,A)", advance="no") &
                        "ME1(", eval%pairing_array(i)%i1(j), ")"
                    if (conjugate) then
                        write (u, "(A)", advance="no") "* x"
                    else
                        write (u, "(A)", advance="no") " x"
                    end if
                end if
            end do
        end do
    end if

```



```

        end if
        write (u, "(1x,A,I0,A)", advance="no") &
            "ME2(", eval%pairing_array(i)%i2(j), ") "
    else if (square) then
        write (u, "(1x,A)", advance="no") " | "
        write (u, "(A,I0,A)", advance="no") &
            "ME1(", eval%pairing_array(i)%i1(j), ") "
        write (u, "(A)", advance="no") "|^2"
    else
        write (u, "(1x,A,I0,A)", advance="no") &
            "ME1(", eval%pairing_array(i)%i1(j), ") "
    end if
    if (allocated (eval%pairing_array(i)%factor)) then
        write (u, "(1x,A)", advance="no") "x"
        write (u, "(1x,'('," // FMT_19 // ",',''," // FMT_19 // &
            ",')')") eval%pairing_array(i)%factor(j)
    else
        write (u, *)
    end if
end do
end do
end if
end subroutine evaluator_write_pairing_array

```

Assignment: Deep copy of the interaction component.

(Evaluators: public) +=

```
public :: assignment(=)
```

(Evaluators: interfaces) ≡

```
interface assignment(=)
    module procedure evaluator_assign
end interface

```

(Evaluators: procedures) +=

```

subroutine evaluator_assign (eval_out, eval_in)
    type(evaluator_t), intent(out) :: eval_out
    type(evaluator_t), intent(in) :: eval_in
    eval_out%type = eval_in%type
    eval_out%int_in1 => eval_in%int_in1
    eval_out%int_in2 => eval_in%int_in2
    eval_out%interaction_t = eval_in%interaction_t
    if (allocated (eval_in%pairing_array)) then
        allocate (eval_out%pairing_array (size (eval_in%pairing_array)))
        eval_out%pairing_array = eval_in%pairing_array
    end if
end subroutine evaluator_assign

```

12.3.3 Auxiliary structures for evaluator creation

Creating an evaluator that properly handles all quantum numbers requires some bookkeeping. In this section, we define several auxiliary types and methods that

organize and simplify this task. More structures are defined within the specific initializers (as local types and internal subroutines).

These types are currently implemented in a partial object-oriented way: We define some basic methods for initialization etc. here, but the evaluator routines below do access their internals as well. This simplifies some things such as index addressing using array slices, at the expense of losing some clarity.

Index mapping

Index mapping are abundant when constructing an evaluator. To have arrays of index mappings, we define this:

```

(Evaluators: types)+≡
  type :: index_map_t
    integer, dimension(:), allocatable :: entry
  end type index_map_t

(Evaluators: procedures)+≡
  elemental subroutine index_map_init (map, n)
    type(index_map_t), intent(out) :: map
    integer, intent(in) :: n
    allocate (map%entry (n))
    map%entry = 0
  end subroutine index_map_init

(Evaluators: procedures)+≡
  function index_map_exists (map) result (flag)
    logical :: flag
    type(index_map_t), intent(in) :: map
    flag = allocated (map%entry)
  end function index_map_exists

(Evaluators: interfaces)+≡
  interface size
    module procedure index_map_size
  end interface

(Evaluators: procedures)+≡
  function index_map_size (map) result (s)
    integer :: s
    type(index_map_t), intent(in) :: map
    if (allocated (map%entry)) then
      s = size (map%entry)
    else
      s = 0
    end if
  end function index_map_size

(Evaluators: interfaces)+≡
  interface assignment(=)
    module procedure index_map_assign_int
    module procedure index_map_assign_array

```

```

end interface

<Evaluators: procedures>+=
  elemental subroutine index_map_assign_int (map, ival)
    type(index_map_t), intent(inout) :: map
    integer, intent(in) :: ival
    map%entry = ival
  end subroutine index_map_assign_int

  subroutine index_map_assign_array (map, array)
    type(index_map_t), intent(inout) :: map
    integer, dimension(:), intent(in) :: array
    map%entry = array
  end subroutine index_map_assign_array

  <Evaluators: procedures>+=
    elemental subroutine index_map_set_entry (map, i, ival)
      type(index_map_t), intent(inout) :: map
      integer, intent(in) :: i
      integer, intent(in) :: ival
      map%entry(i) = ival
    end subroutine index_map_set_entry

  <Evaluators: procedures>+=
    elemental function index_map_get_entry (map, i) result (ival)
      integer :: ival
      type(index_map_t), intent(in) :: map
      integer, intent(in) :: i
      ival = map%entry(i)
    end function index_map_get_entry

```

Index mapping (two-dimensional)

This is a variant with a square matrix instead of an array.

```

<Evaluators: types>+=
  type :: index_map2_t
    integer :: s = 0
    integer, dimension(:,:), allocatable :: entry
  end type index_map2_t

  <Evaluators: procedures>+=
    elemental subroutine index_map2_init (map, n)
      type(index_map2_t), intent(out) :: map
      integer, intent(in) :: n
      map%s = n
      allocate (map%entry (n, n))
    end subroutine index_map2_init

```

```

<Evaluators: procedures>+≡
function index_map2_exists (map) result (flag)
    logical :: flag
    type(index_map2_t), intent(in) :: map
    flag = allocated (map%entry)
end function index_map2_exists

<Evaluators: interfaces>+≡
interface size
    module procedure index_map2_size
end interface

<Evaluators: procedures>+≡
function index_map2_size (map) result (s)
    integer :: s
    type(index_map2_t), intent(in) :: map
    s = map%s
end function index_map2_size

<Evaluators: interfaces>+≡
interface assignment(=)
    module procedure index_map2_assign_int
end interface

<Evaluators: procedures>+≡
elemental subroutine index_map2_assign_int (map, ival)
    type(index_map2_t), intent(inout) :: map
    integer, intent(in) :: ival
    map%entry = ival
end subroutine index_map2_assign_int

<Evaluators: procedures>+≡
elemental subroutine index_map2_set_entry (map, i, j, ival)
    type(index_map2_t), intent(inout) :: map
    integer, intent(in) :: i, j
    integer, intent(in) :: ival
    map%entry(i,j) = ival
end subroutine index_map2_set_entry

<Evaluators: procedures>+≡
elemental function index_map2_get_entry (map, i, j) result (ival)
    integer :: ival
    type(index_map2_t), intent(in) :: map
    integer, intent(in) :: i, j
    ival = map%entry(i,j)
end function index_map2_get_entry

```

Auxiliary structures: particle mask

This is a simple container of a logical array.

```

<Evaluators: types>+≡

```

```

type :: prt_mask_t
    logical, dimension(:), allocatable :: entry
end type prt_mask_t

<Evaluators: procedures>+≡
subroutine prt_mask_init (mask, n)
    type(prt_mask_t), intent(out) :: mask
    integer, intent(in) :: n
    allocate (mask%entry (n))
end subroutine prt_mask_init

<Evaluators: interfaces>+≡
interface size
    module procedure prt_mask_size
end interface

<Evaluators: procedures>+≡
function prt_mask_size (mask) result (s)
    integer :: s
    type(prt_mask_t), intent(in) :: mask
    s = size (mask%entry)
end function prt_mask_size

```

Quantum number containers

Trivial transparent containers:

```

<Evaluators: types>+≡
type :: qn_list_t
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
end type qn_list_t

type :: qn_mask_array_t
    type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
end type qn_mask_array_t

```

Auxiliary structures: connection entries

This type is used as intermediate storage when computing the product of two evaluators or the square of an evaluator. The quantum-number array `qn` corresponds to the particles common to both interactions, but irrelevant quantum numbers (color) masked out. The index arrays `index_in` determine the entries in the input interactions that contribute to this connection. `n_index` is the size of these arrays, and `count` is used while filling the entries. Finally, the quantum-number arrays `qn_in_list` are the actual entries in the input interaction that contribute. In the product case, they exclude the connected quantum numbers.

Each evaluator has its own `connection_table` which contains an array of `connection_entry` objects, but also has stuff that specifically applies to the evaluator type. Hence, we do not generalize the `connection_table_t` type.

The filling procedure `connection_entry_add_state` is specific to the various evaluator types.

(Evaluators: types)+≡

```

type :: connection_entry_t
  type(quantum_numbers_t), dimension(:), allocatable :: qn_conn
  integer, dimension(:), allocatable :: n_index
  integer, dimension(:), allocatable :: count
  type(index_map_t), dimension(:), allocatable :: index_in
  type(qn_list_t), dimension(:), allocatable :: qn_in_list
end type connection_entry_t

```

(Evaluators: procedures)+≡

```

subroutine connection_entry_init &
  (entry, n_count, n_map, qn_conn, count, n_rest)
  type(connection_entry_t), intent(out) :: entry
  integer, intent(in) :: n_count, n_map
  type(quantum_numbers_t), dimension(:), intent(in) :: qn_conn
  integer, dimension(n_count), intent(in) :: count
  integer, dimension(n_count), intent(in) :: n_rest
  integer :: i
  allocate (entry%qn_conn (size (qn_conn)))
  allocate (entry%n_index (n_count))
  allocate (entry%count (n_count))
  allocate (entry%index_in (n_map))
  allocate (entry%qn_in_list (n_count))
  entry%qn_conn = qn_conn
  entry%n_index = count
  entry%count = 0
  if (size (entry%index_in) == size (count)) then
    call index_map_init (entry%index_in, count)
  else
    call index_map_init (entry%index_in, count(1))
  end if
  do i = 1, n_count
    allocate (entry%qn_in_list(i)%qn (n_rest(i), count(i)))
  end do
end subroutine connection_entry_init

```

(Evaluators: procedures)+≡

```

subroutine connection_entry_write (entry, unit)
  type(connection_entry_t), intent(in) :: entry
  integer, intent(in), optional :: unit
  integer :: i, j
  integer :: u
  u = given_output_unit (unit)
  call quantum_numbers_write (entry%qn_conn, unit)
  write (u, *)
  do i = 1, size (entry%n_index)
    write (u, *) "Input interaction", i
    do j = 1, entry%n_index(i)
      if (size (entry%n_index) == size (entry%index_in)) then
        write (u, "(2x,I0,4x,I0,2x)", advance = "no") &
          j, index_map_get_entry (entry%index_in(i), j)
      end if
    end do
  end do

```

```

else
  write (u, "(2x,I0,4x,I0,2x,I0,2x)", advance = "no") &
    j, index_map_get_entry (entry%index_in(1), j), &
    index_map_get_entry (entry%index_in(2), j)
end if
call quantum_numbers_write (entry%qn_in_list(i)%qn(:,j), unit)
write (u, *)
end do
end do
end subroutine connection_entry_write

```

Color handling

For managing color-factor computation, we introduce this local type. The `index` is the index in the color table that corresponds to a given matrix element index in the input interaction. The `col` array stores the color assignments in rows. The `factor` array associates a complex number with each pair of arrays in the color table. The `factor_is_known` array reveals whether a given factor is known already or still has to be computed.

(Evaluators: types)+≡

```

type :: color_table_t
  integer, dimension(:), allocatable :: index
  type(color_t), dimension(:, :), allocatable :: col
  logical, dimension(:, :), allocatable :: factor_is_known
  complex(default), dimension(:, :), allocatable :: factor
end type color_table_t

```

This is the initializer. We extract the color states from the given state matrices, establish index mappings between the two states (implemented by the array `me_index`), make an array of color states, and initialize the color-factor table. The latter is two-dimensional (includes interference) and not yet filled.

(Evaluators: procedures)+≡

```

subroutine color_table_init (color_table, state, n_tot)
  type(color_table_t), intent(out) :: color_table
  type(state_matrix_t), intent(in) :: state
  integer, intent(in) :: n_tot
  type(state_iterator_t) :: it
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  type(state_matrix_t) :: state_col
  integer :: index, n_col_state
  allocate (color_table%index (state%get_n_matrix_elements ()))
  color_table%index = 0
  allocate (qn (n_tot))
  call state_col%init ()
  call it%init (state)
  do while (it%is_valid ())
    index = it%get_me_index ()
    call qn%init (col = it%get_color ())
    call state_col%add_state (qn, me_index = color_table%index(index))
    call it%advance ()
  end do
end subroutine color_table_init

```

```

n_col_state = state_col%get_n_matrix_elements ()
allocate (color_table%col (n_tot, n_col_state))
call it%init (state_col)
do while (it%is_valid ())
    index = it%get_me_index ()
    color_table%col(:,index) = it%get_color ()
    call it%advance ()
end do
call state_col%final ()
allocate (color_table%factor_is_known (n_col_state, n_col_state))
allocate (color_table%factor (n_col_state, n_col_state))
color_table%factor_is_known = .false.
end subroutine color_table_init

```

Output (debugging use):

(Evaluators: procedures) +=

```

subroutine color_table_write (color_table, unit)
    type(color_table_t), intent(in) :: color_table
    integer, intent(in), optional :: unit
    integer :: i, j
    integer :: u
    u = given_output_unit (unit)
    write (u, *) "Color table:"
    if (allocated (color_table%index)) then
        write (u, *) "  Index mapping state => color table:"
        do i = 1, size (color_table%index)
            write (u, "(3x,I0,2x,I0,2x)") i, color_table%index(i)
        end do
        write (u, *) "  Color table:"
        do i = 1, size (color_table%col, 2)
            write (u, "(3x,I0,2x)", advance = "no") i
            call color_write (color_table%col(:,i), unit)
            write (u, *)
        end do
        write (u, *) "  Defined color factors:"
        do i = 1, size (color_table%factor, 1)
            do j = 1, size (color_table%factor, 2)
                if (color_table%factor_is_known(i,j)) then
                    write (u, *) i, j, color_table%factor(i,j)
                end if
            end do
        end do
    end if
end subroutine color_table_write

```

This subroutine sets color factors, based on information from the hard matrix element: the list of pairs of color-flow indices (in the basis of the matrix element code), the list of corresponding factors, and the list of mappings from the matrix element index in the input interaction to the color-flow index in the hard matrix element object.

We first determine the mapping of color-flow indices from the hard matrix element code to the current color table. The mapping could be nontrivial because the latter is derived from iterating over a state matrix, which may return

states in non-canonical order. The translation table can be determined because we have, for the complete state matrix, both the mapping to the hard interaction (the input `col_index_hi`) and the mapping to the current color table (the component `color_table%index`).

Once this mapping is known, we scan the list of index pairs `color_flow_index` and translate them to valid color-table index pairs. For this pair, the color factor is set using the corresponding entry in the list `col_factor`.

(*Evaluators: procedures*) +=

```
subroutine color_table_set_color_factors (color_table, &
    col_flow_index, col_factor, col_index_hi)
    type(color_table_t), intent(inout) :: color_table
    integer, dimension(:,:), intent(in) :: col_flow_index
    complex(default), dimension(:), intent(in) :: col_factor
    integer, dimension(:), intent(in) :: col_index_hi
    integer, dimension(:), allocatable :: hi_to_ct
    integer :: n_cflow
    integer :: hi_index, me_index, ct_index, cf_index
    integer, dimension(2) :: hi_index_pair, ct_index_pair
    n_cflow = size (col_index_hi)
    if (size (color_table%index) /= n_cflow) &
        call msg_bug ("Mismatch between hard matrix element and color table")
    allocate (hi_to_ct (n_cflow))
    do me_index = 1, size (color_table%index)
        ct_index = color_table%index(me_index)
        hi_index = col_index_hi(me_index)
        hi_to_ct(hi_index) = ct_index
    end do
    do cf_index = 1, size (col_flow_index, 2)
        hi_index_pair = col_flow_index(:,cf_index)
        ct_index_pair = hi_to_ct(hi_index_pair)
        color_table%factor(ct_index_pair(1), ct_index_pair(2)) = &
            col_factor(cf_index)
        color_table%factor_is_known(ct_index_pair(1), ct_index_pair(2)) = .true.
    end do
end subroutine color_table_set_color_factors
```

This function returns a color factor, given two indices which point to the matrix elements of the initial state matrix. Internally, we can map them to the corresponding indices in the color table. As a side effect, we store the color factor in the color table for later lookup. (I.e., this function is impure.)

(*Evaluators: procedures*) +=

```
function color_table_get_color_factor (color_table, index1, index2, nc) &
    result (factor)
    real(default) :: factor
    type(color_table_t), intent(inout) :: color_table
    integer, intent(in) :: index1, index2
    integer, intent(in), optional :: nc
    integer :: i1, i2
    i1 = color_table%index(index1)
    i2 = color_table%index(index2)
    if (color_table%factor_is_known(i1,i2)) then
        factor = real(color_table%factor(i1,i2), kind=default)
    else
```

```

        factor = compute_color_factor &
            (color_table%col(:,i1), color_table%col(:,i2), nc)
        color_table%factor(i1,i2) = factor
        color_table%factor_is_known(i1,i2) = .true.
    end if
end function color_table_get_color_factor

```

12.3.4 Creating an evaluator: Matrix multiplication

The evaluator for matrix multiplication is the most complicated variant.

The initializer takes two input interactions and constructs the result evaluator, which consists of the interaction and the multiplication table for the product (or convolution) of the two. Normally, the input interactions are connected by one or more common particles (e.g., decay, structure function convolution).

In the result interaction, quantum numbers of the connections can be summed over. This is determined by the `qn_mask_conn` argument. The `qn_mask_rest` argument is its analog for the other particles within the result interaction. (E.g., for the trace of the state matrix, all quantum numbers are summed over.)

Finally, the `connections_are_resonant` argument tells whether the connecting particles should be marked as resonant in the final event record. If true, this also implies that the second interaction is not the hard process, so any corresponding tags should be removed from the outgoing particles. This applies to decays.

The algorithm consists of the following steps:

1. **find.connections:** Find the particles which are connected, i.e., common to both input interactions. Either they are directly linked, or both are linked to a common source.
2. **compute_index_bounds_and_mappings:** Compute the mappings of particle indices from the input interactions to the result interaction. There is a separate mapping for the connected particles.
3. **accumulate_connected_states:** Create an auxiliary state matrix which lists the possible quantum numbers for the connected particles. When building this matrix, count the number of times each assignment is contained in any of the input states and, for each of the input states, record the index of the matrix element within the new state matrix. For the connected particles, reassign color indices such that no color state is present twice in different color-index assignment. Note that helicity assignments of the connected state can be (and will be) off-diagonal, so no spin correlations are lost in decays.
Do this for both input interactions.
4. **allocate_connection_entries:** Allocate a table of connections. Each table row corresponds to one state in the auxiliary matrix, and to multiple states of the input interactions. It collects all states of the unconnected particles in the two input interactions that are associated with the particular state (quantum-number assignment) of the connected particles.

5. **fill_connection_table**: Fill the table of connections by scanning both input interactions. When copying states, reassign color indices for the unconnected particles such that they match between all involved particle sets (interaction 1, interaction 2, and connected particles).
6. **make_product_interaction**: Scan the table of connections we have just built. For each entry, construct all possible pairs of states of the unconnected particles and combine them with the specific connected-particle state. This is a possible quantum-number assignment of the result interaction. Now mask all quantum numbers that should be summed over, and append this to the result state matrix. Record the matrix element index of the result. We now have the result interaction.
7. **make_pairing_array**: First allocate the pairing array with the number of entries of the result interaction. Then scan the table of connections again. For each entry, record the indices of the matrix elements which have to be multiplied and summed over in order to compute this particular matrix element. This makes up the multiplication table.
8. **record_links**: Transfer all source pointers from the input interactions to the result interaction. Do the same for the internal parent-child relations and resonance assignments. For the connected particles, make up appropriate additional parent-child relations. This allows for fetching momenta from other interactions when a new event is filled, and to reconstruct the event history when the event is analyzed.

After all this is done, for each event, we just have to evaluate the pairing arrays (multiplication tables) in order to compute the result matrix elements in their proper positions. The quantum-number assignments remain fixed from now on.

```

(Evaluators: evaluator: TBP)+≡
  procedure :: init_product => evaluator_init_product

(Evaluators: procedures)+≡
  subroutine evaluator_init_product &
    (eval, int_in1, int_in2, qn_mask_conn, qn_filter_conn, qn_mask_rest, &
     connections_are_resonant, ignore_sub_for_qn)

    class(evaluator_t), intent(out), target :: eval
    class(interaction_t), intent(in), target :: int_in1, int_in2
    type(quantum_numbers_mask_t), intent(in) :: qn_mask_conn
    type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
    type(quantum_numbers_mask_t), intent(in), optional :: qn_mask_rest
    logical, intent(in), optional :: connections_are_resonant
    logical, intent(in), optional :: ignore_sub_for_qn

    type(qn_mask_array_t), dimension(2) :: qn_mask_in
    type(state_matrix_t), pointer :: state_in1, state_in2

    type :: connection_table_t
      integer :: n_conn = 0
      integer, dimension(2) :: n_rest = 0
      integer :: n_tot = 0

```

```

integer :: n_me_conn = 0
type(state_matrix_t) :: state
type(index_map_t), dimension(:), allocatable :: index_conn
type(connection_entry_t), dimension(:), allocatable :: entry
type(index_map_t) :: index_result
end type connection_table_t
type(connection_table_t) :: connection_table

integer :: n_in, n_vir, n_out, n_tot
integer, dimension(2) :: n_rest
integer :: n_conn

integer, dimension(:,:), allocatable :: connection_index
type(index_map_t), dimension(2) :: prt_map_in
type(index_map_t) :: prt_map_conn
type(prt_mask_t), dimension(2) :: prt_is_connected
type(quantum_numbers_mask_t), dimension(:), allocatable :: &
    qn_mask_conn_initial, int_in1_mask, int_in2_mask

integer :: i

eval%type = EVAL_PRODUCT
eval%int_in1 => int_in1
eval%int_in2 => int_in2

state_in1 => int_in1%get_state_matrix_ptr ()
state_in2 => int_in2%get_state_matrix_ptr ()

call find_connections (int_in1, int_in2, n_conn, connection_index)
if (n_conn == 0) then
    call msg_message ("First interaction:")
    call int_in1%basic_write (col_verbose=.true.)
    call msg_message ("Second interaction:")
    call int_in2%basic_write (col_verbose=.true.)
    call msg_fatal ("Evaluator product: no connections found between factors")
end if
call compute_index_bounds_and_mappings &
    (int_in1, int_in2, n_conn, &
     n_in, n_vir, n_out, n_tot, &
     n_rest, prt_map_in, prt_map_conn)

call prt_mask_init (prt_is_connected(1), int_in1%get_n_tot ())
call prt_mask_init (prt_is_connected(2), int_in2%get_n_tot ())
do i = 1, 2
    prt_is_connected(i)%entry = .true.
    prt_is_connected(i)%entry(connection_index(:,i)) = .false.
end do
allocate (qn_mask_conn_initial (n_conn), &
    int_in1_mask (n_conn), int_in2_mask (n_conn))
int_in1_mask = int_in1%get_mask (connection_index(:,1))
int_in2_mask = int_in2%get_mask (connection_index(:,2))
do i = 1, n_conn
    qn_mask_conn_initial(i) = int_in1_mask(i) .or. int_in2_mask(i)
end do

```

```

allocate (qn_mask_in(1)%mask (int_in1%get_n_tot ()))
allocate (qn_mask_in(2)%mask (int_in2%get_n_tot ()))
qn_mask_in(1)%mask = int_in1%get_mask ()
qn_mask_in(2)%mask = int_in2%get_mask ()
call connection_table_init (connection_table, &
    state_in1, state_in2, &
    qn_mask_conn_initial, &
    n_conn, connection_index, n_rest, &
    qn_filter_conn, ignore_sub_for_qn)
call connection_table_fill (connection_table, &
    state_in1, state_in2, &
    connection_index, prt_is_connected)
call make_product_interaction (eval%interaction_t, &
    n_in, n_vir, n_out, &
    connection_table, &
    prt_map_in, prt_is_connected, &
    qn_mask_in, qn_mask_conn_initial, &
    qn_mask_conn, qn_filter_conn, qn_mask_rest)
call make_pairing_array (eval%pairing_array, &
    eval%get_n_matrix_elements (), &
    connection_table)
call record_links (eval%interaction_t, &
    int_in1, int_in2, connection_index, prt_map_in, prt_map_conn, &
    prt_is_connected, connections_are_resonant)
call connection_table_final (connection_table)

if (eval%get_n_matrix_elements () == 0) then
    print *, "Evaluator product"
    print *, "First interaction"
    call int_in1%basic_write (col_verbose=.true.)
    print *
    print *, "Second interaction"
    call int_in2%basic_write (col_verbose=.true.)
    print *
    call msg_fatal ("Product of density matrices is empty", &
        [var_str (" -----"), &
        var_str ("This happens when two density matrices are convoluted "), &
        var_str ("but the processes they belong to (e.g., production "), &
        var_str ("and decay) do not match. This could happen if the "), &
        var_str ("beam specification does not match the hard "), &
        var_str ("process. Or it may indicate a WHIZARD bug.")])
end if

contains

subroutine compute_index_bounds_and_mappings &
    (int1, int2, n_conn, &
    n_in, n_vir, n_out, n_tot, &
    n_rest, prt_map_in, prt_map_conn)
class(interaction_t), intent(in) :: int1, int2
integer, intent(in) :: n_conn
integer, intent(out) :: n_in, n_vir, n_out, n_tot
integer, dimension(2), intent(out) :: n_rest
type(index_map_t), dimension(2), intent(out) :: prt_map_in

```

```

type(index_map_t), intent(out) :: prt_map_conn
integer, dimension(:), allocatable :: index
integer :: n_in1, n_vir1, n_out1
integer :: n_in2, n_vir2, n_out2
integer :: k
n_in1 = int1%get_n_in ()
n_vir1 = int1%get_n_vir ()
n_out1 = int1%get_n_out () - n_conn
n_rest(1) = n_in1 + n_vir1 + n_out1
n_in2 = int2%get_n_in () - n_conn
n_vir2 = int2%get_n_vir ()
n_out2 = int2%get_n_out ()
n_rest(2) = n_in2 + n_vir2 + n_out2
n_in = n_in1 + n_in2
n_vir = n_vir1 + n_vir2 + n_conn
n_out = n_out1 + n_out2
n_tot = n_in + n_vir + n_out
call index_map_init (prt_map_in, n_rest)
call index_map_init (prt_map_conn, n_conn)
allocate (index (n_tot))
index = [ (i, i = 1, n_tot) ]
prt_map_in(1)%entry(1 : n_in1) = index( 1 : n_in1)
k = n_in1
prt_map_in(2)%entry(1 : n_in2) = index(k + 1 : k + n_in2)
k = k + n_in2
prt_map_in(1)%entry(n_in1 + 1 : n_in1 + n_vir1) = index(k + 1 : k + n_vir1)
k = k + n_vir1
prt_map_in(2)%entry(n_in2 + 1 : n_in2 + n_vir2) = index(k + 1 : k + n_vir2)
k = k + n_vir2
prt_map_conn%entry = index(k + 1 : k + n_conn)
k = k + n_conn
prt_map_in(1)%entry(n_in1 + n_vir1 + 1 : n_rest(1)) = index(k + 1 : k + n_out1)
k = k + n_out1
prt_map_in(2)%entry(n_in2 + n_vir2 + 1 : n_rest(2)) = index(k + 1 : k + n_out2)
end subroutine compute_index_bounds_and_mappings

subroutine connection_table_init &
  (connection_table, state_in1, state_in2, qn_mask_conn, &
   n_conn, connection_index, n_rest, &
   qn_filter_conn, ignore_sub_for_qn_in)
type(connection_table_t), intent(out) :: connection_table
type(state_matrix_t), intent(in), target :: state_in1, state_in2
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_conn
integer, intent(in) :: n_conn
integer, dimension(:,:), intent(in) :: connection_index
integer, dimension(2), intent(in) :: n_rest
type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
logical, intent(in), optional :: ignore_sub_for_qn_in
integer, dimension(2) :: n_me_in
type(state_iterator_t) :: it
type(quantum_numbers_t), dimension(n_conn) :: qn
integer :: i, me_index_in, me_index_conn, n_me_conn
integer, dimension(2) :: me_count
logical :: ignore_sub_for_qn, has_sub_qn

```

```

integer :: i_beam_sub
connection_table%n_conn = n_conn
connection_table%n_rest = n_rest
n_me_in(1) = state_in1%get_n_matrix_elements ()
n_me_in(2) = state_in2%get_n_matrix_elements ()
allocate (connection_table%index_conn (2))
call index_map_init (connection_table%index_conn, n_me_in)
connection_table%index_conn = 0
call connection_table%state%init (n_counters = 2)
do i = 1, 2
  select case (i)
    case (1); call it%init (state_in1)
    case (2); call it%init (state_in2)
  end select
  do while (it%is_valid ())
    qn = it%get_quantum_numbers (connection_index(:,i))
    call qn%undefine (qn_mask_conn)
    if (present (qn_filter_conn)) then
      if (.not. all (qn .match. qn_filter_conn)) then
        call it%advance (); cycle
      end if
    end if
    call quantum_numbers_canonicalize_color (qn)
    me_index_in = it%get_me_index ()
    ignore_sub_for_qn = .false.; if (present (ignore_sub_for_qn_in)) ignore_sub_for_qn = i
    has_sub_qn = .false.
    do i_beam_sub = 1, n_beams_rescaled
      has_sub_qn = has_sub_qn .or. any (qn%get_sub () == i_beam_sub)
    end do
    call connection_table%state%add_state (qn, &
      counter_index = i, &
      ignore_sub_for_qn = .not. (ignore_sub_for_qn .and. has_sub_qn), &
      me_index = me_index_conn)
    call index_map_set_entry (connection_table%index_conn(i), &
      me_index_in, me_index_conn)
    call it%advance ()
  end do
end do
n_me_conn = connection_table%state%get_n_matrix_elements ()
connection_table%n_me_conn = n_me_conn
allocate (connection_table%entry (n_me_conn))
call it%init (connection_table%state)
do while (it%is_valid ())
  i = it%get_me_index ()
  me_count = it%get_me_count ()
  call connection_entry_init (connection_table%entry(i), 2, 2, &
    it%get_quantum_numbers (), me_count, n_rest)
  call it%advance ()
end do
end subroutine connection_table_init

subroutine connection_table_final (connection_table)
  type(connection_table_t), intent(inout) :: connection_table
  call connection_table%state%final ()

```

```

end subroutine connection_table_final

subroutine connection_table_write (connection_table, unit)
  type(connection_table_t), intent(in) :: connection_table
  integer, intent(in), optional :: unit
  integer :: i, j
  integer :: u
  u = given_output_unit (unit)
  write (u, *) "Connection table:"
  call connection_table%state%write (unit)
  if (allocated (connection_table%index_conn)) then
    write (u, *) "  Index mapping input => connection table:"
    do i = 1, size (connection_table%index_conn)
      write (u, *) "    Input state", i
      do j = 1, size (connection_table%index_conn(i))
        write (u, *)      j, &
          index_map_get_entry (connection_table%index_conn(i), j)
      end do
    end do
  end if
  if (allocated (connection_table%entry)) then
    write (u, *) "  Connection table contents:"
    do i = 1, size (connection_table%entry)
      call connection_entry_write (connection_table%entry(i), unit)
    end do
  end if
  if (index_map_exists (connection_table%index_result)) then
    write (u, *) "  Index mapping connection table => output:"
    do i = 1, size (connection_table%index_result)
      write (u, *)      i, &
        index_map_get_entry (connection_table%index_result, i)
    end do
  end if
end subroutine connection_table_write

subroutine connection_table_fill &
  (connection_table, state_in1, state_in2, &
   connection_index, prt_is_connected)
  type(connection_table_t), intent(inout) :: connection_table
  type(state_matrix_t), intent(in), target :: state_in1, state_in2
  integer, dimension(:, :), intent(in) :: connection_index
  type(prt_mask_t), dimension(2), intent(in) :: prt_is_connected
  type(state_iterator_t) :: it
  integer :: index_in, index_conn
  integer :: color_offset
  integer :: n_result_entries
  integer :: i, k
  color_offset = connection_table%state%get_max_color_value ()
  do i = 1, 2
    select case (i)
      case (1); call it%init (state_in1)
      case (2); call it%init (state_in2)
    end select
    do while (it%is_valid ())

```



```

        index_in = it%get_me_index ()
        index_conn = index_map_get_entry &
            (connection_table%index_conn(i), index_in)
        if (index_conn /= 0) then
            call connection_entry_add_state &
                (connection_table%entry(index_conn), i, &
                index_in, it%get_quantum_numbers (), &
                connection_index(:,i), prt_is_connected(i), &
                color_offset)
        end if
        call it%advance ()
    end do
    color_offset = color_offset + state_in1%get_max_color_value ()
end do
n_result_entries = 0
do k = 1, size (connection_table%entry)
    n_result_entries = &
        n_result_entries + product (connection_table%entry(k)%n_index)
end do
call index_map_init (connection_table%index_result, n_result_entries)
end subroutine connection_table_fill

subroutine connection_entry_add_state &
    (entry, i, index_in, qn_in, connection_index, prt_is_connected, &
    color_offset)
    type(connection_entry_t), intent(inout) :: entry
    integer, intent(in) :: i
    integer, intent(in) :: index_in
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
    integer, dimension(:), intent(in) :: connection_index
    type(prt_mask_t), intent(in) :: prt_is_connected
    integer, intent(in) :: color_offset
    integer :: c
    integer, dimension(:,:), allocatable :: color_map
    entry%count(i) = entry%count(i) + 1
    c = entry%count(i)
    call make_color_map (color_map, &
        qn_in(connection_index), entry%qn_conn)
    call index_map_set_entry (entry%index_in(i), c, index_in)
    entry%qn_in_list(i)%qn(:,c) = pack (qn_in, prt_is_connected%entry)
    call quantum_numbers_translate_color &
        (entry%qn_in_list(i)%qn(:,c), color_map, color_offset)
end subroutine connection_entry_add_state

subroutine make_product_interaction (int, &
    n_in, n_vir, n_out, &
    connection_table, &
    prt_map_in, prt_is_connected, &
    qn_mask_in, qn_mask_conn_initial, &
    qn_mask_conn, qn_filter_conn, qn_mask_rest)
    type(interaction_t), intent(out), target :: int
    integer, intent(in) :: n_in, n_vir, n_out
    type(connection_table_t), intent(inout), target :: connection_table
    type(index_map_t), dimension(2), intent(in) :: prt_map_in

```

```

type(prt_mask_t), dimension(2), intent(in) :: prt_is_connected
type(qn_mask_array_t), dimension(2), intent(in) :: qn_mask_in
type(quantum_numbers_mask_t), dimension(:), intent(in) :: &
    qn_mask_conn_initial
type(quantum_numbers_mask_t), intent(in) :: qn_mask_conn
type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
type(quantum_numbers_mask_t), intent(in), optional :: qn_mask_rest
type(index_map_t), dimension(2) :: prt_index_in
type(index_map_t) :: prt_index_conn
integer :: n_tot, n_conn
integer, dimension(2) :: n_rest
integer :: i, j, k, m
type(quantum_numbers_t), dimension(:), allocatable :: qn
type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
type(connection_entry_t), pointer :: entry
integer :: result_index
n_conn = connection_table%n_conn
n_rest = connection_table%n_rest
n_tot = sum (n_rest) + n_conn
allocate (qn (n_tot), qn_mask (n_tot))
do i = 1, 2
    call index_map_init (prt_index_in(i), n_rest(i))
    prt_index_in(i) = &
        prt_map_in(i)%entry ([ (j, j = 1, n_rest(i)) ])
end do
call index_map_init (prt_index_conn, n_conn)
prt_index_conn = prt_map_conn%entry ([ (j, j = 1, n_conn) ])
do i = 1, 2
    if (present (qn_mask_rest)) then
        qn_mask(prt_index_in(i)%entry) = &
            pack (qn_mask_in(i)%mask, prt_is_connected(i)%entry) &
            .or. qn_mask_rest
    else
        qn_mask(prt_index_in(i)%entry) = &
            pack (qn_mask_in(i)%mask, prt_is_connected(i)%entry)
    end if
end do
qn_mask(prt_index_conn%entry) = qn_mask_conn_initial .or. qn_mask_conn
call eval%interaction_t%basic_init (n_in, n_vir, n_out, mask = qn_mask)
m = 1
do i = 1, connection_table%n_me_conn
    entry => connection_table%entry(i)
    qn(prt_index_conn%entry) = &
        quantum_numbers_undefined (entry%qn_conn, qn_mask_conn)
    if (present (qn_filter_conn)) then
        if (.not. all (qn(prt_index_conn%entry) .match. qn_filter_conn)) &
            cycle
    end if
    do j = 1, entry%n_index(1)
        qn(prt_index_in(1)%entry) = entry%qn_in_list(1)%qn(:,j)
        do k = 1, entry%n_index(2)
            qn(prt_index_in(2)%entry) = entry%qn_in_list(2)%qn(:,k)
            call int%add_state (qn, me_index = result_index)
            call index_map_set_entry &

```

```

        (connection_table%index_result, m, result_index)
        m = m + 1
    end do
end do
    call int%freeze ()
end subroutine make_product_interaction

subroutine make_pairing_array (pa, n_matrix_elements, connection_table)
    type(pairing_array_t), dimension(:), intent(out), allocatable :: pa
    integer, intent(in) :: n_matrix_elements
    type(connection_table_t), intent(in), target :: connection_table
    type(connection_entry_t), pointer :: entry
    integer, dimension(:), allocatable :: n_entries
    integer :: i, j, k, m, r
    allocate (pa (n_matrix_elements))
    allocate (n_entries (n_matrix_elements))
    n_entries = 0
    do m = 1, size (connection_table%index_result)
        r = index_map_get_entry (connection_table%index_result, m)
        n_entries(r) = n_entries(r) + 1
    end do
    call pairing_array_init &
        (pa, n_entries, has_i2=.true., has_factor=.false.)
    m = 1
    n_entries = 0
    do i = 1, connection_table%n_me_conn
        entry => connection_table%entry(i)
        do j = 1, entry%n_index(1)
            do k = 1, entry%n_index(2)
                r = index_map_get_entry (connection_table%index_result, m)
                n_entries(r) = n_entries(r) + 1
                pa(r)%i1(n_entries(r)) = &
                    index_map_get_entry (entry%index_in(1), j)
                pa(r)%i2(n_entries(r)) = &
                    index_map_get_entry (entry%index_in(2), k)
                m = m + 1
            end do
        end do
    end do
end subroutine make_pairing_array

subroutine record_links (int, &
    int_in1, int_in2, connection_index, prt_map_in, prt_map_conn, &
    prt_is_connected, connections_are_resonant)
    class(interaction_t), intent(inout) :: int
    class(interaction_t), intent(in), target :: int_in1, int_in2
    integer, dimension(:,:), intent(in) :: connection_index
    type(index_map_t), dimension(2), intent(in) :: prt_map_in
    type(index_map_t), intent(in) :: prt_map_conn
    type(prt_mask_t), dimension(2), intent(in) :: prt_is_connected
    logical, intent(in), optional :: connections_are_resonant
    type(index_map_t), dimension(2) :: prt_map_all
    integer :: i, j, k, ival

```

```

call index_map_init (prt_map_all(1), size (prt_is_connected(1)))
k = 0
j = 0
do i = 1, size (prt_is_connected(1))
  if (prt_is_connected(1)%entry(i)) then
    j = j + 1
    ival = index_map_get_entry (prt_map_in(1), j)
    call index_map_set_entry (prt_map_all(1), i, ival)
  else
    k = k + 1
    ival = index_map_get_entry (prt_map_conn, k)
    call index_map_set_entry (prt_map_all(1), i, ival)
  end if
  call int%set_source_link (ival, int_in1, i)
end do
call int_in1%transfer_relations (int, prt_map_all(1)%entry)
call index_map_init (prt_map_all(2), size (prt_is_connected(2)))
j = 0
do i = 1, size (prt_is_connected(2))
  if (prt_is_connected(2)%entry(i)) then
    j = j + 1
    ival = index_map_get_entry (prt_map_in(2), j)
    call index_map_set_entry (prt_map_all(2), i, ival)
    call int%set_source_link (ival, int_in2, i)
  else
    call index_map_set_entry (prt_map_all(2), i, 0)
  end if
end do
call int_in2%transfer_relations (int, prt_map_all(2)%entry)
call int%relate_connections &
  (int_in2, connection_index(:,2), prt_map_all(2)%entry, &
  prt_map_conn%entry, connections_are_resonant)
end subroutine record_links

end subroutine evaluator_init_product

```

12.3.5 Creating an evaluator: square

The generic initializer for an evaluator that squares a matrix element. Depending on the provided mask, we select the appropriate specific initializer for either diagonal or non-diagonal helicity density matrices.

(Evaluators: evaluator: TBP)+≡

```
procedure :: init_square => evaluator_init_square
```

(Evaluators: procedures)+≡

```

subroutine evaluator_init_square (eval, int_in, qn_mask, &
  col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
class(evaluator_t), intent(out), target :: eval
class(interaction_t), intent(in), target :: int_in
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
integer, dimension(:, :), intent(in), optional :: col_flow_index
complex(default), dimension(:), intent(in), optional :: col_factor
integer, dimension(:), intent(in), optional :: col_index_hi

```

```

logical, intent(in), optional :: expand_color_flows
integer, intent(in), optional :: nc
if (all (qn_mask%diagonal_helicity ())) then
    call eval%init_square_diag (int_in, qn_mask, &
        col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
else
    call eval%init_square_nondiag (int_in, qn_mask, &
        col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)
end if
end subroutine evaluator_init_square

```

Color-summed squared matrix (diagonal helicities)

The initializer for an evaluator that squares a matrix element, including color factors. The mask must be such that off-diagonal matrix elements are excluded.

If `color_flows` is set, the evaluator keeps color-flow entries separate and drops all interfering color structures. The color factors are set to unity in this case.

There is only one input interaction. The quantum-number mask is an array, one entry for each particle, so they can be treated individually. For academic purposes, we allow for the number of colors being different from three (but 3 is the default).

The algorithm is analogous to multiplication, with a few notable differences:

1. The connected particles are known, the correspondence is one-to-one. All particles are connected, and the mapping of indices is trivial, which simplifies the following steps.
2. **accumulate_connected_states**: The matrix of connected states encompasses all particles, but color indices are removed. However, ghost states are still kept separate from physical color states. No color-index reassignment is necessary.
3. The table of connections contains single index and quantum-number arrays instead of pairs of them. They are paired with themselves in all possible ways.
4. **make_squared_interaction**: Now apply the predefined quantum-numbers mask, which usually collects all color states (physical and ghosts), and possibly a helicity sum.
5. **make_pairing_array**: For each pair of input states, compute the color factor (including a potential ghost-parity sign) and store this in the pairing array together with the matrix-element indices for multiplication.
6. **record_links**: This is again trivial due to the one-to-one correspondence.

(Evaluators: evaluator: TBP)+≡

```

procedure :: init_square_diag => evaluator_init_square_diag

```

```

(Evaluators: procedures)+≡
subroutine evaluator_init_square_diag (eval, int_in, qn_mask, &
    col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)

class(evaluator_t), intent(out), target :: eval
class(interaction_t), intent(in), target :: int_in
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
integer, dimension(:,:), intent(in), optional :: col_flow_index
complex(default), dimension(:), intent(in), optional :: col_factor
integer, dimension(:), intent(in), optional :: col_index_hi
logical, intent(in), optional :: expand_color_flows
integer, intent(in), optional :: nc

integer :: n_in, n_vir, n_out, n_tot
type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask_initial
type(state_matrix_t), pointer :: state_in

type :: connection_table_t
    integer :: n_tot = 0
    integer :: n_me_conn = 0
    type(state_matrix_t) :: state
    type(index_map_t) :: index_conn
    type(connection_entry_t), dimension(:), allocatable :: entry
    type(index_map_t) :: index_result
end type connection_table_t
type(connection_table_t) :: connection_table

logical :: sum_colors
type(color_table_t) :: color_table

if (present (expand_color_flows)) then
    sum_colors = .not. expand_color_flows
else
    sum_colors = .true.
end if

if (sum_colors) then
    eval%type = EVAL_SQUARE_WITH_COLOR_FACTORS
else
    eval%type = EVAL_SQUARED_FLOWS
end if
eval%int_in1 => int_in

n_in = int_in%get_n_in ()
n_vir = int_in%get_n_vir ()
n_out = int_in%get_n_out ()
n_tot = int_in%get_n_tot ()

state_in => int_in%get_state_matrix_ptr ()

allocate (qn_mask_initial (n_tot))
qn_mask_initial = int_in%get_mask ()
call qn_mask_initial%set_color (sum_colors, mask_cg=.false.)
if (sum_colors) then

```

```

    call color_table_init (color_table, state_in, n_tot)
    if (present (col_flow_index) .and. present (col_factor) &
        .and. present (col_index_hi)) then
        call color_table_set_color_factors &
            (color_table, col_flow_index, col_factor, col_index_hi)
    end if
end if

call connection_table_init (connection_table, state_in, &
    qn_mask_initial, qn_mask, n_tot)
call connection_table_fill (connection_table, state_in)
call make_squared_interaction (eval%interaction_t, &
    n_in, n_vir, n_out, n_tot, &
    connection_table, sum_colors, qn_mask_initial .or. qn_mask)
call make_pairing_array (eval%pairing_array, &
    eval%get_n_matrix_elements (), &
    connection_table, sum_colors, color_table, n_in, n_tot, nc)
call record_links (eval, int_in, n_tot)
call connection_table_final (connection_table)

contains

subroutine connection_table_init &
    (connection_table, state_in, qn_mask_in, qn_mask, n_tot)
    type(connection_table_t), intent(out) :: connection_table
    type(state_matrix_t), intent(in), target :: state_in
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    integer, intent(in) :: n_tot
    type(quantum_numbers_t), dimension(n_tot) :: qn
    type(state_iterator_t) :: it
    integer :: i, n_me_in, me_index_in
    integer :: me_index_conn, n_me_conn
    integer, dimension(1) :: me_count
    logical :: qn_passed
    connection_table%n_tot = n_tot
    n_me_in = state_in%get_n_matrix_elements ()
    call index_map_init (connection_table%index_conn, n_me_in)
    connection_table%index_conn = 0
    call connection_table%state%init (n_counters=1)
    call it%init (state_in)
    do while (it%is_valid ())
        qn = it%get_quantum_numbers ()
        if (all (quantum_numbers_are_physical (qn, qn_mask))) then
            call qn%undefine (qn_mask_in)
            qn_passed = .true.
            if (qn_passed) then
                me_index_in = it%get_me_index ()
                call connection_table%state%add_state (qn, &
                    counter_index = 1, me_index = me_index_conn)
                call index_map_set_entry (connection_table%index_conn, &
                    me_index_in, me_index_conn)
            end if
        end if
    end if
end if

```

```

        call it%advance ()
    end do
    n_me_conn = connection_table%state%get_n_matrix_elements ()
    connection_table%n_me_conn = n_me_conn
    allocate (connection_table%entry (n_me_conn))
    call it%init (connection_table%state)
    do while (it%is_valid ())
        i = it%get_me_index ()
        me_count = it%get_me_count ()
        call connection_entry_init (connection_table%entry(i), 1, 2, &
            it%get_quantum_numbers (), me_count, [n_tot])
        call it%advance ()
    end do
end subroutine connection_table_init

subroutine connection_table_final (connection_table)
    type(connection_table_t), intent(inout) :: connection_table
    call connection_table%state%final ()
end subroutine connection_table_final

subroutine connection_table_write (connection_table, unit)
    type(connection_table_t), intent(in) :: connection_table
    integer, intent(in), optional :: unit
    integer :: i
    integer :: u
    u = given_output_unit (unit)
    write (u, *) "Connection table:"
    call connection_table%state%write (unit)
    if (index_map_exists (connection_table%index_conn)) then
        write (u, *) "  Index mapping input => connection table:"
        do i = 1, size (connection_table%index_conn)
            write (u, *) i, &
                index_map_get_entry (connection_table%index_conn, i)
        end do
    end if
    if (allocated (connection_table%entry)) then
        write (u, *) "  Connection table contents"
        do i = 1, size (connection_table%entry)
            call connection_entry_write (connection_table%entry(i), unit)
        end do
    end if
    if (index_map_exists (connection_table%index_result)) then
        write (u, *) "  Index mapping connection table => output"
        do i = 1, size (connection_table%index_result)
            write (u, *) i, &
                index_map_get_entry (connection_table%index_result, i)
        end do
    end if
end subroutine connection_table_write

subroutine connection_table_fill (connection_table, state)
    type(connection_table_t), intent(inout) :: connection_table
    type(state_matrix_t), intent(in), target :: state
    integer :: index_in, index_conn, n_result_entries

```



```

type(state_iterator_t) :: it
integer :: k
call it%init (state)
do while (it%is_valid ())
    index_in = it%get_me_index ()
    index_conn = &
        index_map_get_entry (connection_table%index_conn, index_in)
    if (index_conn /= 0) then
        call connection_entry_add_state &
            (connection_table%entry(index_conn), &
            index_in, it%get_quantum_numbers ())
    end if
    call it%advance ()
end do
n_result_entries = 0
do k = 1, size (connection_table%entry)
    n_result_entries = &
        n_result_entries + connection_table%entry(k)%n_index(1) ** 2
end do
call index_map_init (connection_table%index_result, n_result_entries)
connection_table%index_result = 0
end subroutine connection_table_fill

subroutine connection_entry_add_state (entry, index_in, qn_in)
    type(connection_entry_t), intent(inout) :: entry
    integer, intent(in) :: index_in
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
    integer :: c
    entry%count = entry%count + 1
    c = entry%count(1)
    call index_map_set_entry (entry%index_in(1), c, index_in)
    entry%qn_in_list(1)%qn(:,c) = qn_in
end subroutine connection_entry_add_state

subroutine make_squared_interaction (int, &
    n_in, n_vir, n_out, n_tot, &
    connection_table, sum_colors, qn_mask)
    type(interaction_t), intent(out), target :: int
    integer, intent(in) :: n_in, n_vir, n_out, n_tot
    type(connection_table_t), intent(inout), target :: connection_table
    logical, intent(in) :: sum_colors
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    type(connection_entry_t), pointer :: entry
    integer :: result_index, n_contrib
    integer :: i, m
    type(quantum_numbers_t), dimension(n_tot) :: qn
    call eval%interaction_t%basic_init (n_in, n_vir, n_out, mask=qn_mask)
    m = 0
    do i = 1, connection_table%n_me_conn
        entry => connection_table%entry(i)
        qn = quantum_numbers_undefined (entry%qn_conn, qn_mask)
        if (.not. sum_colors) call qn(1:n_in)%invert_color ()
        call int%add_state (qn, me_index = result_index)
        n_contrib = entry%n_index(1) ** 2
    end do

```

```

        connection_table%index_result%entry(m+1:m+n_contrib) = result_index
        m = m + n_contrib
    end do
    call int%freeze ()
end subroutine make_squared_interaction

subroutine make_pairing_array (pa, &
    n_matrix_elements, connection_table, sum_colors, color_table, &
    n_in, n_tot, nc)
    type(pairing_array_t), dimension(:), intent(out), allocatable :: pa
    integer, intent(in) :: n_matrix_elements
    type(connection_table_t), intent(in), target :: connection_table
    logical, intent(in) :: sum_colors
    type(color_table_t), intent(inout) :: color_table
    type(connection_entry_t), pointer :: entry
    integer, intent(in) :: n_in, n_tot
    integer, intent(in), optional :: nc
    integer, dimension(:), allocatable :: n_entries
    integer :: i, k, l, ks, ls, m, r
    integer :: color_multiplicity_in
    allocate (pa (n_matrix_elements))
    allocate (n_entries (n_matrix_elements))
    n_entries = 0
    do m = 1, size (connection_table%index_result)
        r = index_map_get_entry (connection_table%index_result, m)
        n_entries(r) = n_entries(r) + 1
    end do
    call pairing_array_init &
        (pa, n_entries, has_i2 = sum_colors, has_factor = sum_colors)
    m = 1
    n_entries = 0
    do i = 1, connection_table%n_me_conn
        entry => connection_table%entry(i)
        do k = 1, entry%n_index(1)
            if (sum_colors) then
                color_multiplicity_in = product (abs &
                    (entry%qn_in_list(1)%qn(:n_in, k)%get_color_type ()))
            do l = 1, entry%n_index(1)
                r = index_map_get_entry (connection_table%index_result, m)
                n_entries(r) = n_entries(r) + 1
                ks = index_map_get_entry (entry%index_in(1), k)
                ls = index_map_get_entry (entry%index_in(1), l)
                pa(r)%i1(n_entries(r)) = ks
                pa(r)%i2(n_entries(r)) = ls
                pa(r)%factor(n_entries(r)) = &
                    color_table_get_color_factor (color_table, ks, ls, nc) &
                    / color_multiplicity_in
                m = m + 1
            end do
        else
            r = index_map_get_entry (connection_table%index_result, m)
            n_entries(r) = n_entries(r) + 1
            ks = index_map_get_entry (entry%index_in(1), k)
            pa(r)%i1(n_entries(r)) = ks

```

```

        m = m + 1
    end if
end do
end subroutine make_pairing_array

subroutine record_links (int, int_in, n_tot)
    class(interaction_t), intent(inout) :: int
    class(interaction_t), intent(in), target :: int_in
    integer, intent(in) :: n_tot
    integer, dimension(n_tot) :: map
    integer :: i
    do i = 1, n_tot
        call int%set_source_link (i, int_in, i)
    end do
    map = [ (i, i = 1, n_tot) ]
    call int_in%transfer_relations (int, map)
end subroutine record_links

end subroutine evaluator_init_square_diag

```

Color-summed squared matrix (support nodiagonal helicities)

The initializer for an evaluator that squares a matrix element, including color factors. Unless requested otherwise by the quantum-number mask, the result contains off-diagonal matrix elements. (The input interaction must be diagonal since it represents an amplitude, not a density matrix.)

There is only one input interaction. The quantum-number mask is an array, one entry for each particle, so they can be treated individually. For academic purposes, we allow for the number of colors being different from three (but 3 is the default).

The algorithm is analogous to the previous one, with some additional complications due to the necessity to loop over two helicity indices.

(Evaluators: evaluator: TBP)+≡

```

    procedure :: init_square_nondiag => evaluator_init_square_nondiag

```

(Evaluators: procedures)+≡

```

    subroutine evaluator_init_square_nondiag (eval, int_in, qn_mask, &
        col_flow_index, col_factor, col_index_hi, expand_color_flows, nc)

        class(evaluator_t), intent(out), target :: eval
        class(interaction_t), intent(in), target :: int_in
        type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
        integer, dimension(:,:), intent(in), optional :: col_flow_index
        complex(default), dimension(:), intent(in), optional :: col_factor
        integer, dimension(:), intent(in), optional :: col_index_hi
        logical, intent(in), optional :: expand_color_flows
        integer, intent(in), optional :: nc

        integer :: n_in, n_vir, n_out, n_tot
        type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask_initial
        type(state_matrix_t), pointer :: state_in

```

```

type :: connection_table_t
  integer :: n_tot = 0
  integer :: n_me_conn = 0
  type(state_matrix_t) :: state
  type(index_map2_t) :: index_conn
  type(connection_entry_t), dimension(:), allocatable :: entry
  type(index_map_t) :: index_result
end type connection_table_t
type(connection_table_t) :: connection_table

logical :: sum_colors
type(color_table_t) :: color_table

if (present (expand_color_flows)) then
  sum_colors = .not. expand_color_flows
else
  sum_colors = .true.
end if

if (sum_colors) then
  eval%type = EVAL_SQUARE_WITH_COLOR_FACTORS
else
  eval%type = EVAL_SQUARED_FLOWS
end if
eval%int_in1 => int_in

n_in = int_in%get_n_in ()
n_vir = int_in%get_n_vir ()
n_out = int_in%get_n_out ()
n_tot = int_in%get_n_tot ()

state_in => int_in%get_state_matrix_ptr ()

allocate (qn_mask_initial (n_tot))
qn_mask_initial = int_in%get_mask ()
call qn_mask_initial%set_color (sum_colors, mask_cg=.false.)
if (sum_colors) then
  call color_table_init (color_table, state_in, n_tot)
  if (present (col_flow_index) .and. present (col_factor) &
    .and. present (col_index_hi)) then
    call color_table_set_color_factors &
      (color_table, col_flow_index, col_factor, col_index_hi)
  end if
end if

call connection_table_init (connection_table, state_in, &
  qn_mask_initial, qn_mask, n_tot)
call connection_table_fill (connection_table, state_in)
call make_squared_interaction (eval%interaction_t, &
  n_in, n_vir, n_out, n_tot, &
  connection_table, sum_colors, qn_mask_initial .or. qn_mask)
call make_pairing_array (eval%pairing_array, &
  eval%get_n_matrix_elements (), &

```

```

        connection_table, sum_colors, color_table, n_in, n_tot, nc)
call record_links (eval, int_in, n_tot)
call connection_table_final (connection_table)

```

contains

```

subroutine connection_table_init &
    (connection_table, state_in, qn_mask_in, qn_mask, n_tot)
type(connection_table_t), intent(out) :: connection_table
type(state_matrix_t), intent(in), target :: state_in
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
integer, intent(in) :: n_tot
type(quantum_numbers_t), dimension(n_tot) :: qn1, qn2, qn
type(state_iterator_t) :: it1, it2, it
integer :: i, n_me_in, me_index_in1, me_index_in2
integer :: me_index_conn, n_me_conn
integer, dimension(1) :: me_count
logical :: qn_passed
connection_table%n_tot = n_tot
n_me_in = state_in%get_n_matrix_elements ()
call index_map2_init (connection_table%index_conn, n_me_in)
connection_table%index_conn = 0
call connection_table%state%init (n_counters=1)
call it1%init (state_in)
do while (it1%is_valid ())
    qn1 = it1%get_quantum_numbers ()
    me_index_in1 = it1%get_me_index ()
    call it2%init (state_in)
    do while (it2%is_valid ())
        qn2 = it2%get_quantum_numbers ()
        if (all (quantum_numbers_are_compatible (qn1, qn2, qn_mask))) then
            qn = qn1 .merge. qn2
            call qn%undefine (qn_mask_in)
            qn_passed = .true.
            if (qn_passed) then
                me_index_in2 = it2%get_me_index ()
                call connection_table%state%add_state (qn, &
                    counter_index = 1, me_index = me_index_conn)
                call index_map2_set_entry (connection_table%index_conn, &
                    me_index_in1, me_index_in2, me_index_conn)
            end if
        end if
        call it2%advance ()
    end do
    call it1%advance ()
end do
n_me_conn = connection_table%state%get_n_matrix_elements ()
connection_table%n_me_conn = n_me_conn
allocate (connection_table%entry (n_me_conn))
call it%init (connection_table%state)
do while (it%is_valid ())
    i = it%get_me_index ()
    me_count = it%get_me_count ()

```

```

        call connection_entry_init (connection_table%entry(i), 1, 2, &
            it%get_quantum_numbers (), me_count, [n_tot])
        call it%advance ()
    end do
end subroutine connection_table_init

subroutine connection_table_final (connection_table)
    type(connection_table_t), intent(inout) :: connection_table
    call connection_table%state%final ()
end subroutine connection_table_final

subroutine connection_table_write (connection_table, unit)
    type(connection_table_t), intent(in) :: connection_table
    integer, intent(in), optional :: unit
    integer :: i, j
    integer :: u
    u = given_output_unit (unit)
    write (u, *) "Connection table:"
    call connection_table%state%write (unit)
    if (index_map2_exists (connection_table%index_conn)) then
        write (u, *) "  Index mapping input => connection table:"
        do i = 1, size (connection_table%index_conn)
            do j = 1, size (connection_table%index_conn)
                write (u, *)  i, j, &
                    index_map2_get_entry (connection_table%index_conn, i, j)
            end do
        end do
    end if
    if (allocated (connection_table%entry)) then
        write (u, *) "  Connection table contents"
        do i = 1, size (connection_table%entry)
            call connection_entry_write (connection_table%entry(i), unit)
        end do
    end if
    if (index_map_exists (connection_table%index_result)) then
        write (u, *) "  Index mapping connection table => output"
        do i = 1, size (connection_table%index_result)
            write (u, *)  i, &
                index_map_get_entry (connection_table%index_result, i)
        end do
    end if
end subroutine connection_table_write

subroutine connection_table_fill (connection_table, state)
    type(connection_table_t), intent(inout), target :: connection_table
    type(state_matrix_t), intent(in), target :: state
    integer :: index1_in, index2_in, index_conn, n_result_entries
    type(state_iterator_t) :: it1, it2
    integer :: k
    call it1%init (state)
    do while (it1%is_valid ())
        index1_in = it1%get_me_index ()
        call it2%init (state)
        do while (it2%is_valid ())

```

```

        index2_in = it2%get_me_index ()
        index_conn = index_map2_get_entry &
            (connection_table%index_conn, index1_in, index2_in)
        if (index_conn /= 0) then
            call connection_entry_add_state &
                (connection_table%entry(index_conn), &
                    index1_in, index2_in, &
                    it1%get_quantum_numbers () &
                    .merge. &
                    it2%get_quantum_numbers ())
        end if
        call it2%advance ()
    end do
    call it1%advance ()
end do
n_result_entries = 0
do k = 1, size (connection_table%entry)
    n_result_entries = &
        n_result_entries + connection_table%entry(k)%n_index(1)
end do
call index_map_init (connection_table%index_result, n_result_entries)
connection_table%index_result = 0
end subroutine connection_table_fill

subroutine connection_entry_add_state (entry, index1_in, index2_in, qn_in)
    type(connection_entry_t), intent(inout) :: entry
    integer, intent(in) :: index1_in, index2_in
    type(quantum_numbers_t), dimension(:), intent(in) :: qn_in
    integer :: c
    entry%count = entry%count + 1
    c = entry%count(1)
    call index_map_set_entry (entry%index_in(1), c, index1_in)
    call index_map_set_entry (entry%index_in(2), c, index2_in)
    entry%qn_in_list(1)%qn(:,c) = qn_in
end subroutine connection_entry_add_state

subroutine make_squared_interaction (int, &
    n_in, n_vir, n_out, n_tot, &
    connection_table, sum_colors, qn_mask)
    type(interaction_t), intent(out), target :: int
    integer, intent(in) :: n_in, n_vir, n_out, n_tot
    type(connection_table_t), intent(inout), target :: connection_table
    logical, intent(in) :: sum_colors
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    type(connection_entry_t), pointer :: entry
    integer :: result_index
    integer :: i, k, m
    type(quantum_numbers_t), dimension(n_tot) :: qn
    call eval%interaction_t%basic_init (n_in, n_vir, n_out, mask=qn_mask)
    m = 0
    do i = 1, connection_table%n_me_conn
        entry => connection_table%entry(i)
        do k = 1, size (entry%qn_in_list(1)%qn, 2)
            qn = quantum_numbers_undefined &

```

```

        (entry%qn_in_list(1)%qn(:,k), qn_mask)
    if (.not. sum_colors) call qn(1:n_in)%invert_color ()
    call int%add_state (qn, me_index = result_index)
    call index_map_set_entry (connection_table%index_result, m + 1, &
        result_index)
    m = m + 1
end do
end do
call int%freeze ()
end subroutine make_squared_interaction

subroutine make_pairing_array (pa, &
    n_matrix_elements, connection_table, sum_colors, color_table, &
    n_in, n_tot, nc)
    type(pairing_array_t), dimension(:), intent(out), allocatable :: pa
    integer, intent(in) :: n_matrix_elements
    type(connection_table_t), intent(in), target :: connection_table
    logical, intent(in) :: sum_colors
    type(color_table_t), intent(inout) :: color_table
    type(connection_entry_t), pointer :: entry
    integer, intent(in) :: n_in, n_tot
    integer, intent(in), optional :: nc
    integer, dimension(:), allocatable :: n_entries
    integer :: i, k, k1s, k2s, m, r
    integer :: color_multiplicity_in
    allocate (pa (n_matrix_elements))
    allocate (n_entries (n_matrix_elements))
    n_entries = 0
    do m = 1, size (connection_table%index_result)
        r = index_map_get_entry (connection_table%index_result, m)
        n_entries(r) = n_entries(r) + 1
    end do
    call pairing_array_init &
        (pa, n_entries, has_i2 = sum_colors, has_factor = sum_colors)
    m = 1
    n_entries = 0
    do i = 1, connection_table%n_me_conn
        entry => connection_table%entry(i)
        do k = 1, entry%n_index(1)
            r = index_map_get_entry (connection_table%index_result, m)
            n_entries(r) = n_entries(r) + 1
            if (sum_colors) then
                k1s = index_map_get_entry (entry%index_in(1), k)
                k2s = index_map_get_entry (entry%index_in(2), k)
                pa(r)%i1(n_entries(r)) = k1s
                pa(r)%i2(n_entries(r)) = k2s
                color_multiplicity_in = product (abs &
                    (entry%qn_in_list(1)%qn(:,n_in, k)%get_color_type ()))
                pa(r)%factor(n_entries(r)) = &
                    color_table_get_color_factor (color_table, k1s, k2s, nc) &
                    / color_multiplicity_in
            else
                k1s = index_map_get_entry (entry%index_in(1), k)
                pa(r)%i1(n_entries(r)) = k1s
            end if
        end do
    end do
end subroutine

```



```

        end if
        m = m + 1
    end do
end do
end subroutine make_pairing_array

subroutine record_links (int, int_in, n_tot)
    class(interaction_t), intent(inout) :: int
    class(interaction_t), intent(in), target :: int_in
    integer, intent(in) :: n_tot
    integer, dimension(n_tot) :: map
    integer :: i
    do i = 1, n_tot
        call int%set_source_link (i, int_in, i)
    end do
    map = [ (i, i = 1, n_tot) ]
    call int_in%transfer_relations (int, map)
end subroutine record_links

end subroutine evaluator_init_square_nondiag

```

Copy with additional contracted color states

This evaluator involves no square or multiplication, its matrix elements are just copies of the (single) input interaction. However, the state matrix of the interaction contains additional states that have color indices contracted. This is used for copies of the beam or structure-function interactions that need to match the hard interaction also in the case where its color indices coincide.

(Evaluators: evaluator: TBP)+≡

```
procedure :: init_color_contractions => evaluator_init_color_contractions
```

(Evaluators: procedures)+≡

```

subroutine evaluator_init_color_contractions (eval, int_in)
    class(evaluator_t), intent(out), target :: eval
    type(interaction_t), intent(in), target :: int_in
    integer :: n_in, n_vir, n_out, n_tot
    type(state_matrix_t) :: state_with_contractions
    integer, dimension(:), allocatable :: me_index
    integer, dimension(:), allocatable :: result_index
    eval%type = EVAL_COLOR_CONTRACTION
    eval%int_in1 => int_in
    n_in = int_in%get_n_in ()
    n_vir = int_in%get_n_vir ()
    n_out = int_in%get_n_out ()
    n_tot = int_in%get_n_tot ()
    state_with_contractions = int_in%get_state_matrix_ptr ()
    call state_with_contractions%add_color_contractions ()
    call make_contracted_interaction (eval%interaction_t, &
        me_index, result_index, &
        n_in, n_vir, n_out, n_tot, &
        state_with_contractions, int_in%get_mask ())
    call make_pairing_array (eval%pairing_array, me_index, result_index)
    call record_links (eval, int_in, n_tot)

```

```

call state_with_contractions%final ()

contains

subroutine make_contracted_interaction (int, &
    me_index, result_index, &
    n_in, n_vir, n_out, n_tot, state, qn_mask)
    type(interaction_t), intent(out), target :: int
    integer, dimension(:), intent(out), allocatable :: me_index
    integer, dimension(:), intent(out), allocatable :: result_index
    integer, intent(in) :: n_in, n_vir, n_out, n_tot
    type(state_matrix_t), intent(in) :: state
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    type(state_iterator_t) :: it
    integer :: n_me, i
    type(quantum_numbers_t), dimension(n_tot) :: qn
    call int%basic_init (n_in, n_vir, n_out, mask=qn_mask)
    n_me = state%get_n_leaves ()
    allocate (me_index (n_me))
    allocate (result_index (n_me))
    call it%init (state)
    i = 0
    do while (it%is_valid ())
        i = i + 1
        me_index(i) = it%get_me_index ()
        qn = it%get_quantum_numbers ()
        call int%add_state (qn, me_index = result_index(i))
        call it%advance ()
    end do
    call int%freeze ()
end subroutine make_contracted_interaction

subroutine make_pairing_array (pa, me_index, result_index)
    type(pairing_array_t), dimension(:), intent(out), allocatable :: pa
    integer, dimension(:), intent(in) :: me_index, result_index
    integer, dimension(:), allocatable :: n_entries
    integer :: n_matrix_elements, r, i, k
    !!! The result indices of the appended color contracted states
    !!! start counting from 1 again. For the pairing array, we currently
    !!! only take the first part of ascending indices into account
    !!! excluding the color contracted states.
    n_matrix_elements = size (me_index)
    k = 0
    do i = 1, n_matrix_elements
        r = result_index(i)
        if (r < i) exit
        k = r
    end do
    allocate (pa (k))
    allocate (n_entries (k))
    n_entries = 1
    call pairing_array_init &
        (pa, n_entries, has_i2=.false., has_factor=.false.)
    do i = 1, k

```

```

        r = result_index(i)
        pa(r)%i1(1) = me_index(i)
    end do
end subroutine make_pairing_array

subroutine record_links (int, int_in, n_tot)
    class(interaction_t), intent(inout) :: int
    class(interaction_t), intent(in), target :: int_in
    integer, intent(in) :: n_tot
    integer, dimension(n_tot) :: map
    integer :: i
    do i = 1, n_tot
        call int%set_source_link (i, int_in, i)
    end do
    map = [ (i, i = 1, n_tot) ]
    call int_in%transfer_relations (int, map)
end subroutine record_links

end subroutine evaluator_init_color_contractions

```

Auxiliary procedure for initialization

This will become a standard procedure in F2008. The result is true if the number of true values in the mask is odd. We use the function for determining the ghost parity of a quantum-number array.

[tho:] It's not used anymore and `mod (count (mask), 2) == 1` is a cooler implementation anyway.

```

<(UNUSED) Evaluators: procedures>≡
function parity (mask)
    logical :: parity
    logical, dimension(:) :: mask
    integer :: i
    parity = .false.
    do i = 1, size (mask)
        if (mask(i)) parity = .not. parity
    end do
end function parity

```

Reassign external source links from one to another.

```

<Evaluators: public>+≡
    public :: evaluator_reassign_links

<Evaluators: interfaces>+≡
    interface evaluator_reassign_links
        module procedure evaluator_reassign_links_eval
        module procedure evaluator_reassign_links_int
    end interface

<Evaluators: procedures>+≡
    subroutine evaluator_reassign_links_eval (eval, eval_src, eval_target)
        type(evaluator_t), intent(inout) :: eval
        type(evaluator_t), intent(in) :: eval_src
    end subroutine evaluator_reassign_links_eval

```

```

type(evaluator_t), intent(in), target :: eval_target
if (associated (eval%int_in1)) then
  if (eval%int_in1%get_tag () == eval_src%get_tag ()) then
    eval%int_in1 => eval_target%interaction_t
  end if
end if
if (associated (eval%int_in2)) then
  if (eval%int_in2%get_tag () == eval_src%get_tag ()) then
    eval%int_in2 => eval_target%interaction_t
  end if
end if
call interaction_reassign_links &
  (eval%interaction_t, eval_src%interaction_t, &
  eval_target%interaction_t)
end subroutine evaluator_reassign_links_eval

subroutine evaluator_reassign_links_int (eval, int_src, int_target)
  type(evaluator_t), intent(inout) :: eval
  type(interaction_t), intent(in) :: int_src
  type(interaction_t), intent(in), target :: int_target
  if (associated (eval%int_in1)) then
    if (eval%int_in1%get_tag () == int_src%get_tag ()) then
      eval%int_in1 => int_target
    end if
  end if
  if (associated (eval%int_in2)) then
    if (eval%int_in2%get_tag () == int_src%get_tag ()) then
      eval%int_in2 => int_target
    end if
  end if
  call interaction_reassign_links (eval%interaction_t, int_src, int_target)
end subroutine evaluator_reassign_links_int

```

Return flavor, momentum, and position of the first unstable particle present in the interaction.

(Evaluators: public)+≡

```
public :: evaluator_get_unstable_particle
```

(Evaluators: procedures)+≡

```

subroutine evaluator_get_unstable_particle (eval, flv, p, i)
  type(evaluator_t), intent(in) :: eval
  type(flavor_t), intent(out) :: flv
  type(vector4_t), intent(out) :: p
  integer, intent(out) :: i
  call interaction_get_unstable_particle (eval%interaction_t, flv, p, i)
end subroutine evaluator_get_unstable_particle

```

(Evaluators: public)+≡

```
public :: evaluator_get_int_in_ptr
```

(Evaluators: procedures)+≡

```

function evaluator_get_int_in_ptr (eval, i) result (int_in)
  class(interaction_t), pointer :: int_in
  type(evaluator_t), intent(in), target :: eval

```

```

integer, intent(in) :: i
if (i == 1) then
    int_in => eval%int_in1
else if (i == 2) then
    int_in => eval%int_in2
else
    int_in => null ()
end if
end function evaluator_get_int_in_ptr

```

12.3.6 Creating an evaluator: identity

The identity evaluator creates a copy of the first input evaluator; the second input is not used.

All particles link back to the input evaluator and the internal relations are copied. As evaluation does take a shortcut by cloning the matrix elements, the pairing array is not used and does not have to be set up.

```

(Evaluators: evaluator: TBP)+≡
    procedure :: init_identity => evaluator_init_identity

(Evaluators: procedures)+≡
    subroutine evaluator_init_identity (eval, int)
        class(evaluator_t), intent(out), target :: eval
        class(interaction_t), intent(in), target :: int
        integer :: n_in, n_out, n_vir, n_tot
        integer :: i
        integer, dimension(:), allocatable :: map
        type(state_matrix_t), pointer :: state
        type(state_iterator_t) :: it
        eval%type = EVAL_IDENTITY
        eval%int_in1 => int
        nullify (eval%int_in2)
        n_in = int%get_n_in ()
        n_out = int%get_n_out ()
        n_vir = int%get_n_vir ()
        n_tot = int%get_n_tot ()
        call eval%interaction_t%basic_init (n_in, n_vir, n_out, &
            mask = int%get_mask (), &
            resonant = int%get_resonance_flags ())
        do i = 1, n_tot
            call eval%set_source_link (i, int, i)
        end do
        allocate (map(n_tot))
        map = [(i, i = 1, n_tot)]
        call int%transfer_relations (eval, map)
        state => int%get_state_matrix_ptr ()
        call it%init (state)
        do while (it%is_valid ())
            call eval%add_state (it%get_quantum_numbers (), &
                it%get_me_index ())
            call it%advance ()
        end do
    end subroutine

```

```

call eval%freeze ()

end subroutine evaluator_init_identity

```

12.3.7 Creating an evaluator: quantum number sum

This evaluator operates on the diagonal of a density matrix and sums over the quantum numbers specified by the mask. The optional argument **drop** allows to drop a particle from the resulting density matrix. The handling of virtuals is not completely sane, especially in connection with dropping particles.

When summing over matrix element entries, we keep the separation into entries and normalization (in the corresponding evaluation routine below).

```

(Evaluators: evaluator: TBP)+≡
  procedure :: init_qn_sum => evaluator_init_qn_sum

(Evaluators: procedures)+≡
  subroutine evaluator_init_qn_sum (eval, int, qn_mask, drop)
    class(evaluator_t), intent(out), target :: eval
    class(interaction_t), target, intent(in) :: int
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask
    logical, intent(in), optional, dimension(:) :: drop
    type(state_iterator_t) :: it_old, it_new
    integer, dimension(:), allocatable :: pairing_size, pairing_target, i_new
    integer, dimension(:), allocatable :: map
    integer :: n_in, n_out, n_vir, n_tot, n_me_old, n_me_new
    integer :: i, j
    type(state_matrix_t), pointer :: state_new, state_old
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    logical :: matched
    logical, dimension(size (qn_mask)) :: dropped
    integer :: ndropped
    integer, dimension(:), allocatable :: inotdropped
    type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
    logical, dimension(:), allocatable :: resonant

    eval%type = EVAL_QN_SUM
    eval%int_in1 => int
    nullify (eval%int_in2)
    if (present (drop)) then
      dropped = drop
    else
      dropped = .false.
    end if
    ndropped = count (dropped)

    n_in = int%get_n_in ()
    n_out = int%get_n_out () - ndropped
    n_vir = int%get_n_vir ()
    n_tot = int%get_n_tot () - ndropped

    allocate (inotdropped (n_tot))
    i = 1

```

```

do j = 1, n_tot + ndropped
  if (dropped(j)) cycle
    inotdropped(i) = j
    i = i + 1
end do

allocate (mask(n_tot + ndropped))
mask = int%get_mask ()
allocate (resonant(n_tot + ndropped))
resonant = int%get_resonance_flags ()
call eval%interaction_t%basic_init (n_in, n_vir, n_out, &
  mask = mask(inotdropped) .or. qn_mask(inotdropped), &
  resonant = resonant(inotdropped))
i = 1
do j = 1, n_tot + ndropped
  if (dropped(j)) cycle
    call eval%set_source_link (i, int, j)
    i = i + 1
end do
allocate (map(n_tot + ndropped))
i = 1
do j = 1, n_tot + ndropped
  if (dropped(j)) then
    map(j) = 0
  else
    map(j) = i
    i = i + 1
  end if
end do
call int%transfer_relations (eval, map)

n_me_old = int%get_n_matrix_elements ()
allocate (pairing_size (n_me_old), source = 0)
allocate (pairing_target (n_me_old), source = 0)
pairing_size = 0
state_old => int%get_state_matrix_ptr ()
state_new => eval%get_state_matrix_ptr ()
call it_old%init (state_old)
allocate (qn(n_tot + ndropped))
do while (it_old%is_valid ())
  qn = it_old%get_quantum_numbers ()
  if (.not. all (qn%are_diagonal ())) then
    call it_old%advance ()
    cycle
  end if
  matched = .false.
  call it_new%init (state_new)
  if (eval%get_n_matrix_elements () > 0) then
    do while (it_new%is_valid ())
      if (all (qn(inotdropped) .match. &
        it_new%get_quantum_numbers ())) &
      then
        matched = .true.
        i = it_new%get_me_index ()

```

```

        exit
    end if
    call it_new%advance ()
end do
end if
if (.not. matched) then
    call eval%add_state (qn(inotdropped))
    i = eval%get_n_matrix_elements ()
end if
pairing_size(i) = pairing_size(i) + 1
pairing_target(it_old%get_me_index ()) = i
call it_old%advance ()
end do
call eval%freeze ()

n_me_new = eval%get_n_matrix_elements ()
allocate (eval%pairing_array (n_me_new))
do i = 1, n_me_new
    call pairing_array_init (eval%pairing_array(i), &
        pairing_size(i), .false., .false.)
end do

allocate (i_new (n_me_new), source = 0)
do i = 1, n_me_old
    j = pairing_target(i)
    if (j > 0) then
        i_new(j) = i_new(j) + 1
        eval%pairing_array(j)%i1(i_new(j)) = i
    end if
end do

end subroutine evaluator_init_qn_sum

```

12.3.8 Evaluation

When the input interactions (which are pointed to in the pairings stored within the evaluator) are filled with values, we can activate the evaluator, i.e., calculate the result values which are stored in the interaction.

The evaluation of matrix elements can be done in parallel. A `forall` construct is not appropriate, however. We would need `do concurrent` here. Nevertheless, the evaluation functions are marked as `pure`.

```

<Evaluators: evaluator: TBP>+≡
    procedure :: evaluate => evaluator_evaluate

<Evaluators: procedures>+≡
    subroutine evaluator_evaluate (eval)
        class(evaluator_t), intent(inout), target :: eval
        integer :: i
        select case (eval%type)
        case (EVAL_PRODUCT)
            do i = 1, size(eval%pairing_array)
                call eval%evaluate_product (i, &

```



```

        eval%int_in1, eval%int_in2, &
        eval%pairing_array(i)%i1, eval%pairing_array(i)%i2)
    if (debug2_active (D_QFT)) then
        print *, 'eval%pairing_array(i)%i1, eval%pairing_array(i)%i2 = ', &
            eval%pairing_array(i)%i1, eval%pairing_array(i)%i2
        print *, 'MEs = ', &
            eval%int_in1%get_matrix_element (eval%pairing_array(i)%i1), &
            eval%int_in2%get_matrix_element (eval%pairing_array(i)%i2)
    end if
end do
case (EVAL_SQUARE_WITH_COLOR_FACTORS)
do i = 1, size(eval%pairing_array)
    call eval%evaluate_product_cf (i, &
        eval%int_in1, eval%int_in1, &
        eval%pairing_array(i)%i1, eval%pairing_array(i)%i2, &
        eval%pairing_array(i)%factor)
end do
case (EVAL_SQUARED_FLOWS)
do i = 1, size(eval%pairing_array)
    call eval%evaluate_square_c (i, &
        eval%int_in1, &
        eval%pairing_array(i)%i1)
end do
case (EVAL_COLOR_CONTRACTION)
do i = 1, size(eval%pairing_array)
    call eval%evaluate_sum (i, &
        eval%int_in1, &
        eval%pairing_array(i)%i1)
end do
case (EVAL_IDENTITY)
    call eval%set_matrix_element (eval%int_in1)
case (EVAL_QN_SUM)
do i = 1, size (eval%pairing_array)
    call eval%evaluate_me_sum (i, &
        eval%int_in1, eval%pairing_array(i)%i1)
    call eval%set_norm (eval%int_in1%get_norm ())
end do
end select
end subroutine evaluator_evaluate

```

12.3.9 Unit tests

Test module, followed by the corresponding implementation module.

(evaluators_ut.f90)≡
⟨File header⟩

```

module evaluators_ut
    use unit_tests
    use evaluators_uti

```

⟨Standard module head⟩

```

    <Evaluators: public test>

contains

    <Evaluators: test driver>

    end module evaluators_ut
<evaluators_uti.f90>≡
    <File header>

    module evaluators_uti

    <Use kinds>
        use lorentz
        use flavors
        use colors
        use helicities
        use quantum_numbers
        use interactions
        use model_data

        use evaluators

    <Standard module head>

    <Evaluators: test declarations>

contains

    <Evaluators: tests>

    end module evaluators_uti
API: driver for the unit tests below.
<Evaluators: public test>≡
    public :: evaluator_test
<Evaluators: test driver>≡
    subroutine evaluator_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Evaluators: execute tests>
    end subroutine evaluator_test

```

Test: Create two interactions. The interactions are twofold connected. The first connection has a helicity index that is kept, the second connection has a helicity index that is summed over. Concatenate the interactions in an evaluator, which thus contains a result interaction. Fill the input interactions with values, activate the evaluator and print the result.

```

<Evaluators: execute tests>≡
    call test (evaluator_1, "evaluator_1", &
        "check evaluators (1)", &
        u, results)

```

```

<Evaluators: test declarations>≡
    public :: evaluator_1

<Evaluators: tests>≡
    subroutine evaluator_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(interaction_t), target :: int_qqtt, int_tbw, int1, int2
        type(flavor_t), dimension(:), allocatable :: flv
        type(color_t), dimension(:), allocatable :: col
        type(helicity_t), dimension(:), allocatable :: hel
        type(quantum_numbers_t), dimension(:), allocatable :: qn
        integer :: f, c, h1, h2, h3
        type(vector4_t), dimension(4) :: p
        type(vector4_t), dimension(2) :: q
        type(quantum_numbers_mask_t) :: qn_mask_conn
        type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask2
        type(evaluator_t), target :: eval, eval2, eval3

        call model%init_sm_test ()

        write (u, "(A)")    "*** Evaluator for matrix product"
        write (u, "(A)")    "***   Construct interaction for qq -> tt"
        write (u, "(A)")
        call int_qqtt%basic_init (2, 0, 2, set_relations=.true.)
        allocate (flv (4), col (4), hel (4), qn (4))
        allocate (qn_mask2 (4))
        do c = 1, 2
            select case (c)
            case (1)
                call col%init_col_acl ([1, 0, 1, 0], [0, 2, 0, 2])
            case (2)
                call col%init_col_acl ([1, 0, 2, 0], [0, 1, 0, 2])
            end select
            do f = 1, 2
                call flv%init ([f, -f, 6, -6], model)
                do h1 = -1, 1, 2
                    call hel(3)%init (h1)
                    do h2 = -1, 1, 2
                        call hel(4)%init (h2)
                        call qn%init (flv, col, hel)
                        call int_qqtt%add_state (qn)
                    end do
                end do
            end do
        end do
        call int_qqtt%freeze ()
        deallocate (flv, col, hel, qn)
        write (u, "(A)")    "***   Construct interaction for t -> bW"
        call int_tbw%basic_init (1, 0, 2, set_relations=.true.)
        allocate (flv (3), col (3), hel (3), qn (3))
        call flv%init ([6, 5, 24], model)
        call col%init_col_acl ([1, 1, 0], [0, 0, 0])
        do h1 = -1, 1, 2
            call hel(1)%init (h1)
        end do
    end subroutine evaluator_1

```

```

do h2 = -1, 1, 2
  call hel(2)%init (h2)
do h3 = -1, 1
  call hel(3)%init (h3)
  call qn%init (flv, col, hel)
  call int_tbw%add_state (qn)
end do
end do
end do
call int_tbw%freeze ()
deallocate (flv, col, hel, qn)
write (u, "(A)")  "***  Link interactions"
call int_tbw%set_source_link (1, int_qqtt, 3)
qn_mask_conn = quantum_numbers_mask (.false.,.false.,.true.)
write (u, "(A)")
write (u, "(A)")  "***  Show input"
call int_qqtt%basic_write (unit = u)
write (u, "(A)")
call int_tbw%basic_write (unit = u)
write (u, "(A)")
write (u, "(A)")  "***  Evaluate product"
call eval%init_product (int_qqtt, int_tbw, qn_mask_conn)
call eval%write (unit = u)

call int1%basic_init (2, 0, 2, set_relations=.true.)
call int2%basic_init (1, 0, 2, set_relations=.true.)
p(1) = vector4_moving (1000._default, 1000._default, 3)
p(2) = vector4_moving (200._default, 200._default, 2)
p(3) = vector4_moving (100._default, 200._default, 1)
p(4) = p(1) - p(2) - p(3)
call int1%set_momenta (p)
q(1) = vector4_moving (50._default,-50._default, 3)
q(2) = p(2) + p(4) - q(1)
call int2%set_momenta (q, outgoing=.true.)
call int1%set_matrix_element ([ (2._default,0._default), &
  (4._default,1._default), (-3._default,0._default)])
call int2%set_matrix_element ([ (-3._default,0._default), &
  (0._default,1._default), (1._default,2._default)])
call eval%receive_momenta ()
call eval%evaluate ()
call int1%basic_write (unit = u)
write (u, "(A)")
call int2%basic_write (unit = u)
write (u, "(A)")
call eval%write (unit = u)
write (u, "(A)")
call int1%final ()
call int2%final ()
call eval%final ()

write (u, "(A)")
write (u, "(A)")  "*** Evaluator for matrix square"
allocate (flv(4), col(4), qn(4))
call int1%basic_init (2, 0, 2, set_relations=.true.)

```

```

call flv%init ([1, -1, 21, 21], model)
call col(1)%init ([1])
call col(2)%init ([-2])
call col(3)%init ([2, -3])
call col(4)%init ([3, -1])
call qn%init (flv, col)
call int1%add_state (qn)
call col(3)%init ([3, -1])
call col(4)%init ([2, -3])
call qn%init (flv, col)
call int1%add_state (qn)
call col(3)%init ([2, -1])
call col(4)%init (.true.)
call qn%init (flv, col)
call int1%add_state (qn)
call int1%freeze ()
! [qn_mask2 not set since default is false]
call eval%init_square (int1, qn_mask2, nc=3)
call eval2%init_square_nondiag (int1, qn_mask2)
qn_mask2 = quantum_numbers_mask (.false., .true., .true.)
call eval3%init_square_diag (eval, qn_mask2)
call int1%set_matrix_element &
  ((2._default,0._default), &
  (4._default,1._default), (-3._default,0._default))]
call int1%set_momenta (p)
call int1%basic_write (unit = u)
write (u, "(A)")
call eval%receive_momenta ()
call eval%evaluate ()
call eval%write (unit = u)
write (u, "(A)")
call eval2%receive_momenta ()
call eval2%evaluate ()
call eval2%write (unit = u)
write (u, "(A)")
call eval3%receive_momenta ()
call eval3%evaluate ()
call eval3%write (unit = u)
call int1%final ()
call eval%final ()
call eval2%final ()
call eval3%final ()

call model%final ()
end subroutine evaluator_1

```

```

<Evaluators: execute tests>+≡
call test (evaluator_2, "evaluator_2", &
  "check evaluators (2)", &
  u, results)

```

```

<Evaluators: test declarations>+≡
public :: evaluator_2

```

```

<Evaluators: tests>+≡

```

```

subroutine evaluator_2 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(interaction_t), target :: int
  integer :: h1, h2, h3, h4
  type(helicity_t), dimension(4) :: hel
  type(color_t), dimension(4) :: col
  type(flavor_t), dimension(4) :: flv
  type(quantum_numbers_t), dimension(4) :: qn
  type(vector4_t), dimension(4) :: p
  type(evaluator_t) :: eval
  integer :: i

  call model%init_sm_test ()

  write (u, "(A)") "*** Creating interaction for e+ e- -> W+ W-"
  write (u, "(A)")

  call flv%init ([11, -11, 24, -24], model)
  do i = 1, 4
    call col(i)%init ()
  end do
  call int%basic_init (2, 0, 2, set_relations=.true.)
  do h1 = -1, 1, 2
    call hel(1)%init (h1)
    do h2 = -1, 1, 2
      call hel(2)%init (h2)
      do h3 = -1, 1
        call hel(3)%init (h3)
        do h4 = -1, 1
          call hel(4)%init (h4)
          call qn%init (flv, col, hel)
          call int%add_state (qn)
        end do
      end do
    end do
  end do
  call int%freeze ()
  call int%set_matrix_element &
    ([ (cmplx (i, kind=default), i = 1, 36)])
  p(1) = vector4_moving (1000._default, 1000._default, 3)
  p(2) = vector4_moving (1000._default, -1000._default, 3)
  p(3) = vector4_moving (1000._default, &
    sqrt (1E6_default - 80._default**2), 3)
  p(4) = p(1) + p(2) - p(3)
  call int%set_momenta (p)
  write (u, "(A)") "*** Setting up evaluator"
  write (u, "(A)")

  call eval%init_identity (int)
  write (u, "(A)") "*** Transferring momenta and evaluating"
  write (u, "(A)")

  call eval%receive_momenta ()

```

```

call eval%evaluate ()
write (u, "(A)") "*****"
write (u, "(A)") "  Interaction dump"
write (u, "(A)") "*****"
call int%basic_write (unit = u)
write (u, "(A)")
write (u, "(A)") "*****"
write (u, "(A)") "  Evaluator dump"
write (u, "(A)") "*****"
call eval%write (unit = u)
write (u, "(A)")
write (u, "(A)") "*** cleaning up"
call int%final ()
call eval%final ()

call model%final ()
end subroutine evaluator_2

```

<Evaluators: execute tests>+≡

```

call test (evaluator_3, "evaluator_3", &
  "check evaluators (3)", &
  u, results)

```

<Evaluators: test declarations>+≡

```

public :: evaluator_3

```

<Evaluators: tests>+≡

```

subroutine evaluator_3 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(interaction_t), target :: int
  integer :: h1, h2, h3, h4
  type(helicity_t), dimension(4) :: hel
  type(color_t), dimension(4) :: col
  type(flavor_t), dimension(4) :: flv1, flv2
  type(quantum_numbers_t), dimension(4) :: qn
  type(vector4_t), dimension(4) :: p
  type(evaluator_t) :: eval1, eval2, eval3
  type(quantum_numbers_mask_t), dimension(4) :: qn_mask
  integer :: i

  call model%init_sm_test ()

  write (u, "(A)") "*** Creating interaction for e+/mu+ e-/mu- -> W+ W-"
  call flv1%init ([11, -11, 24, -24], model)
  call flv2%init ([13, -13, 24, -24], model)
  do i = 1, 4
    call col (i)%init ()
  end do
  call int%basic_init (2, 0, 2, set_relations=.true.)
  do h1 = -1, 1, 2
    call hel(1)%init (h1)
    do h2 = -1, 1, 2
      call hel(2)%init (h2)
      do h3 = -1, 1

```

```

        call hel(3)%init (h3)
        do h4 = -1, 1
            call hel(4)%init (h4)
            call qn%init (flv1, col, hel)
            call int%add_state (qn)
            call qn%init (flv2, col, hel)
            call int%add_state (qn)
        end do
    end do
end do
call int%freeze ()
call int%set_matrix_element &
    ([[cplx (1, kind=default), i = 1, 72]])
p(1) = vector4_moving (1000._default, 1000._default, 3)
p(2) = vector4_moving (1000._default, -1000._default, 3)
p(3) = vector4_moving (1000._default, &
    sqrt (1E6_default - 80._default**2), 3)
p(4) = p(1) + p(2) - p(3)
call int%set_momenta (p)
write (u, "(A)")  "*** Setting up evaluators"
call qn_mask%init (.false., .true., .true.)
call eval1%init_qn_sum (int, qn_mask)
call qn_mask%init (.true., .true., .true.)
call eval2%init_qn_sum (int, qn_mask)
call qn_mask%init (.false., .true., .false.)
call eval3%init_qn_sum (int, qn_mask, &
    [.false., .false., .false., .true.])
write (u, "(A)")  "*** Transferring momenta and evaluating"
call eval1%receive_momenta ()
call eval1%evaluate ()
call eval2%receive_momenta ()
call eval2%evaluate ()
call eval3%receive_momenta ()
call eval3%evaluate ()
write (u, "(A)")  "*****"
write (u, "(A)")  "  Interaction dump"
write (u, "(A)")  "*****"
call int%basic_write (unit = u)
write (u, "(A)")
write (u, "(A)")  "*****"
write (u, "(A)")  "  Evaluator dump --- spin sum"
write (u, "(A)")  "*****"
call eval1%write (unit = u)
call eval1%basic_write (unit = u)
write (u, "(A)")  "*****"
write (u, "(A)")  "  Evaluator dump --- spin / flavor sum"
write (u, "(A)")  "*****"
call eval2%write (unit = u)
call eval2%basic_write (unit = u)
write (u, "(A)")  "*****"
write (u, "(A)")  "  Evaluator dump --- flavor sum, drop last W"
write (u, "(A)")  "*****"
call eval3%write (unit = u)

```



```

call eval3%basic_write (unit = u)
write (u, "(A)")
write (u, "(A)")  "*** cleaning up"
call int%final ()
call eval1%final ()
call eval2%final ()
call eval3%final ()

call model%final ()
end subroutine evaluator_3

```

This test evaluates a product with different quantum-number masks and filters for the linked entry.

```

<Evaluators: execute tests>+≡
call test (evaluator_4, "evaluator_4", &
  "check evaluator product with filter", &
  u, results)

<Evaluators: test declarations>+≡
public :: evaluator_4

<Evaluators: tests>+≡
subroutine evaluator_4 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(interaction_t), target :: int1, int2
  integer :: h1, h2, h3
  type(helicity_t), dimension(3) :: hel
  type(color_t), dimension(3) :: col
  type(flavor_t), dimension(2) :: flv1, flv2
  type(flavor_t), dimension(3) :: flv3, flv4
  type(quantum_numbers_t), dimension(3) :: qn
  type(evaluator_t) :: eval1, eval2, eval3, eval4
  type(quantum_numbers_mask_t) :: qn_mask
  type(flavor_t) :: flv_filter
  type(helicity_t) :: hel_filter
  type(color_t) :: col_filter
  type(quantum_numbers_t) :: qn_filter
  integer :: i

  write (u, "(A)")  "* Test output: evaluator_4"
  write (u, "(A)")  "* Purpose: test evaluator products &
    &with mask and filter"
  write (u, "(A)")

  call model%init_sm_test ()

  write (u, "(A)")  "* Creating interaction for e- -> W+/Z"
  write (u, "(A)")

  call flv1%init ([11, 24], model)
  call flv2%init ([11, 23], model)
  do i = 1, 3
    call col(i)%init ()
  end do

```

```

call int1%basic_init (1, 0, 1, set_relations=.true.)
do h1 = -1, 1, 2
  call hel(1)%init (h1)
  do h2 = -1, 1
    call hel(2)%init (h2)
    call qn(:2)%init (flv1, col(:2), hel(:2))
    call int1%add_state (qn(:2))
    call qn(:2)%init (flv2, col(:2), hel(:2))
    call int1%add_state (qn(:2))
  end do
end do
call int1%freeze ()
call int1%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Creating interaction for W+/Z -> u ubar/dbar"
write (u, "(A)")

call flv3%init ([24, 2, -1], model)
call flv4%init ([23, 2, -2], model)

call int2%basic_init (1, 0, 2, set_relations=.true.)
do h1 = -1, 1
  call hel(1)%init (h1)
  do h2 = -1, 1, 2
    call hel(2)%init (h2)
    do h3 = -1, 1, 2
      call hel(3)%init (h3)
      call qn(:3)%init (flv3, col(:3), hel(:3))
      call int2%add_state (qn(:3))
      call qn(:3)%init (flv4, col(:3), hel(:3))
      call int2%add_state (qn(:3))
    end do
  end do
end do
call int2%freeze ()

call int2%set_source_link (1, int1, 2)
call int2%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Product evaluator"
write (u, "(A)")

call qn_mask%init (.false., .false., .false.)
call eval1%init_product (int1, int2, qn_mask_conn = qn_mask)
call eval1%write (u)

write (u, "(A)")
write (u, "(A)")  "* Product evaluator with helicity mask"
write (u, "(A)")

call qn_mask%init (.false., .false., .true.)
call eval2%init_product (int1, int2, qn_mask_conn = qn_mask)

```

```

call eval2%write (u)

write (u, "(A)")
write (u, "(A)")  "* Product with flavor filter and helicity mask"
write (u, "(A)")

call qn_mask%init (.false., .false., .true.)
call flv_filter%init (24, model)
call hel_filter%init ()
call col_filter%init ()
call qn_filter%init (flv_filter, col_filter, hel_filter)
call eval3%init_product (int1, int2, &
    qn_mask_conn = qn_mask, qn_filter_conn = qn_filter)
call eval3%write (u)

write (u, "(A)")
write (u, "(A)")  "* Product with helicity filter and mask"
write (u, "(A)")

call qn_mask%init (.false., .false., .true.)
call flv_filter%init ()
call hel_filter%init (0)
call col_filter%init ()
call qn_filter%init (flv_filter, col_filter, hel_filter)
call eval4%init_product (int1, int2, &
    qn_mask_conn = qn_mask, qn_filter_conn = qn_filter)
call eval4%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eval1%final ()
call eval2%final ()
call eval3%final ()
call eval4%final ()

call int1%final ()
call int2%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: evaluator_4"

end subroutine evaluator_4

```

Chapter 13

Sindarin Built-In Types

Here, we define a couple of types and objects which are useful both internally for WHIZARD, and visible to the user, so they correspond to Sindarin types.

particle_specifiers Expressions for particles and particle alternatives, involving particle names.

pdg_arrays Integer (PDG) codes for particles. Useful for particle aliases (e.g., 'quark' for u, d, s etc.).

jets Define (pseudo)jets as objects. Functional only if the **fastjet** library is linked. (This may change in the future.)

subevents Particle collections built from event records, for use in analysis and other Sindarin expressions

analysis Observables, histograms, and plots.

13.1 Particle Specifiers

In this module we introduce a type for specifying a particle or particle alternative. In addition to the particle specifiers (strings separated by colons), the type contains an optional flag **polarized** and a string **decay**. If the **polarized** flag is set, particle polarization information should be kept when generating events for this process. If the **decay** string is set, it is the ID of a decay process which should be applied to this particle when generating events.

In input/output form, the **polarized** flag is indicated by an asterisk (*) in brackets, and the **decay** is indicated by its ID in brackets.

The **read** and **write** procedures in this module are not type-bound but generic procedures which handle scalar and array arguments.

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

```
module particle_specifiers
```

```
<Use strings>
```

```
  use io_units
```

```
  use diagnostics
```

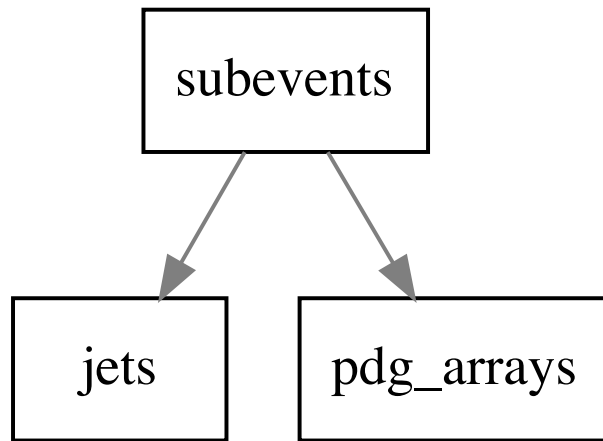


Figure 13.1: Module dependencies in `src/types`.

```

⟨Standard module head⟩

⟨Particle specifiers: public⟩

⟨Particle specifiers: types⟩

⟨Particle specifiers: interfaces⟩

contains

⟨Particle specifiers: procedures⟩

end module particle_specifiers

```

13.1.1 Base type

This is an abstract type which can hold a single particle or an expression.

```

⟨Particle specifiers: types⟩≡
  type, abstract :: prt_spec_expr_t
  contains
    ⟨Particle specifiers: prt spec expr: TBP⟩
  end type prt_spec_expr_t

```

Output, as a string.

```

⟨Particle specifiers: prt spec expr: TBP⟩≡
  procedure (prt_spec_expr_to_string), deferred :: to_string

⟨Particle specifiers: interfaces⟩≡
  abstract interface
    function prt_spec_expr_to_string (object) result (string)
      import
        class(prt_spec_expr_t), intent(in) :: object
        type(string_t) :: string
      end function prt_spec_expr_to_string
  end interface

```

Call an `expand` method for all enclosed subexpressions (before handling the current expression).

```

⟨Particle specifiers: prt spec expr: TBP⟩+≡
  procedure (prt_spec_expr_expand_sub), deferred :: expand_sub

⟨Particle specifiers: interfaces⟩+≡
  abstract interface
    subroutine prt_spec_expr_expand_sub (object)
      import
        class(prt_spec_expr_t), intent(inout) :: object
      end subroutine prt_spec_expr_expand_sub
  end interface

```

13.1.2 Wrapper type

This wrapper can hold a particle expression of any kind. We need it so we can make variadic arrays.

```
<Particle specifiers: public>≡
    public :: prt_expr_t
<Particle specifiers: types>+≡
    type :: prt_expr_t
        class(prt_spec_expr_t), allocatable :: x
        contains
        <Particle specifiers: prt expr: TBP>
    end type prt_expr_t
```

Output as a string: delegate.

```
<Particle specifiers: prt expr: TBP>≡
    procedure :: to_string => prt_expr_to_string
<Particle specifiers: procedures>≡
    recursive function prt_expr_to_string (object) result (string)
        class(prt_expr_t), intent(in) :: object
        type(string_t) :: string
        if (allocated (object%x)) then
            string = object%x%to_string ()
        else
            string = ""
        end if
    end function prt_expr_to_string
```

Allocate the expression as a particle specifier and copy the value.

```
<Particle specifiers: prt expr: TBP>+≡
    procedure :: init_spec => prt_expr_init_spec
<Particle specifiers: procedures>+≡
    subroutine prt_expr_init_spec (object, spec)
        class(prt_expr_t), intent(out) :: object
        type(prt_spec_t), intent(in) :: spec
        allocate (prt_spec_t :: object%x)
        select type (x => object%x)
        type is (prt_spec_t)
            x = spec
        end select
    end subroutine prt_expr_init_spec
```

Allocate as a list/sum and allocate for a given length

```
<Particle specifiers: prt expr: TBP>+≡
    procedure :: init_list => prt_expr_init_list
    procedure :: init_sum => prt_expr_init_sum
<Particle specifiers: procedures>+≡
    subroutine prt_expr_init_list (object, n)
        class(prt_expr_t), intent(out) :: object
        integer, intent(in) :: n
        allocate (prt_spec_list_t :: object%x)
```

```

        select type (x => object%x)
        type is (prt_spec_list_t)
            allocate (x%expr (n))
        end select
    end subroutine prt_expr_init_list

    subroutine prt_expr_init_sum (object, n)
        class(prt_expr_t), intent(out) :: object
        integer, intent(in) :: n
        allocate (prt_spec_sum_t :: object%x)
        select type (x => object%x)
        type is (prt_spec_sum_t)
            allocate (x%expr (n))
        end select
    end subroutine prt_expr_init_sum

```

Return the number of terms. This is unity, except if the expression is a sum.

```

<Particle specifiers: prt expr: TBP>+≡
    procedure :: get_n_terms => prt_expr_get_n_terms

<Particle specifiers: procedures>+≡
    function prt_expr_get_n_terms (object) result (n)
        class(prt_expr_t), intent(in) :: object
        integer :: n
        if (allocated (object%x)) then
            select type (x => object%x)
            type is (prt_spec_sum_t)
                n = size (x%expr)
            class default
                n = 1
            end select
        else
            n = 0
        end if
    end function prt_expr_get_n_terms

```

Transform one of the terms, as returned by the previous method, to an array of particle specifiers. The array has more than one entry if the selected term is a list. This makes sense only if the expression has been completely expanded, so the list contains only atoms.

```

<Particle specifiers: prt expr: TBP>+≡
    procedure :: term_to_array => prt_expr_term_to_array

<Particle specifiers: procedures>+≡
    recursive subroutine prt_expr_term_to_array (object, array, i)
        class(prt_expr_t), intent(in) :: object
        type(prt_spec_t), dimension(:), intent(inout), allocatable :: array
        integer, intent(in) :: i
        integer :: j
        if (allocated (array)) deallocate (array)
        select type (x => object%x)
        type is (prt_spec_t)
            allocate (array (1))
            array(1) = x

```



```

type is (prt_spec_list_t)
  allocate (array (size (x%expr)))
  do j = 1, size (array)
    select type (y => x%expr(j)%x)
      type is (prt_spec_t)
        array(j) = y
    end select
  end do
type is (prt_spec_sum_t)
  call x%expr(i)%term_to_array (array, 1)
end select
end subroutine prt_expr_term_to_array

```

13.1.3 The atomic type

The trivial case is a single particle, including optional decay and polarization attributes.

Definition

The particle is unstable if the **decay** array is allocated. The **polarized** flag and decays may not be set simultaneously.

```

<Particle specifiers: public>+≡
  public :: prt_spec_t

<Particle specifiers: types>+≡
  type, extends (prt_spec_expr_t) :: prt_spec_t
    private
    type(string_t) :: name
    logical :: polarized = .false.
    type(string_t), dimension(:), allocatable :: decay
  contains
    <Particle specifiers: prt spec: TBP>
  end type prt_spec_t

```

I/O

Output. Old-style subroutines.

```

<Particle specifiers: public>+≡
  public :: prt_spec_write

<Particle specifiers: interfaces>+≡
  interface prt_spec_write
    module procedure prt_spec_write1
    module procedure prt_spec_write2
  end interface prt_spec_write

<Particle specifiers: procedures>+≡
  subroutine prt_spec_write1 (object, unit, advance)
    type(prt_spec_t), intent(in) :: object
    integer, intent(in), optional :: unit
    character(len=*), intent(in), optional :: advance

```

```

character(3) :: adv
integer :: u
u = given_output_unit (unit)
adv = "yes"; if (present (advance)) adv = advance
write (u, "(A)", advance = adv) char (object%to_string ())
end subroutine prt_spec_write1

```

Write an array as a list of particle specifiers.

```

<Particle specifiers: procedures>+≡
subroutine prt_spec_write2 (prt_spec, unit, advance)
  type(prt_spec_t), dimension(:), intent(in) :: prt_spec
  integer, intent(in), optional :: unit
  character(len=*), intent(in), optional :: advance
  character(3) :: adv
  integer :: u, i
  u = given_output_unit (unit)
  adv = "yes"; if (present (advance)) adv = advance
  do i = 1, size (prt_spec)
    if (i > 1) write (u, "(A)", advance="no") " ", "
    call prt_spec_write (prt_spec(i), u, advance="no")
  end do
  write (u, "(A)", advance = adv)
end subroutine prt_spec_write2

```

Read. Input may be string or array of strings.

```

<Particle specifiers: public>+≡
public :: prt_spec_read

<Particle specifiers: interfaces>+≡
interface prt_spec_read
  module procedure prt_spec_read1
  module procedure prt_spec_read2
end interface prt_spec_read

```

Read a single particle specifier

```

<Particle specifiers: procedures>+≡
pure subroutine prt_spec_read1 (prt_spec, string)
  type(prt_spec_t), intent(out) :: prt_spec
  type(string_t), intent(in) :: string
  type(string_t) :: arg, buffer
  integer :: b1, b2, c, n, i
  b1 = scan (string, "(")
  b2 = scan (string, ")")
  if (b1 == 0) then
    prt_spec%name = trim (adjustl (string))
  else
    prt_spec%name = trim (adjustl (extract (string, 1, b1-1)))
    arg = trim (adjustl (extract (string, b1+1, b2-1)))
    if (arg == "*") then
      prt_spec%polarized = .true.
    else
      n = 0
      buffer = arg
      do

```

```

        if (verify (buffer, " ") == 0) exit
        n = n + 1
        c = scan (buffer, "+")
        if (c == 0) exit
        buffer = extract (buffer, c+1)
    end do
    allocate (prt_spec%decay (n))
    buffer = arg
    do i = 1, n
        c = scan (buffer, "+")
        if (c == 0) c = len (buffer) + 1
        prt_spec%decay(i) = trim (adjustl (extract (buffer, 1, c-1)))
        buffer = extract (buffer, c+1)
    end do
end if
end if
end subroutine prt_spec_read1

```

Read a particle specifier array, given as a single string. The array is allocated to the correct size.

(Particle specifiers: procedures)+≡

```

pure subroutine prt_spec_read2 (prt_spec, string)
    type(prt_spec_t), dimension(:), intent(out), allocatable :: prt_spec
    type(string_t), intent(in) :: string
    type(string_t) :: buffer
    integer :: c, i, n
    n = 0
    buffer = string
    do
        n = n + 1
        c = scan (buffer, ",")
        if (c == 0) exit
        buffer = extract (buffer, c+1)
    end do
    allocate (prt_spec (n))
    buffer = string
    do i = 1, size (prt_spec)
        c = scan (buffer, ",")
        if (c == 0) c = len (buffer) + 1
        call prt_spec_read (prt_spec(i), &
            trim (adjustl (extract (buffer, 1, c-1))))
        buffer = extract (buffer, c+1)
    end do
end subroutine prt_spec_read2

```

Constructor

Initialize a particle specifier.

(Particle specifiers: public)+≡

```

public :: new_prt_spec

```

(Particle specifiers: interfaces)+≡

```

interface new_prt_spec
  module procedure new_prt_spec
  module procedure new_prt_spec_polarized
  module procedure new_prt_spec_unstable
end interface new_prt_spec

<Particle specifiers: procedures>+≡
elemental function new_prt_spec (name) result (prt_spec)
  type(string_t), intent(in) :: name
  type(prt_spec_t) :: prt_spec
  prt_spec%name = name
end function new_prt_spec

elemental function new_prt_spec_polarized (name, polarized) result (prt_spec)
  type(string_t), intent(in) :: name
  logical, intent(in) :: polarized
  type(prt_spec_t) :: prt_spec
  prt_spec%name = name
  prt_spec%polarized = polarized
end function new_prt_spec_polarized

pure function new_prt_spec_unstable (name, decay) result (prt_spec)
  type(string_t), intent(in) :: name
  type(string_t), dimension(:), intent(in) :: decay
  type(prt_spec_t) :: prt_spec
  prt_spec%name = name
  allocate (prt_spec%decay (size (decay)))
  prt_spec%decay = decay
end function new_prt_spec_unstable

```

Access Methods

Return the particle name without qualifiers

```

<Particle specifiers: prt spec: TBP>≡
  procedure :: get_name => prt_spec_get_name

<Particle specifiers: procedures>+≡
  elemental function prt_spec_get_name (prt_spec) result (name)
    class(prt_spec_t), intent(in) :: prt_spec
    type(string_t) :: name
    name = prt_spec%name
  end function prt_spec_get_name

```

Return the name with qualifiers

```

<Particle specifiers: prt spec: TBP>+≡
  procedure :: to_string => prt_spec_to_string

<Particle specifiers: procedures>+≡
  function prt_spec_to_string (object) result (string)
    class(prt_spec_t), intent(in) :: object
    type(string_t) :: string
    integer :: i
    string = object%name
  end function prt_spec_to_string

```

```

if (allocated (object%decay)) then
  string = string // "("
  do i = 1, size (object%decay)
    if (i > 1) string = string // " + "
    string = string // object%decay(i)
  end do
  string = string // ")"
else if (object%polarized) then
  string = string // "(*)"
end if
end function prt_spec_to_string

```

Return the polarization flag

```

⟨Particle specifiers: prt spec: TBP⟩+≡
  procedure :: is_polarized => prt_spec_is_polarized

⟨Particle specifiers: procedures⟩+≡
  elemental function prt_spec_is_polarized (prt_spec) result (flag)
    class(prt_spec_t), intent(in) :: prt_spec
    logical :: flag
    flag = prt_spec%polarized
  end function prt_spec_is_polarized

```

The particle is unstable if there is a decay array.

```

⟨Particle specifiers: prt spec: TBP⟩+≡
  procedure :: is_unstable => prt_spec_is_unstable

⟨Particle specifiers: procedures⟩+≡
  elemental function prt_spec_is_unstable (prt_spec) result (flag)
    class(prt_spec_t), intent(in) :: prt_spec
    logical :: flag
    flag = allocated (prt_spec%decay)
  end function prt_spec_is_unstable

```

Return the number of decay channels

```

⟨Particle specifiers: prt spec: TBP⟩+≡
  procedure :: get_n_decays => prt_spec_get_n_decays

⟨Particle specifiers: procedures⟩+≡
  elemental function prt_spec_get_n_decays (prt_spec) result (n)
    class(prt_spec_t), intent(in) :: prt_spec
    integer :: n
    if (allocated (prt_spec%decay)) then
      n = size (prt_spec%decay)
    else
      n = 0
    end if
  end function prt_spec_get_n_decays

```

Return the decay channels

```

⟨Particle specifiers: prt spec: TBP⟩+≡
  procedure :: get_decays => prt_spec_get_decays

```

```

⟨Particle specifiers: procedures⟩+≡
  subroutine prt_spec_get_decays (prt_spec, decay)
    class(prt_spec_t), intent(in) :: prt_spec
    type(string_t), dimension(:), allocatable, intent(out) :: decay
    if (allocated (prt_spec%decay)) then
      allocate (decay (size (prt_spec%decay)))
      decay = prt_spec%decay
    else
      allocate (decay (0))
    end if
  end subroutine prt_spec_get_decays

```

Miscellaneous

There is nothing to expand here:

```

⟨Particle specifiers: prt spec: TBP⟩+≡
  procedure :: expand_sub => prt_spec_expand_sub

⟨Particle specifiers: procedures⟩+≡
  subroutine prt_spec_expand_sub (object)
    class(prt_spec_t), intent(inout) :: object
  end subroutine prt_spec_expand_sub

```

13.1.4 List

A list of particle specifiers, indicating, e.g., the final state of a process.

```

⟨Particle specifiers: public⟩+≡
  public :: prt_spec_list_t

⟨Particle specifiers: types⟩+≡
  type, extends (prt_spec_expr_t) :: prt_spec_list_t
    type(prt_spec_expr_t), dimension(:), allocatable :: expr
  contains
    ⟨Particle specifiers: prt spec list: TBP⟩
  end type prt_spec_list_t

```

Output: Concatenate the components. Insert brackets if the component is also a list. The components of the `expr` array, if any, should all be filled.

```

⟨Particle specifiers: prt spec list: TBP⟩≡
  procedure :: to_string => prt_spec_list_to_string

⟨Particle specifiers: procedures⟩+≡
  recursive function prt_spec_list_to_string (object) result (string)
    class(prt_spec_list_t), intent(in) :: object
    type(string_t) :: string
    integer :: i
    string = ""
    if (allocated (object%expr)) then
      do i = 1, size (object%expr)
        if (i > 1) string = string // ", "
        select type (x => object%expr(i)%x)

```

```

        type is (prt_spec_list_t)
        string = string // "(" // x%to_string () // ")"
    class default
        string = string // x%to_string ()
    end select
end do
end if
end function prt_spec_list_to_string

```

Flatten: if there is a subexpression which is also a list, include the components as direct members of the current list.

(Particle specifiers: prt spec list: TBP)+≡

```

    procedure :: flatten => prt_spec_list_flatten

```

(Particle specifiers: procedures)+≡

```

    subroutine prt_spec_list_flatten (object)
        class(prt_spec_list_t), intent(inout) :: object
        type(prt_expr_t), dimension(:), allocatable :: tmp_expr
        integer :: i, n_flat, i_flat
        n_flat = 0
        do i = 1, size (object%expr)
            select type (y => object%expr(i)%x)
            type is (prt_spec_list_t)
                n_flat = n_flat + size (y%expr)
            class default
                n_flat = n_flat + 1
            end select
        end do
        if (n_flat > size (object%expr)) then
            allocate (tmp_expr (n_flat))
            i_flat = 0
            do i = 1, size (object%expr)
                select type (y => object%expr(i)%x)
                type is (prt_spec_list_t)
                    tmp_expr (i_flat + 1 : i_flat + size (y%expr)) = y%expr
                    i_flat = i_flat + size (y%expr)
                class default
                    tmp_expr (i_flat + 1) = object%expr(i)
                    i_flat = i_flat + 1
                end select
            end do
        end if
        if (allocated (tmp_expr)) &
            call move_alloc (from = tmp_expr, to = object%expr)
    end subroutine prt_spec_list_flatten

```

Convert a list of sums into a sum of lists. (Subexpressions which are not sums are left untouched.)

(Particle specifiers: procedures)+≡

```

    subroutine distribute_prt_spec_list (object)
        class(prt_spec_expr_t), intent(inout), allocatable :: object
        class(prt_spec_expr_t), allocatable :: new_object
        integer, dimension(:), allocatable :: n, ii

```

```

integer :: k, n_expr, n_terms, i_term
select type (object)
type is (prt_spec_list_t)
  n_expr = size (object%expr)
  allocate (n (n_expr), source = 1)
  allocate (ii (n_expr), source = 1)
  do k = 1, size (object%expr)
    select type (y => object%expr(k)%x)
    type is (prt_spec_sum_t)
      n(k) = size (y%expr)
    end select
  end do
  n_terms = product (n)
  if (n_terms > 1) then
    allocate (prt_spec_sum_t :: new_object)
    select type (new_object)
    type is (prt_spec_sum_t)
      allocate (new_object%expr (n_terms))
      do i_term = 1, n_terms
        allocate (prt_spec_list_t :: new_object%expr(i_term)%x)
        select type (x => new_object%expr(i_term)%x)
        type is (prt_spec_list_t)
          allocate (x%expr (n_expr))
          do k = 1, n_expr
            select type (y => object%expr(k)%x)
            type is (prt_spec_sum_t)
              x%expr(k) = y%expr(ii(k))
            class default
              x%expr(k) = object%expr(k)
            end select
          end do
        end select
        INCR_INDEX: do k = n_expr, 1, -1
          if (ii(k) < n(k)) then
            ii(k) = ii(k) + 1
            exit INCR_INDEX
          else
            ii(k) = 1
          end if
        end do INCR_INDEX
      end do
    end select
  end if
end select
if (allocated (new_object)) call move_alloc (from = new_object, to = object)
end subroutine distribute_prt_spec_list

```

Apply expand to all components of the list.

```

<Particle specifiers: prt spec list: TBP>+≡
  procedure :: expand_sub => prt_spec_list_expand_sub

<Particle specifiers: procedures>+≡
  recursive subroutine prt_spec_list_expand_sub (object)
    class(prt_spec_list_t), intent(inout) :: object

```



```

integer :: i
if (allocated (object%expr)) then
  do i = 1, size (object%expr)
    call object%expr(i)%expand ()
  end do
end if
end subroutine prt_spec_list_expand_sub

```

13.1.5 Sum

A sum of particle specifiers, indicating, e.g., a sum of final states.

```

⟨Particle specifiers: public⟩+≡
  public :: prt_spec_sum_t

⟨Particle specifiers: types⟩+≡
  type, extends (prt_spec_expr_t) :: prt_spec_sum_t
    type(prt_spec_expr_t), dimension(:), allocatable :: expr
    contains
    ⟨Particle specifiers: prt spec sum: TBP⟩
  end type prt_spec_sum_t

```

Output: Concatenate the components. Insert brackets if the component is a list or also a sum. The components of the `expr` array, if any, should all be filled.

```

⟨Particle specifiers: prt spec sum: TBP⟩≡
  procedure :: to_string => prt_spec_sum_to_string

⟨Particle specifiers: procedures⟩+≡
  recursive function prt_spec_sum_to_string (object) result (string)
    class(prt_spec_sum_t), intent(in) :: object
    type(string_t) :: string
    integer :: i
    string = ""
    if (allocated (object%expr)) then
      do i = 1, size (object%expr)
        if (i > 1) string = string // " + "
        select type (x => object%expr(i)%x)
          type is (prt_spec_list_t)
            string = string // "(" // x%to_string () // ")"
          type is (prt_spec_sum_t)
            string = string // "(" // x%to_string () // ")"
          class default
            string = string // x%to_string ()
        end select
      end do
    end if
  end function prt_spec_sum_to_string

```

Flatten: if there is a subexpression which is also a sum, include the components as direct members of the current sum.

This is identical to `prt_spec_list_flatten` above, except for the type.

```

⟨Particle specifiers: prt spec sum: TBP⟩+≡
  procedure :: flatten => prt_spec_sum_flatten

```

<Particle specifiers: procedures>+≡

```

subroutine prt_spec_sum_flatten (object)
  class(prt_spec_sum_t), intent(inout) :: object
  type(prt_expr_t), dimension(:), allocatable :: tmp_expr
  integer :: i, n_flat, i_flat
  n_flat = 0
  do i = 1, size (object%expr)
    select type (y => object%expr(i)%x)
      type is (prt_spec_sum_t)
        n_flat = n_flat + size (y%expr)
      class default
        n_flat = n_flat + 1
    end select
  end do
  if (n_flat > size (object%expr)) then
    allocate (tmp_expr (n_flat))
    i_flat = 0
    do i = 1, size (object%expr)
      select type (y => object%expr(i)%x)
        type is (prt_spec_sum_t)
          tmp_expr (i_flat + 1 : i_flat + size (y%expr)) = y%expr
          i_flat = i_flat + size (y%expr)
        class default
          tmp_expr (i_flat + 1) = object%expr(i)
          i_flat = i_flat + 1
        end select
      end do
    end if
    if (allocated (tmp_expr)) &
      call move_alloc (from = tmp_expr, to = object%expr)
  end subroutine prt_spec_sum_flatten

```

Apply expand to all terms in the sum.

<Particle specifiers: prt spec sum: TBP>+≡

```

procedure :: expand_sub => prt_spec_sum_expand_sub

```

<Particle specifiers: procedures>+≡

```

recursive subroutine prt_spec_sum_expand_sub (object)
  class(prt_spec_sum_t), intent(inout) :: object
  integer :: i
  if (allocated (object%expr)) then
    do i = 1, size (object%expr)
      call object%expr(i)%expand ()
    end do
  end if
end subroutine prt_spec_sum_expand_sub

```

13.1.6 Expression Expansion

The `expand` method transforms each particle specifier expression into a sum of lists, according to the rules

$$a, (b, c) \rightarrow a, b, c \quad (13.1)$$

$$a + (b + c) \rightarrow a + b + c \quad (13.2)$$

$$a, b + c \rightarrow (a, b) + (a, c) \quad (13.3)$$

Note that the precedence of comma and plus are opposite to this expansion, so the parentheses in the final expression are necessary.

We assume that subexpressions are filled, i.e., arrays are allocated.

```
<Particle specifiers: prt expr: TBP>+≡
  procedure :: expand => prt_expr_expand

<Particle specifiers: procedures>+≡
  recursive subroutine prt_expr_expand (expr)
    class(prt_expr_t), intent(inout) :: expr
    if (allocated (expr%x)) then
      call distribute_prt_spec_list (expr%x)
      call expr%x%expand_sub ()
      select type (x => expr%x)
        type is (prt_spec_list_t)
          call x%flatten ()
        type is (prt_spec_sum_t)
          call x%flatten ()
      end select
    end if
  end subroutine prt_expr_expand
```

13.1.7 Unit Tests

Test module, followed by the corresponding implementation module.

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

  module particle_specifiers_ut
    use unit_tests
    use particle_specifiers_uti

<Standard module head>

<Particle specifiers: public test>

  contains

<Particle specifiers: test driver>

  end module particle_specifiers_ut
```

```

<particle_specifiers_util.f90>≡
  <File header>

  module particle_specifiers_util

    <Use strings>

    use particle_specifiers

    <Standard module head>

    <Particle specifiers: test declarations>

    contains

    <Particle specifiers: tests>

  end module particle_specifiers_util
API: driver for the unit tests below.
<Particle specifiers: public test>≡
  public :: particle_specifiers_test
<Particle specifiers: test driver>≡
  subroutine particle_specifiers_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Particle specifiers: execute tests>
  end subroutine particle_specifiers_test

```

Particle specifier array

Define, read and write an array of particle specifiers.

```

<Particle specifiers: execute tests>≡
  call test (particle_specifiers_1, "particle_specifiers_1", &
    "Handle particle specifiers", &
    u, results)
<Particle specifiers: test declarations>≡
  public :: particle_specifiers_1
<Particle specifiers: tests>≡
  subroutine particle_specifiers_1 (u)
    integer, intent(in) :: u
    type(prt_spec_t), dimension(:), allocatable :: prt_spec
    type(string_t), dimension(:), allocatable :: decay
    type(string_t), dimension(0) :: no_decay
    integer :: i, j

    write (u, "(A)")  "*" Test output: particle_specifiers_1"
    write (u, "(A)")  "*" Purpose: Read and write a particle specifier array"
    write (u, "(A)")

    allocate (prt_spec (5))
    prt_spec = [ &

```

```

        new_prt_spec (var_str ("a")), &
        new_prt_spec (var_str ("b"), .true.), &
        new_prt_spec (var_str ("c"), [var_str ("dec1")]), &
        new_prt_spec (var_str ("d"), [var_str ("dec1"), var_str ("dec2")]), &
        new_prt_spec (var_str ("e"), no_decay) &
    ]
do i = 1, size (prt_spec)
    write (u, "(A)") char (prt_spec(i)%to_string ())
end do
write (u, "(A)")

call prt_spec_read (prt_spec, &
    var_str (" a, b( *), c( dec1), d (dec1 + dec2 ), e()"))
call prt_spec_write (prt_spec, u)

do i = 1, size (prt_spec)
    write (u, "(A)")
    write (u, "(A,A)") char (prt_spec(i)%get_name ()), ":"
    write (u, "(A,L1)") "polarized = ", prt_spec(i)%is_polarized ()
    write (u, "(A,L1)") "unstable = ", prt_spec(i)%is_unstable ()
    write (u, "(A,I0)") "n_decays = ", prt_spec(i)%get_n_decays ()
    call prt_spec(i)%get_decays (decay)
    write (u, "(A)", advance="no") "decays      ="
    do j = 1, size (decay)
        write (u, "(1x,A)", advance="no") char (decay(j))
    end do
    write (u, "(A)")
end do

write (u, "(A)")
write (u, "(A)")  "* Test output end: particle_specifiers_1"
end subroutine particle_specifiers_1

```

Particle specifier expressions

Nested expressions (only basic particles, no decay specs).

(Particle specifiers: execute tests)+≡

```

call test (particle_specifiers_2, "particle_specifiers_2", &
    "Particle specifier expressions", &
    u, results)

```

(Particle specifiers: test declarations)+≡

```

public :: particle_specifiers_2

```

(Particle specifiers: tests)+≡

```

subroutine particle_specifiers_2 (u)
    integer, intent(in) :: u
    type(prt_spec_t) :: a, b, c, d, e, f
    type(prt_expr_t) :: pe1, pe2, pe3
    type(prt_expr_t) :: pe4, pe5, pe6, pe7, pe8, pe9
    integer :: i
    type(prt_spec_t), dimension(:), allocatable :: pa

    write (u, "(A)")  "* Test output: particle_specifiers_2"

```

```

write (u, "(A)")  "*"   Purpose: Create and display particle expressions"
write (u, "(A)")

write (u, "(A)")  "*" Basic expressions"
write (u, *)

a = new_prt_spec (var_str ("a"))
b = new_prt_spec (var_str ("b"))
c = new_prt_spec (var_str ("c"))
d = new_prt_spec (var_str ("d"))
e = new_prt_spec (var_str ("e"))
f = new_prt_spec (var_str ("f"))

call pe1%init_spec (a)
write (u, "(A)")  char (pe1%to_string ())

call pe2%init_sum (2)
select type (x => pe2%x)
type is (prt_spec_sum_t)
    call x%expr(1)%init_spec (a)
    call x%expr(2)%init_spec (b)
end select
write (u, "(A)")  char (pe2%to_string ())

call pe3%init_list (2)
select type (x => pe3%x)
type is (prt_spec_list_t)
    call x%expr(1)%init_spec (a)
    call x%expr(2)%init_spec (b)
end select
write (u, "(A)")  char (pe3%to_string ())

write (u, *)
write (u, "(A)")  "*" Nested expressions"
write (u, *)

call pe4%init_list (2)
select type (x => pe4%x)
type is (prt_spec_list_t)
    call x%expr(1)%init_sum (2)
    select type (y => x%expr(1)%x)
    type is (prt_spec_sum_t)
        call y%expr(1)%init_spec (a)
        call y%expr(2)%init_spec (b)
    end select
    call x%expr(2)%init_spec (c)
end select
write (u, "(A)")  char (pe4%to_string ())

call pe5%init_list (2)
select type (x => pe5%x)
type is (prt_spec_list_t)
    call x%expr(1)%init_list (2)
    select type (y => x%expr(1)%x)

```

```

        type is (prt_spec_list_t)
        call y%expr(1)%init_spec (a)
        call y%expr(2)%init_spec (b)
    end select
    call x%expr(2)%init_spec (c)
end select
write (u, "(A)")  char (pe5%to_string ())

call pe6%init_sum (2)
select type (x => pe6%x)
type is (prt_spec_sum_t)
    call x%expr(1)%init_spec (a)
    call x%expr(2)%init_sum (2)
    select type (y => x%expr(2)%x)
    type is (prt_spec_sum_t)
        call y%expr(1)%init_spec (b)
        call y%expr(2)%init_spec (c)
    end select
end select
write (u, "(A)")  char (pe6%to_string ())

call pe7%init_list (2)
select type (x => pe7%x)
type is (prt_spec_list_t)
    call x%expr(1)%init_sum (2)
    select type (y => x%expr(1)%x)
    type is (prt_spec_sum_t)
        call y%expr(1)%init_spec (a)
        call y%expr(2)%init_list (2)
        select type (z => y%expr(2)%x)
        type is (prt_spec_list_t)
            call z%expr(1)%init_spec (b)
            call z%expr(2)%init_spec (c)
        end select
    end select
    call x%expr(2)%init_spec (d)
end select
write (u, "(A)")  char (pe7%to_string ())

call pe8%init_sum (2)
select type (x => pe8%x)
type is (prt_spec_sum_t)
    call x%expr(1)%init_list (2)
    select type (y => x%expr(1)%x)
    type is (prt_spec_list_t)
        call y%expr(1)%init_spec (a)
        call y%expr(2)%init_spec (b)
    end select
    call x%expr(2)%init_list (2)
    select type (y => x%expr(2)%x)
    type is (prt_spec_list_t)
        call y%expr(1)%init_spec (c)
        call y%expr(2)%init_spec (d)
    end select

```

```

end select
write (u, "(A)") char (pe8%to_string ())

call pe9%init_list (3)
select type (x => pe9%x)
type is (prt_spec_list_t)
    call x%expr(1)%init_sum (2)
    select type (y => x%expr(1)%x)
    type is (prt_spec_sum_t)
        call y%expr(1)%init_spec (a)
        call y%expr(2)%init_spec (b)
    end select
    call x%expr(2)%init_spec (c)
    call x%expr(3)%init_sum (3)
    select type (y => x%expr(3)%x)
    type is (prt_spec_sum_t)
        call y%expr(1)%init_spec (d)
        call y%expr(2)%init_spec (e)
        call y%expr(3)%init_spec (f)
    end select
end select
write (u, "(A)") char (pe9%to_string ())

write (u, *)
write (u, "(A)")  "* Expand as sum"
write (u, *)

call pe1%expand ()
write (u, "(A)") char (pe1%to_string ())

call pe4%expand ()
write (u, "(A)") char (pe4%to_string ())

call pe5%expand ()
write (u, "(A)") char (pe5%to_string ())

call pe6%expand ()
write (u, "(A)") char (pe6%to_string ())

call pe7%expand ()
write (u, "(A)") char (pe7%to_string ())

call pe8%expand ()
write (u, "(A)") char (pe8%to_string ())

call pe9%expand ()
write (u, "(A)") char (pe9%to_string ())

write (u, *)
write (u, "(A)")  "* Transform to arrays:"

write (u, "(A)")  "* Atomic specifier"
do i = 1, pe1%get_n_terms ()
    call pe1%term_to_array (pa, i)

```



```

        call prt_spec_write (pa, u)
    end do

    write (u, *)
    write (u, "(A)")  "* List"
    do i = 1, pe5%get_n_terms ()
        call pe5%term_to_array (pa, i)
        call prt_spec_write (pa, u)
    end do

    write (u, *)
    write (u, "(A)")  "* Sum of atoms"
    do i = 1, pe6%get_n_terms ()
        call pe6%term_to_array (pa, i)
        call prt_spec_write (pa, u)
    end do

    write (u, *)
    write (u, "(A)")  "* Sum of lists"
    do i = 1, pe9%get_n_terms ()
        call pe9%term_to_array (pa, i)
        call prt_spec_write (pa, u)
    end do

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: particle_specifiers_2"
end subroutine particle_specifiers_2

```

13.2 PDG arrays

For defining aliases, we introduce a special type which holds a set of (integer) PDG codes.

`<pdg_arrays.f90>`≡
<File header>

`module pdg_arrays`

```

    use io_units
    use sorting
    use physics_defs

```

<Standard module head>

<PDG arrays: public>

<PDG arrays: types>

<PDG arrays: interfaces>

`contains`

```

    <PDG arrays: procedures>

```

```

end module pdg_arrays

```

13.2.1 Type definition

Using an allocatable array eliminates the need for initializer and/or finalizer.

```

<PDG arrays: public>≡
    public :: pdg_array_t
<PDG arrays: types>≡
    type :: pdg_array_t
        private
            integer, dimension(:), allocatable :: pdg
        contains
            <PDG arrays: pdg array: TBP>
        end type pdg_array_t

```

Output

```

<PDG arrays: public>+≡
    public :: pdg_array_write
<PDG arrays: pdg array: TBP>≡
    procedure :: write => pdg_array_write
<PDG arrays: procedures>≡
    subroutine pdg_array_write (aval, unit)
        class(pdg_array_t), intent(in) :: aval
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(A)", advance="no") "PDG("
        if (allocated (aval%pdg)) then
            do i = 1, size (aval%pdg)
                if (i > 1) write (u, "(A)", advance="no") ", "
                write (u, "(I0)", advance="no") aval%pdg(i)
            end do
        end if
        write (u, "(A)", advance="no") ")"
    end subroutine pdg_array_write

```

```

<PDG arrays: public>+≡
    public :: pdg_array_write_set
<PDG arrays: procedures>+≡
    subroutine pdg_array_write_set (aval, unit)
        type(pdg_array_t), intent(in), dimension(:) :: aval
        integer, intent(in), optional :: unit
        integer :: i
        do i = 1, size (aval)
            call aval(i)%write (unit)
            print *, ''
        end do
    end subroutine pdg_array_write_set

```

13.2.2 Basic operations

Assignment. We define assignment from and to an integer array. Note that the integer array, if it is the l.h.s., must be declared allocatable by the caller.

```
<PDG arrays: public>+≡
    public :: assignment(=)

<PDG arrays: interfaces>≡
    interface assignment(=)
        module procedure pdg_array_from_int_array
        module procedure pdg_array_from_int
        module procedure int_array_from_pdg_array
    end interface

<PDG arrays: procedures>+≡
    subroutine pdg_array_from_int_array (aval, iarray)
        type(pdg_array_t), intent(out) :: aval
        integer, dimension(:), intent(in) :: iarray
        allocate (aval%pdg (size (iarray)))
        aval%pdg = iarray
    end subroutine pdg_array_from_int_array

    elemental subroutine pdg_array_from_int (aval, int)
        type(pdg_array_t), intent(out) :: aval
        integer, intent(in) :: int
        allocate (aval%pdg (1))
        aval%pdg = int
    end subroutine pdg_array_from_int

    subroutine int_array_from_pdg_array (iarray, aval)
        integer, dimension(:), allocatable, intent(out) :: iarray
        type(pdg_array_t), intent(in) :: aval
        if (allocated (aval%pdg)) then
            allocate (iarray (size (aval%pdg)))
            iarray = aval%pdg
        else
            allocate (iarray (0))
        end if
    end subroutine int_array_from_pdg_array
```

Allocate space for a PDG array

```
<PDG arrays: public>+≡
    public :: pdg_array_init

<PDG arrays: procedures>+≡
    subroutine pdg_array_init (aval, n_elements)
        type(pdg_array_t), intent(inout) :: aval
        integer, intent(in) :: n_elements
        allocate(aval%pdg(n_elements))
    end subroutine pdg_array_init
```

Deallocate a previously allocated pdg array

```
<PDG arrays: public>+≡
    public :: pdg_array_delete
```

```

(PDG arrays: procedures)+≡
  subroutine pdg_array_delete (aval)
    type(pdg_array_t), intent(inout) :: aval
    if (allocated (aval%pdg)) deallocate (aval%pdg)
  end subroutine pdg_array_delete

```

Merge two pdg arrays, i.e. append a particle string to another leaving out doublettes

```

(PDG arrays: public)+≡
  public :: pdg_array_merge

(PDG arrays: procedures)+≡
  subroutine pdg_array_merge (aval1, aval2)
    type(pdg_array_t), intent(inout) :: aval1
    type(pdg_array_t), intent(in) :: aval2
    type(pdg_array_t) :: aval
    if (allocated (aval1%pdg) .and. allocated (aval2%pdg)) then
      if (.not. any (aval1%pdg == aval2%pdg)) aval = aval1 // aval2
    else if (allocated (aval1%pdg)) then
      aval = aval1
    else if (allocated (aval2%pdg)) then
      aval = aval2
    end if
    call pdg_array_delete (aval1)
    aval1 = aval%pdg
  end subroutine pdg_array_merge

```

Length of the array.

```

(PDG arrays: public)+≡
  public :: pdg_array_get_length

(PDG arrays: pdg array: TBP)+≡
  procedure :: get_length => pdg_array_get_length

(PDG arrays: procedures)+≡
  elemental function pdg_array_get_length (aval) result (n)
    class(pdg_array_t), intent(in) :: aval
    integer :: n
    if (allocated (aval%pdg)) then
      n = size (aval%pdg)
    else
      n = 0
    end if
  end function pdg_array_get_length

```

Return the element with index i.

```

(PDG arrays: public)+≡
  public :: pdg_array_get

(PDG arrays: pdg array: TBP)+≡
  procedure :: get => pdg_array_get

```

```

(PDG arrays: procedures)+≡
elemental function pdg_array_get (aval, i) result (pdg)
  class(pdg_array_t), intent(in) :: aval
  integer, intent(in), optional :: i
  integer :: pdg
  if (present (i)) then
    pdg = aval%pdg(i)
  else
    pdg = aval%pdg(1)
  end if
end function pdg_array_get

```

Explicitly set the element with index i.

```

(PDG arrays: pdg array: TBP)+≡
procedure :: set => pdg_array_set

```

```

(PDG arrays: procedures)+≡
subroutine pdg_array_set (aval, i, pdg)
  class(pdg_array_t), intent(inout) :: aval
  integer, intent(in) :: i
  integer, intent(in) :: pdg
  aval%pdg(i) = pdg
end subroutine pdg_array_set

```

```

(PDG arrays: pdg array: TBP)+≡
procedure :: add => pdg_array_add

```

```

(PDG arrays: procedures)+≡
function pdg_array_add (aval, aval_add) result (aval_out)
  type(pdg_array_t) :: aval_out
  class(pdg_array_t), intent(in) :: aval
  type(pdg_array_t), intent(in) :: aval_add
  integer :: n, n_add, i
  n = size (aval%pdg)
  n_add = size (aval_add%pdg)
  allocate (aval_out%pdg (n + n_add))
  aval_out%pdg(1:n) = aval%pdg
  do i = 1, n_add
    aval_out%pdg(n+i) = aval_add%pdg(i)
  end do
end function pdg_array_add

```

Replace element with index i by a new array of elements.

```

(PDG arrays: public)+≡
public :: pdg_array_replace

```

```

(PDG arrays: pdg array: TBP)+≡
procedure :: replace => pdg_array_replace

```

```

(PDG arrays: procedures)+≡
function pdg_array_replace (aval, i, pdg_new) result (aval_new)
  class(pdg_array_t), intent(in) :: aval
  integer, intent(in) :: i
  integer, dimension(:), intent(in) :: pdg_new

```

```

type(pdg_array_t) :: aval_new
integer :: n, l
n = size (aval%pdg)
l = size (pdg_new)
allocate (aval_new%pdg (n + l - 1))
aval_new%pdg(:i-1) = aval%pdg(:i-1)
aval_new%pdg(i:i+l-1) = pdg_new
aval_new%pdg(i+l:) = aval%pdg(i+l:)
end function pdg_array_replace

```

Concatenate two PDG arrays

```

(PDG arrays: public)+≡
public :: operator(//)

(PDG arrays: interfaces)+≡
interface operator(//)
module procedure concat_pdg_arrays
end interface

(PDG arrays: procedures)+≡
function concat_pdg_arrays (aval1, aval2) result (aval)
type(pdg_array_t) :: aval
type(pdg_array_t), intent(in) :: aval1, aval2
integer :: n1, n2
if (allocated (aval1%pdg) .and. allocated (aval2%pdg)) then
n1 = size (aval1%pdg)
n2 = size (aval2%pdg)
allocate (aval%pdg (n1 + n2))
aval%pdg(:n1) = aval1%pdg
aval%pdg(n1+1:) = aval2%pdg
else if (allocated (aval1%pdg)) then
aval = aval1
else if (allocated (aval2%pdg)) then
aval = aval2
end if
end function concat_pdg_arrays

```

13.2.3 Matching

A PDG array matches a given PDG code if the code is present within the array. If either one is zero (UNDEFINED), the match also succeeds.

```

(PDG arrays: public)+≡
public :: operator(.match.)

(PDG arrays: interfaces)+≡
interface operator(.match.)
module procedure pdg_array_match_integer
module procedure pdg_array_match_pdg_array
end interface

```

Match a single code against the array.

```
<PDG arrays: procedures>+≡
  elemental function pdg_array_match_integer (aval, pdg) result (flag)
    logical :: flag
    type(pdg_array_t), intent(in) :: aval
    integer, intent(in) :: pdg
    if (allocated (aval%pdg)) then
      flag = pdg == UNDEFINED &
        .or. any (aval%pdg == UNDEFINED) &
        .or. any (aval%pdg == pdg)
    else
      flag = .false.
    end if
  end function pdg_array_match_integer
```

Check if the pdg-number corresponds to a quark

```
<PDG arrays: public>+≡
  public :: is_quark

<PDG arrays: procedures>+≡
  elemental function is_quark (pdg_nr)
    logical :: is_quark
    integer, intent(in) :: pdg_nr
    if (abs (pdg_nr) >= 1 .and. abs (pdg_nr) <= 6) then
      is_quark = .true.
    else
      is_quark = .false.
    end if
  end function is_quark
```

Check if pdg-number corresponds to a gluon

```
<PDG arrays: public>+≡
  public :: is_gluon

<PDG arrays: procedures>+≡
  elemental function is_gluon (pdg_nr)
    logical :: is_gluon
    integer, intent(in) :: pdg_nr
    if (pdg_nr == GLUON) then
      is_gluon = .true.
    else
      is_gluon = .false.
    end if
  end function is_gluon
```

Check if pdg-number corresponds to a photon

```
<PDG arrays: public>+≡
  public :: is_photon

<PDG arrays: procedures>+≡
  elemental function is_photon (pdg_nr)
    logical :: is_photon
    integer, intent(in) :: pdg_nr
```

```

    if (pdg_nr == PHOTON) then
        is_photon = .true.
    else
        is_photon = .false.
    end if
end function is_photon

```

Check if pdg-number corresponds to a colored particle

```

(PDG arrays: public)+≡
    public :: is_colored

(PDG arrays: procedures)+≡
    elemental function is_colored (pdg_nr)
        logical :: is_colored
        integer, intent(in) :: pdg_nr
        is_colored = is_quark (pdg_nr) .or. is_gluon (pdg_nr)
    end function is_colored

```

Check if the pdg-number corresponds to a lepton

```

(PDG arrays: public)+≡
    public :: is_lepton

(PDG arrays: procedures)+≡
    elemental function is_lepton (pdg_nr)
        logical :: is_lepton
        integer, intent(in) :: pdg_nr
        if (abs (pdg_nr) >= ELECTRON .and. &
            abs (pdg_nr) <= TAU_NEUTRINO) then
            is_lepton = .true.
        else
            is_lepton = .false.
        end if
    end function is_lepton

```

```

(PDG arrays: public)+≡
    public :: is_fermion

(PDG arrays: procedures)+≡
    elemental function is_fermion (pdg_nr)
        logical :: is_fermion
        integer, intent(in) :: pdg_nr
        is_fermion = is_lepton(pdg_nr) .or. is_quark(pdg_nr)
    end function is_fermion

```

Check if the pdg-number corresponds to a massless vector boson

```

(PDG arrays: public)+≡
    public :: is_massless_vector

(PDG arrays: procedures)+≡
    elemental function is_massless_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_massless_vector
        if (pdg_nr == GLUON .or. pdg_nr == PHOTON) then

```



```

        is_massless_vector = .true.
    else
        is_massless_vector = .false.
    end if
end function is_massless_vector

```

Check if pdg-number corresponds to a massive vector boson

```

(PDG arrays: public)+≡
    public :: is_massive_vector

(PDG arrays: procedures)+≡
    elemental function is_massive_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_massive_vector
        if (abs (pdg_nr) == Z_BOSON .or. abs (pdg_nr) == W_BOSON) then
            is_massive_vector = .true.
        else
            is_massive_vector = .false.
        end if
    end function is_massive_vector

```

Check if pdg-number corresponds to a vector boson

```

(PDG arrays: public)+≡
    public :: is_vector

(PDG arrays: procedures)+≡
    elemental function is_vector (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_vector
        if (is_massless_vector (pdg_nr) .or. is_massive_vector (pdg_nr)) then
            is_vector = .true.
        else
            is_vector = .false.
        end if
    end function is_vector

```

Check if particle is elementary.

```

(PDG arrays: public)+≡
    public :: is_elementary

(PDG arrays: procedures)+≡
    elemental function is_elementary (pdg_nr)
        integer, intent(in) :: pdg_nr
        logical :: is_elementary
        if (is_vector (pdg_nr) .or. is_fermion (pdg_nr) .or. pdg_nr == 25) then
            is_elementary = .true.
        else
            is_elementary = .false.
        end if
    end function is_elementary

```

Check if particle is an EW boson or scalar.

```

(PDG arrays: public)+≡
    public :: is_ew_boson_scalar

```

```

(PDG arrays: procedures)+≡
elemental function is_ew_boson_scalar (pdg_nr)
integer, intent(in) :: pdg_nr
logical :: is_ew_boson_scalar
if (is_photon (pdg_nr) .or. is_massive_vector (pdg_nr) .or. pdg_nr == 25) then
    is_ew_boson_scalar = .true.
else
    is_ew_boson_scalar = .false.
end if
end function is_ew_boson_scalar

```

Check if particle is strongly interacting

```

(PDG arrays: pdg array: TBP)+≡
procedure :: has_colored_particles => pdg_array_has_colored_particles

(PDG arrays: procedures)+≡
function pdg_array_has_colored_particles (pdg) result (colored)
class(pdg_array_t), intent(in) :: pdg
logical :: colored
integer :: i, pdg_nr
colored = .false.
do i = 1, size (pdg%pdg)
    pdg_nr = pdg%pdg(i)
    if (is_quark (pdg_nr) .or. is_gluon (pdg_nr)) then
        colored = .true.
        exit
    end if
end do
end function pdg_array_has_colored_particles

```

This function is a convenience function for the determination of possible compatibility of flavor structures of processes with certain orders of QCD and QED/EW coupling constants. It assumes the Standard Model (SM) as underlying physics model. The function is based on a naive counting of external particles which are connected to the process by the specific kind of couplings depending on the underlying theory (QCD and/or QED/EW) of which the corresponding particle is a part of. It is constructed in a way that the exclusion of coupling power combinations is well-defined.

```

(PDG arrays: public)+≡
public :: query_coupling_powers

(PDG arrays: procedures)+≡
function query_coupling_powers (flv, a_power, as_power) result (valid)
integer, intent(in), dimension(:) :: flv
integer, dimension(:, :), allocatable :: power_pair_array
integer, dimension(2) :: power_pair_ref
integer, intent(in) :: a_power, as_power
integer :: i, n_legs, n_gluons, n_quarks, n_gamWZH, n_leptons
logical, dimension(:), allocatable :: pairs_included
logical :: valid
integer :: n_bound
power_pair_ref = [a_power, as_power]
n_legs = size (flv)

```

```

allocate (power_pair_array (2, n_legs - 1))
do i = 1, n_legs - 1
  power_pair_array (1, i) = n_legs - 1 - i
  power_pair_array (2, i) = i - 1
end do
allocate (pairs_included (n_legs - 1))
pairs_included = .true.
n_gluons = count (is_gluon (flv))
n_gamWZH = count (is_ew_boson_scalar (flv))
n_quarks = count (is_quark (flv))
n_leptons = count (is_lepton (flv))
if (n_gluons >= 1 .and. n_gluons <= 3) then
  do i = 1, n_gluons
    pairs_included (i) = .false.
  end do
else if (n_gluons > 2 .and. n_quarks <= 2 .and. n_gluons + n_quarks == n_legs) then
  do i = 1, n_legs - 2
    pairs_included (i) = .false.
  end do
end if
n_bound = 0
if (n_gamWZH + n_leptons == n_legs) then
  n_bound = n_gamWZH + n_leptons - 2
else if (n_quarks == 2 .and. n_leptons + n_quarks + n_gamWZH == n_legs) then
  n_bound = n_legs - 2
else if (n_gamWZH + n_leptons > 0) then
  n_bound = int (n_leptons/2.) + n_gamWZH
end if
if (n_bound > 0) then
  do i = 1, n_bound
    pairs_included (n_legs - i) = .false.
  end do
end if
if (n_quarks == 4 .and. .not. qcd_ew_interferences (flv)) then
  do i = 1, 2
    pairs_included (n_legs - i) = .false.
  end do
end if
valid = .false.
do i = 1, n_legs - 1
  if (all (power_pair_array (:, i) == power_pair_ref) .and. pairs_included (i)) then
    valid = .true.
    exit
  end if
end do
end function query_coupling_powers

```

This function checks if there is a flavor structure which possibly can induce QCD-EW interference amplitudes. It evaluates to **true** if there are at least 2 quark pairs whereby the quarks of at least one quark pair must have the same flavor.

(PDG arrays: public)+≡
public :: qcd_ew_interferences

```

(PDG arrays: procedures)+≡
function qcd_ew_interferences (flv) result (valid)
  integer, intent(in), dimension(:) :: flv
  integer :: i, n_pairs
  logical :: valid, qqbar_pair
  n_pairs = 0
  valid = .false.
  qqbar_pair = .false.
  if (count (is_quark (flv)) >= 4) then
    do i = DOWN_Q, TOP_Q
      qqbar_pair = count (abs (flv) == i) >= 2
      if (qqbar_pair) n_pairs = n_pairs + 1
      if (n_pairs > 0) then
        valid = .true.
        exit
      end if
    end do
  end if
end function qcd_ew_interferences

```

Match two arrays. Succeeds if any pair of entries matches.

```

(PDG arrays: procedures)+≡
function pdg_array_match_pdg_array (aval1, aval2) result (flag)
  logical :: flag
  type(pdg_array_t), intent(in) :: aval1, aval2
  if (allocated (aval1%pdg) .and. allocated (aval2%pdg)) then
    flag = any (aval1 .match. aval2%pdg)
  else
    flag = .false.
  end if
end function pdg_array_match_pdg_array

```

Comparison. Here, we take the PDG arrays as-is, assuming that they are sorted.

The ordering is a bit odd: first, we look only at the absolute values of the PDG codes. If they all match, the particle comes before the antiparticle, scanning from left to right.

```

(PDG arrays: public)+≡
public :: operator(<)
public :: operator(>)
public :: operator(<=)
public :: operator(>=)
public :: operator(==)
public :: operator(/=)

(PDG arrays: interfaces)+≡
interface operator(<)
  module procedure pdg_array_lt
end interface
interface operator(>)
  module procedure pdg_array_gt
end interface
interface operator(<=)
  module procedure pdg_array_le
end interface

```

```

end interface
interface operator(>=)
  module procedure pdg_array_ge
end interface
interface operator(==)
  module procedure pdg_array_eq
end interface
interface operator(/=)
  module procedure pdg_array_ne
end interface

```

(PDG arrays: procedures) +=

```

elemental function pdg_array_lt (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  integer :: i
  if (size (aval1%pdg) /= size (aval2%pdg)) then
    flag = size (aval1%pdg) < size (aval2%pdg)
  else
    do i = 1, size (aval1%pdg)
      if (abs (aval1%pdg(i)) /= abs (aval2%pdg(i))) then
        flag = abs (aval1%pdg(i)) < abs (aval2%pdg(i))
        return
      end if
    end do
    do i = 1, size (aval1%pdg)
      if (aval1%pdg(i) /= aval2%pdg(i)) then
        flag = aval1%pdg(i) > aval2%pdg(i)
        return
      end if
    end do
    flag = .false.
  end if
end function pdg_array_lt

elemental function pdg_array_gt (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  flag = .not. (aval1 < aval2 .or. aval1 == aval2)
end function pdg_array_gt

elemental function pdg_array_le (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  flag = aval1 < aval2 .or. aval1 == aval2
end function pdg_array_le

elemental function pdg_array_ge (aval1, aval2) result (flag)
  type(pdg_array_t), intent(in) :: aval1, aval2
  logical :: flag
  flag = .not. (aval1 < aval2)
end function pdg_array_ge

elemental function pdg_array_eq (aval1, aval2) result (flag)

```

```

    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
    if (size (aval1%pdg) /= size (aval2%pdg)) then
        flag = .false.
    else
        flag = all (aval1%pdg == aval2%pdg)
    end if
end function pdg_array_eq

elemental function pdg_array_ne (aval1, aval2) result (flag)
    type(pdg_array_t), intent(in) :: aval1, aval2
    logical :: flag
    flag = .not. (aval1 == aval2)
end function pdg_array_ne

```

Equivalence. Two PDG arrays are equivalent if either one contains UNDEFINED or if each element of array 1 is present in array 2, and vice versa.

```

(PDG arrays: public)+≡
    public :: operator(.eqv.)
    public :: operator(.neqv.)

(PDG arrays: interfaces)+≡
    interface operator(.eqv.)
        module procedure pdg_array_equivalent
    end interface
    interface operator(.neqv.)
        module procedure pdg_array_inequivalent
    end interface

(PDG arrays: procedures)+≡
    elemental function pdg_array_equivalent (aval1, aval2) result (eq)
        logical :: eq
        type(pdg_array_t), intent(in) :: aval1, aval2
        logical, dimension(:), allocatable :: match1, match2
        integer :: i
        if (allocated (aval1%pdg) .and. allocated (aval2%pdg)) then
            eq = any (aval1%pdg == UNDEFINED) &
                .or. any (aval2%pdg == UNDEFINED)
        if (.not. eq) then
            allocate (match1 (size (aval1%pdg)))
            allocate (match2 (size (aval2%pdg)))
            match1 = .false.
            match2 = .false.
            do i = 1, size (aval1%pdg)
                match2 = match2 .or. aval1%pdg(i) == aval2%pdg
            end do
            do i = 1, size (aval2%pdg)
                match1 = match1 .or. aval2%pdg(i) == aval1%pdg
            end do
            eq = all (match1) .and. all (match2)
        end if
    else
        eq = .false.
    end if
end function

```

```

end function pdg_array_equivalent

elemental function pdg_array_inequivalent (aval1, aval2) result (neq)
  logical :: neq
  type(pdg_array_t), intent(in) :: aval1, aval2
  neq = .not. pdg_array_equivalent (aval1, aval2)
end function pdg_array_inequivalent

```

13.2.4 Sorting

Sort a PDG array by absolute value, particle before antiparticle. After sorting, we eliminate double entries.

```

<PDG arrays: public>+≡
  public :: sort_abs

<PDG arrays: interfaces>+≡
  interface sort_abs
    module procedure pdg_array_sort_abs
  end interface

<PDG arrays: pdg array: TBP>+≡
  procedure :: sort_abs => pdg_array_sort_abs

<PDG arrays: procedures>+≡
  function pdg_array_sort_abs (aval1, unique) result (aval2)
    class(pdg_array_t), intent(in) :: aval1
    logical, intent(in), optional :: unique
    type(pdg_array_t) :: aval2
    integer, dimension(:), allocatable :: tmp
    logical, dimension(:), allocatable :: mask
    integer :: i, n
    logical :: uni
    uni = .false.; if (present (unique)) uni = unique
    n = size (aval1%pdg)
    if (uni) then
      allocate (tmp (n), mask(n))
      tmp = sort_abs (aval1%pdg)
      mask(1) = .true.
      do i = 2, n
        mask(i) = tmp(i) /= tmp(i-1)
      end do
      allocate (aval2%pdg (count (mask)))
      aval2%pdg = pack (tmp, mask)
    else
      allocate (aval2%pdg (n))
      aval2%pdg = sort_abs (aval1%pdg)
    end if
  end function pdg_array_sort_abs

<PDG arrays: pdg array: TBP>+≡
  procedure :: intersect => pdg_array_intersect

```

```

(PDG arrays: procedures)+≡
function pdg_array_intersect (aval1, match) result (aval2)
  class(pdg_array_t), intent(in) :: aval1
  integer, dimension(:) :: match
  type(pdg_array_t) :: aval2
  integer, dimension(:), allocatable :: isec
  integer :: i
  isec = pack (aval1%pdg, [(any(aval1%pdg(i) == match), i=1,size(aval1%pdg))])
  aval2 = isec
end function pdg_array_intersect

(PDG arrays: pdg array: TBP)+≡
procedure :: search_for_particle => pdg_array_search_for_particle

(PDG arrays: procedures)+≡
elemental function pdg_array_search_for_particle (pdg, i_part) result (found)
  class(pdg_array_t), intent(in) :: pdg
  integer, intent(in) :: i_part
  logical :: found
  found = any (pdg%pdg == i_part)
end function pdg_array_search_for_particle

(PDG arrays: pdg array: TBP)+≡
procedure :: invert => pdg_array_invert

(PDG arrays: procedures)+≡
function pdg_array_invert (pdg) result (pdg_inverse)
  class(pdg_array_t), intent(in) :: pdg
  type(pdg_array_t) :: pdg_inverse
  integer :: i, n
  n = size (pdg%pdg)
  allocate (pdg_inverse%pdg (n))
  do i = 1, n
    select case (pdg%pdg(i))
    case (GLUON, PHOTON, Z_BOSON, 25)
      pdg_inverse%pdg(i) = pdg%pdg(i)
    case default
      pdg_inverse%pdg(i) = -pdg%pdg(i)
    end select
  end do
end function pdg_array_invert

```

13.2.5 PDG array list

A PDG array list, or PDG list, is an array of PDG-array objects with some convenience methods.

```

(PDG arrays: public)+≡
public :: pdg_list_t

(PDG arrays: types)+≡
type :: pdg_list_t
  type(pdg_array_t), dimension(:), allocatable :: a

```



```

contains
  <PDG arrays: pdg list: TBP>
end type pdg_list_t

```

Output, as a comma-separated list without advancing I/O.

```

<PDG arrays: pdg list: TBP>≡
  procedure :: write => pdg_list_write

<PDG arrays: procedures>+≡
  subroutine pdg_list_write (object, unit)
    class(pdg_list_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    if (allocated (object%a)) then
      do i = 1, size (object%a)
        if (i > 1) write (u, "(A)", advance="no") ", "
        call object%a(i)%write (u)
      end do
    end if
  end subroutine pdg_list_write

```

Initialize for a certain size. The entries are initially empty PDG arrays.

```

<PDG arrays: pdg list: TBP>+≡
  generic :: init => pdg_list_init_size
  procedure, private :: pdg_list_init_size

<PDG arrays: procedures>+≡
  subroutine pdg_list_init_size (pl, n)
    class(pdg_list_t), intent(out) :: pl
    integer, intent(in) :: n
    allocate (pl%a (n))
  end subroutine pdg_list_init_size

```

Initialize with a definite array of PDG codes. That is, each entry in the list becomes a single-particle PDG array.

```

<PDG arrays: pdg list: TBP>+≡
  generic :: init => pdg_list_init_int_array
  procedure, private :: pdg_list_init_int_array

<PDG arrays: procedures>+≡
  subroutine pdg_list_init_int_array (pl, pdg)
    class(pdg_list_t), intent(out) :: pl
    integer, dimension(:), intent(in) :: pdg
    integer :: i
    allocate (pl%a (size (pdg)))
    do i = 1, size (pdg)
      pl%a(i) = pdg(i)
    end do
  end subroutine pdg_list_init_int_array

```

Set one of the entries. No bounds-check.

```

(PDG arrays: pdg list: TBP)+≡
generic :: set => pdg_list_set_int
generic :: set => pdg_list_set_int_array
generic :: set => pdg_list_set_pdg_array
procedure, private :: pdg_list_set_int
procedure, private :: pdg_list_set_int_array
procedure, private :: pdg_list_set_pdg_array

(PDG arrays: procedures)+≡
subroutine pdg_list_set_int (pl, i, pdg)
  class(pdg_list_t), intent(inout) :: pl
  integer, intent(in) :: i
  integer, intent(in) :: pdg
  pl%a(i) = pdg
end subroutine pdg_list_set_int

subroutine pdg_list_set_int_array (pl, i, pdg)
  class(pdg_list_t), intent(inout) :: pl
  integer, intent(in) :: i
  integer, dimension(:), intent(in) :: pdg
  pl%a(i) = pdg
end subroutine pdg_list_set_int_array

subroutine pdg_list_set_pdg_array (pl, i, pa)
  class(pdg_list_t), intent(inout) :: pl
  integer, intent(in) :: i
  type(pdg_array_t), intent(in) :: pa
  pl%a(i) = pa
end subroutine pdg_list_set_pdg_array

```

Array size, not the length of individual entries

```

(PDG arrays: pdg list: TBP)+≡
procedure :: get_size => pdg_list_get_size

(PDG arrays: procedures)+≡
function pdg_list_get_size (pl) result (n)
  class(pdg_list_t), intent(in) :: pl
  integer :: n
  if (allocated (pl%a)) then
    n = size (pl%a)
  else
    n = 0
  end if
end function pdg_list_get_size

```

Return an entry, as a PDG array.

```

(PDG arrays: pdg list: TBP)+≡
procedure :: get => pdg_list_get

(PDG arrays: procedures)+≡
function pdg_list_get (pl, i) result (pa)
  type(pdg_array_t) :: pa
  class(pdg_list_t), intent(in) :: pl

```

```

integer, intent(in) :: i
pa = pl%a(i)
end function pdg_list_get

```

Check if the list entries are all either mutually disjoint or identical. The individual entries (PDG arrays) should already be sorted, so we can test for equality.

```

(PDG arrays: pdg list: TBP)+≡
  procedure :: is_regular => pdg_list_is_regular

(PDG arrays: procedures)+≡
  function pdg_list_is_regular (pl) result (flag)
    class(pdg_list_t), intent(in) :: pl
    logical :: flag
    integer :: i, j, s
    s = pl%get_size ()
    flag = .true.
    do i = 1, s
      do j = i + 1, s
        if (pl%a(i) .match. pl%a(j)) then
          if (pl%a(i) /= pl%a(j)) then
            flag = .false.
            return
          end if
        end if
      end do
    end do
  end function pdg_list_is_regular

```

Sort the list. First, each entry gets sorted, including elimination of doublers. Then, we sort the list, using the first member of each PDG array as the marker. No removal of doublers at this stage.

If `n_in` is supplied, we do not reorder the first `n_in` particle entries.

```

(PDG arrays: pdg list: TBP)+≡
  procedure :: sort_abs => pdg_list_sort_abs

(PDG arrays: procedures)+≡
  function pdg_list_sort_abs (pl, n_in) result (pl_sorted)
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in), optional :: n_in
    type(pdg_list_t) :: pl_sorted
    type(pdg_array_t), dimension(:), allocatable :: pa
    integer, dimension(:), allocatable :: pdg, map
    integer :: i, n0
    call pl_sorted%init (pl%get_size ())
    if (allocated (pl%a)) then
      allocate (pa (size (pl%a)))
      do i = 1, size (pl%a)
        pa(i) = pl%a(i)%sort_abs (unique = .true.)
      end do
      allocate (pdg (size (pa)), source = 0)
      do i = 1, size (pa)
        if (allocated (pa(i)%pdg)) then
          if (size (pa(i)%pdg) > 0) then

```

```

        pdg(i) = pa(i)%pdg(1)
    end if
end if
end do
if (present (n_in)) then
    n0 = n_in
else
    n0 = 0
end if
allocate (map (size (pdg)))
map(:n0) = [(i, i = 1, n0)]
map(n0+1:) = n0 + order_abs (pdg(n0+1:))
do i = 1, size (pa)
    call pl_sorted%set (i, pa(map(i)))
end do
end if
end function pdg_list_sort_abs

```

Compare sorted lists: equality. The result is undefined if some entries are not allocated.

```

(PDG arrays: pdg list: TBP)+≡
generic :: operator (==) => pdg_list_eq
procedure, private :: pdg_list_eq

(PDG arrays: procedures)+≡
function pdg_list_eq (p1, p2) result (flag)
class(pdg_list_t), intent(in) :: p1, p2
logical :: flag
integer :: i
flag = .false.
if (allocated (p1%a) .and. allocated (p2%a)) then
    if (size (p1%a) == size (p2%a)) then
        do i = 1, size (p1%a)
            associate (a1 => p1%a(i), a2 => p2%a(i))
                if (allocated (a1%pdg) .and. allocated (a2%pdg)) then
                    if (size (a1%pdg) == size (a2%pdg)) then
                        if (size (a1%pdg) > 0) then
                            if (a1%pdg(1) /= a2%pdg(1)) return
                        end if
                    else
                        return
                    end if
                end if
            end associate
        end do
        flag = .true.
    end if
end if
end function pdg_list_eq

```

Compare sorted lists. The result is undefined if some entries are not allocated.

The ordering is quite complicated. First, a shorter list comes before a longer list. Comparing entry by entry, a shorter entry comes first. Next, we check the first PDG code within corresponding entries. This is compared by absolute value. If equal, particle comes before antiparticle. Finally, if all is equal, the result is false.

```

(PDG arrays: pdg list: TBP)+≡
  generic :: operator (<) => pdg_list_lt
  procedure, private :: pdg_list_lt

(PDG arrays: procedures)+≡
  function pdg_list_lt (p11, p12) result (flag)
    class(pdg_list_t), intent(in) :: p11, p12
    logical :: flag
    integer :: i
    flag = .false.
    if (allocated (p11%a) .and. allocated (p12%a)) then
      if (size (p11%a) < size (p12%a)) then
        flag = .true.; return
      else if (size (p11%a) > size (p12%a)) then
        return
      else
        do i = 1, size (p11%a)
          associate (a1 => p11%a(i), a2 => p12%a(i))
            if (allocated (a1%pdg) .and. allocated (a2%pdg)) then
              if (size (a1%pdg) < size (a2%pdg)) then
                flag = .true.; return
              else if (size (a1%pdg) > size (a2%pdg)) then
                return
              else
                if (size (a1%pdg) > 0) then
                  if (abs (a1%pdg(1)) < abs (a2%pdg(1))) then
                    flag = .true.; return
                  else if (abs (a1%pdg(1)) > abs (a2%pdg(1))) then
                    return
                  else if (a1%pdg(1) > 0 .and. a2%pdg(1) < 0) then
                    flag = .true.; return
                  else if (a1%pdg(1) < 0 .and. a2%pdg(1) > 0) then
                    return
                  end if
                end if
              end if
            else
              return
            end if
          end associate
        end do
        flag = .false.
      end if
    end if
  end function pdg_list_lt

```

Replace an entry. In the result, the entry #i is replaced by the contents of the second argument. The result is not sorted.

If `n_in` is also set and `i` is less or equal to `n_in`, replace `#i` only by the first entry of `pl_insert`, and insert the remainder after entry `n_in`.

(PDG arrays: pdg list: TBP)+≡

procedure :: replace => pdg_list_replace

(PDG arrays: procedures)+≡

```
function pdg_list_replace (pl, i, pl_insert, n_in) result (pl_out)
  type(pdg_list_t) :: pl_out
  class(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: i
  class(pdg_list_t), intent(in) :: pl_insert
  integer, intent(in), optional :: n_in
  integer :: n, n_insert, n_out, k
  n = pl%get_size ()
  n_insert = pl_insert%get_size ()
  n_out = n + n_insert - 1
  call pl_out%init (n_out)
!   if (allocated (pl%a)) then
!     do k = 1, i - 1
!       pl_out%a(k) = pl%a(k)
!     end do
!   end if
  if (present (n_in)) then
    pl_out%a(i) = pl_insert%a(1)
    do k = i + 1, n_in
      pl_out%a(k) = pl%a(k)
    end do
    do k = 1, n_insert - 1
      pl_out%a(n_in+k) = pl_insert%a(1+k)
    end do
    do k = 1, n - n_in
      pl_out%a(n_in+k+n_insert-1) = pl%a(n_in+k)
    end do
  else
!   if (allocated (pl_insert%a)) then
!     do k = 1, n_insert
!       pl_out%a(i-1+k) = pl_insert%a(k)
!     end do
!   end if
!   if (allocated (pl%a)) then
!     do k = 1, n - i
!       pl_out%a(i+n_insert-1+k) = pl%a(i+k)
!     end do
!   end if
! end if
end function pdg_list_replace
```

(PDG arrays: pdg list: TBP)+≡

procedure :: fusion => pdg_list_fusion

(PDG arrays: procedures)+≡

```
function pdg_list_fusion (pl, pl_insert, i, check_if_existing) result (pl_out)
  type(pdg_list_t) :: pl_out
  class(pdg_list_t), intent(in) :: pl
```

```

type(pdg_list_t), intent(in) :: pl_insert
integer, intent(in) :: i
logical, intent(in) :: check_if_existing
integer :: n, n_insert, k, n_out
logical :: new_pdg
n = pl%get_size ()
n_insert = pl_insert%get_size ()
new_pdg = .not. check_if_existing .or. &
  (.not. any (pl%search_for_particle (pl_insert%a(1)%pdg)))
call pl_out%init (n + n_insert - 1)
do k = 1, n
  if (new_pdg .and. k == i) then
    pl_out%a(k) = pl%a(k)%add (pl_insert%a(1))
  else
    pl_out%a(k) = pl%a(k)
  end if
end do
do k = n + 1, n + n_insert - 1
  pl_out%a(k) = pl_insert%a(k-n)
end do
end function pdg_list_fusion

```

(PDG arrays: pdg list: TBP)+≡
 procedure :: get_pdg_sizes => pdg_list_get_pdg_sizes

(PDG arrays: procedures)+≡
 function pdg_list_get_pdg_sizes (pl) result (i_size)
 integer, dimension(:), allocatable :: i_size
 class(pdg_list_t), intent(in) :: pl
 integer :: i, n
 n = pl%get_size ()
 allocate (i_size (n))
 do i = 1, n
 i_size(i) = size (pl%a(i)%pdg)
 end do
end function pdg_list_get_pdg_sizes

Replace the entries of `pl` by the matching entries of `pl_match`, one by one. This is done in-place. If there is no match, return failure.

(PDG arrays: pdg list: TBP)+≡
 procedure :: match_replace => pdg_list_match_replace

(PDG arrays: procedures)+≡
 subroutine pdg_list_match_replace (pl, pl_match, success)
 class(pdg_list_t), intent(inout) :: pl
 class(pdg_list_t), intent(in) :: pl_match
 logical, intent(out) :: success
 integer :: i, j
 success = .true.
 SCAN_ENTRIES: do i = 1, size (pl%a)
 do j = 1, size (pl_match%a)
 if (pl%a(i) .match. pl_match%a(j)) then
 pl%a(i) = pl_match%a(j)
 cycle SCAN_ENTRIES
 end if
 end do
 end do

```

        end if
    end do
    success = .false.
    return
end do SCAN_ENTRIES
end subroutine pdg_list_match_replace

```

Just check if a PDG array matches any entry in the PDG list. The second version returns the position of the match within the list. An optional mask indicates the list elements that should be checked.

```

(PDG arrays: pdg list: TBP)+≡
generic :: operator (.match.) => pdg_list_match_pdg_array
procedure, private :: pdg_list_match_pdg_array
procedure :: find_match => pdg_list_find_match_pdg_array

(PDG arrays: procedures)+≡
function pdg_list_match_pdg_array (pl, pa) result (flag)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), intent(in) :: pa
    logical :: flag
    flag = pl%find_match (pa) /= 0
end function pdg_list_match_pdg_array

function pdg_list_find_match_pdg_array (pl, pa, mask) result (i)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), intent(in) :: pa
    logical, dimension(:), intent(in), optional :: mask
    integer :: i
    do i = 1, size (pl%a)
        if (present (mask)) then
            if (.not. mask(i)) cycle
        end if
        if (pl%a(i) .match. pa) return
    end do
    i = 0
end function pdg_list_find_match_pdg_array

```

Some old compilers have problems with allocatable arrays as intent(out) or as function result, so be conservative here:

```

(PDG arrays: pdg list: TBP)+≡
procedure :: create_pdg_array => pdg_list_create_pdg_array

(PDG arrays: procedures)+≡
subroutine pdg_list_create_pdg_array (pl, pdg)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_array_t), dimension(:), intent(inout), allocatable :: pdg
    integer :: n_elements
    integer :: i
    associate (a => pl%a)
        n_elements = size (a)
        if (allocated (pdg)) deallocate (pdg)
        allocate (pdg (n_elements))
        do i = 1, n_elements
            pdg(i) = a(i)
        end do
    end associate
end subroutine pdg_list_create_pdg_array

```



```

        end do
    end associate
end subroutine pdg_list_create_pdg_array

```

<PDG arrays: pdg list: TBP>+≡

```

    procedure :: create_antiparticles => pdg_list_create_antiparticles

```

<PDG arrays: procedures>+≡

```

subroutine pdg_list_create_antiparticles (pl, pl_anti, n_new_particles)
    class(pdg_list_t), intent(in) :: pl
    type(pdg_list_t), intent(out) :: pl_anti
    integer, intent(out) :: n_new_particles
    type(pdg_list_t) :: pl_inverse
    integer :: i, n
    integer :: n_identical
    logical, dimension(:), allocatable :: collect
    n = pl%get_size (); n_identical = 0
    allocate (collect (n)); collect = .true.
    call pl_inverse%init (n)
    do i = 1, n
        pl_inverse%a(i) = pl%a(i)%invert()
    end do
    do i = 1, n
        if (any (pl_inverse%a(i) == pl%a)) then
            collect(i) = .false.
            n_identical = n_identical + 1
        end if
    end do
    n_new_particles = n - n_identical
    if (n_new_particles > 0) then
        call pl_anti%init (n_new_particles)
        do i = 1, n
            if (collect (i)) pl_anti%a(i) = pl_inverse%a(i)
        end do
    end if
end subroutine pdg_list_create_antiparticles

```

<PDG arrays: pdg list: TBP>+≡

```

    procedure :: search_for_particle => pdg_list_search_for_particle

```

<PDG arrays: procedures>+≡

```

elemental function pdg_list_search_for_particle (pl, i_part) result (found)
    logical :: found
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: i_part
    integer :: i_pl
    do i_pl = 1, size (pl%a)
        found = pl%a(i_pl)%search_for_particle (i_part)
        if (found) return
    end do
end function pdg_list_search_for_particle

```

<PDG arrays: pdg list: TBP>+≡

```

    procedure :: contains_colored_particles => pdg_list_contains_colored_particles

```

```

<PDG arrays: procedures>+=
  function pdg_list_contains_colored_particles (pl) result (colored)
    class(pdg_list_t), intent(in) :: pl
    logical :: colored
    integer :: i
    colored = .false.
    do i = 1, size (pl%a)
      if (pl%a(i)%has_colored_particles()) then
        colored = .true.
        exit
      end if
    end do
  end function pdg_list_contains_colored_particles

```

13.2.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<pdg_arrays_ut.f90>≡
  <File header>

  module pdg_arrays_ut
    use unit_tests
    use pdg_arrays_uti

    <Standard module head>

    <PDG arrays: public test>

    contains

    <PDG arrays: test driver>

    end module pdg_arrays_ut
  <pdg_arrays_uti.f90>≡
    <File header>

    module pdg_arrays_uti

      use pdg_arrays

      <Standard module head>

      <PDG arrays: test declarations>

      contains

      <PDG arrays: tests>

      end module pdg_arrays_uti
  API: driver for the unit tests below.
  <PDG arrays: public test>≡
    public :: pdg_arrays_test

```

```

(PDG arrays: test driver)≡
  subroutine pdg_arrays_test (u, results)
    integer, intent(in) :: u
    type (test_results_t), intent(inout) :: results
    (PDG arrays: execute tests)
  end subroutine pdg_arrays_test

```

Basic functionality.

```

(PDG arrays: execute tests)≡
  call test (pdg_arrays_1, "pdg_arrays_1", &
    "create and sort PDG array", &
    u, results)

(PDG arrays: test declarations)≡
  public :: pdg_arrays_1

(PDG arrays: tests)≡
  subroutine pdg_arrays_1 (u)
    integer, intent(in) :: u

    type(pdg_array_t) :: pa, pa1, pa2, pa3, pa4, pa5, pa6
    integer, dimension(:), allocatable :: pdg

    write (u, "(A)")  "* Test output: pdg_arrays_1"
    write (u, "(A)")  "* Purpose: create and sort PDG arrays"
    write (u, "(A)")

    write (u, "(A)")  "* Assignment"
    write (u, "(A)")

    call pa%write (u)
    write (u, *)
    write (u, "(A,I0)") "length = ", pa%get_length ()
    pdg = pa
    write (u, "(A,3(1x,I0))") "contents = ", pdg

    write (u, *)
    pa = 1
    call pa%write (u)
    write (u, *)
    write (u, "(A,I0)") "length = ", pa%get_length ()
    pdg = pa
    write (u, "(A,3(1x,I0))") "contents = ", pdg

    write (u, *)
    pa = [1, 2, 3]
    call pa%write (u)
    write (u, *)
    write (u, "(A,I0)") "length = ", pa%get_length ()
    pdg = pa
    write (u, "(A,3(1x,I0))") "contents = ", pdg
    write (u, "(A,I0)") "element #2 = ", pa%get (2)

    write (u, *)
    write (u, "(A)")  "* Replace"

```

```

write (u, *)

pa = pa%replace (2, [-5, 5, -7])
call pa%write (u)
write (u, *)

write (u, *)
write (u, "(A)")  "* Sort"
write (u, *)

pa = [1, -7, 3, -5, 5, 3]
call pa%write (u)
write (u, *)
pa1 = pa%sort_abs ()
pa2 = pa%sort_abs (unique = .true.)
call pa1%write (u)
write (u, *)
call pa2%write (u)
write (u, *)

write (u, *)
write (u, "(A)")  "* Compare"
write (u, *)

pa1 = [1, 3]
pa2 = [1, 2, -2]
pa3 = [1, 2, 4]
pa4 = [1, 2, 4]
pa5 = [1, 2, -4]
pa6 = [1, 2, -3]

write (u, "(A,6(1x,L1))") "< ", &
    pa1 < pa2, pa2 < pa3, pa3 < pa4, pa4 < pa5, pa5 < pa6, pa6 < pa1
write (u, "(A,6(1x,L1))") "> ", &
    pa1 > pa2, pa2 > pa3, pa3 > pa4, pa4 > pa5, pa5 > pa6, pa6 > pa1
write (u, "(A,6(1x,L1))") "<=", &
    pa1 <= pa2, pa2 <= pa3, pa3 <= pa4, pa4 <= pa5, pa5 <= pa6, pa6 <= pa1
write (u, "(A,6(1x,L1))") ">=", &
    pa1 >= pa2, pa2 >= pa3, pa3 >= pa4, pa4 >= pa5, pa5 >= pa6, pa6 >= pa1
write (u, "(A,6(1x,L1))") "==", &
    pa1 == pa2, pa2 == pa3, pa3 == pa4, pa4 == pa5, pa5 == pa6, pa6 == pa1
write (u, "(A,6(1x,L1))") "/=", &
    pa1 /= pa2, pa2 /= pa3, pa3 /= pa4, pa4 /= pa5, pa5 /= pa6, pa6 /= pa1

write (u, *)
pa1 = [0]
pa2 = [1, 2]
pa3 = [1, -2]

write (u, "(A,6(1x,L1))") ".eqv ", &
    pa1 .eqv. pa1, pa1 .eqv. pa2, &
    pa2 .eqv. pa2, pa2 .eqv. pa3

write (u, "(A,6(1x,L1))") ".neqv", &

```

```

        pa1 .neqv. pa1, pa1 .neqv. pa2, &
        pa2 .neqv. pa2, pa2 .neqv. pa3

write (u, *)
write (u, "(A,6(1x,L1))") "match", &
        pa1 .match. 0, pa1 .match. 1, &
        pa2 .match. 0, pa2 .match. 1, pa2 .match. 3

write (u, "(A)")
write (u, "(A)")  "* Test output end: pdg_arrays_1"

end subroutine pdg_arrays_1

```

PDG array list, i.e., arrays of arrays.

```

<PDG arrays: execute tests>+≡
    call test (pdg_arrays_2, "pdg_arrays_2", &
        "create and sort PDG lists", &
        u, results)

<PDG arrays: test declarations>+≡
    public :: pdg_arrays_2

<PDG arrays: tests>+≡
    subroutine pdg_arrays_2 (u)
        integer, intent(in) :: u

        type(pdg_array_t) :: pa
        type(pdg_list_t) :: pl, pl1

        write (u, "(A)")  "* Test output: pdg_arrays_2"
        write (u, "(A)")  "* Purpose: create and sort PDG lists"
        write (u, "(A)")

        write (u, "(A)")  "* Assignment"
        write (u, "(A)")

        call pl%init (3)
        call pl%set (1, 42)
        call pl%set (2, [3, 2])
        pa = [5, -5]
        call pl%set (3, pa)
        call pl%write (u)
        write (u, *)
        write (u, "(A,I0)") "size = ", pl%get_size ()

        write (u, "(A)")
        write (u, "(A)")  "* Sort"
        write (u, "(A)")

        pl = pl%sort_abs ()
        call pl%write (u)
        write (u, *)

        write (u, "(A)")

```

```

write (u, "(A)")  "* Extract item #3"
write (u, "(A)")

pa = pl%get (3)
call pa%write (u)
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Replace item #3"
write (u, "(A)")

call pl1%init (2)
call pl1%set (1, [2, 4])
call pl1%set (2, -7)

pl = pl%replace (3, pl1)
call pl%write (u)
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Test output end: pdg_arrays_2"

end subroutine pdg_arrays_2

```

Check if a (sorted) PDG array lists is regular. The entries (PDG arrays) must not overlap, unless they are identical.

```

<PDG arrays: execute tests>+=
  call test (pdg_arrays_3, "pdg_arrays_3", &
    "check PDG lists", &
    u, results)

<PDG arrays: test declarations>+=
  public :: pdg_arrays_3

<PDG arrays: tests>+=
  subroutine pdg_arrays_3 (u)
    integer, intent(in) :: u

    type(pdg_list_t) :: pl

    write (u, "(A)")  "* Test output: pdg_arrays_3"
    write (u, "(A)")  "* Purpose: check for regular PDG lists"
    write (u, "(A)")

    write (u, "(A)")  "* Regular list"
    write (u, "(A)")

    call pl%init (4)
    call pl%set (1, [1, 2])
    call pl%set (2, [1, 2])
    call pl%set (3, [5, -5])
    call pl%set (4, 42)
    call pl%write (u)
    write (u, *)
    write (u, "(L1)") pl%is_regular ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Irregular list"
write (u, "(A)")

call pl%init (4)
call pl%set (1, [1, 2])
call pl%set (2, [1, 2])
call pl%set (3, [2, 5, -5])
call pl%set (4, 42)
call pl%write (u)
write (u, *)
write (u, "(L1)") pl%is_regular ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: pdg_arrays_3"

end subroutine pdg_arrays_3

```

Compare PDG array lists. The lists must be regular, i.e., sorted and with non-overlapping (or identical) entries.

```

<PDG arrays: execute tests>+≡
call test (pdg_arrays_4, "pdg_arrays_4", &
  "compare PDG lists", &
  u, results)

<PDG arrays: test declarations>+≡
public :: pdg_arrays_4

<PDG arrays: tests>+≡
subroutine pdg_arrays_4 (u)
  integer, intent(in) :: u

  type(pdg_list_t) :: pl1, pl2, pl3

  write (u, "(A)")  "* Test output: pdg_arrays_4"
  write (u, "(A)")  "* Purpose: check for regular PDG lists"
  write (u, "(A)")

  write (u, "(A)")  "* Create lists"
  write (u, "(A)")

  call pl1%init (4)
  call pl1%set (1, [1, 2])
  call pl1%set (2, [1, 2])
  call pl1%set (3, [5, -5])
  call pl1%set (4, 42)
  write (u, "(I1,1x)", advance = "no") 1
  call pl1%write (u)
  write (u, *)

  call pl2%init (2)
  call pl2%set (1, 3)
  call pl2%set (2, [5, -5])
  write (u, "(I1,1x)", advance = "no") 2

```

```

call pl2%write (u)
write (u, *)

call pl3%init (2)
call pl3%set (1, 4)
call pl3%set (2, [5, -5])
write (u, "(I1,1x)", advance = "no") 3
call pl3%write (u)
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* a == b"
write (u, "(A)")

write (u, "(2x,A)") "123"
write (u, *)
write (u, "(I1,1x,4L1)") 1, pl1 == pl1, pl1 == pl2, pl1 == pl3
write (u, "(I1,1x,4L1)") 2, pl2 == pl1, pl2 == pl2, pl2 == pl3
write (u, "(I1,1x,4L1)") 3, pl3 == pl1, pl3 == pl2, pl3 == pl3

write (u, "(A)")
write (u, "(A)")  "* a < b"
write (u, "(A)")

write (u, "(2x,A)") "123"
write (u, *)
write (u, "(I1,1x,4L1)") 1, pl1 < pl1, pl1 < pl2, pl1 < pl3
write (u, "(I1,1x,4L1)") 2, pl2 < pl1, pl2 < pl2, pl2 < pl3
write (u, "(I1,1x,4L1)") 3, pl3 < pl1, pl3 < pl2, pl3 < pl3

write (u, "(A)")
write (u, "(A)")  "* Test output end: pdg_arrays_4"

end subroutine pdg_arrays_4

```

Match-replace: translate all entries in the first list into the matching entries of the second list, if there is a match.

```

<PDG arrays: execute tests>+≡
call test (pdg_arrays_5, "pdg_arrays_5", &
  "match PDG lists", &
  u, results)

<PDG arrays: test declarations>+≡
public :: pdg_arrays_5

<PDG arrays: tests>+≡
subroutine pdg_arrays_5 (u)
  integer, intent(in) :: u

  type(pdg_list_t) :: pl1, pl2, pl3
  logical :: success

  write (u, "(A)")  "* Test output: pdg_arrays_5"
  write (u, "(A)")  "* Purpose: match-replace"
  write (u, "(A)")

```



```

write (u, "(A)")  "* Create lists"
write (u, "(A)")

call pl1%init (2)
call pl1%set (1, [1, 2])
call pl1%set (2, 42)
call pl1%write (u)
write (u, *)
call pl3%init (2)
call pl3%set (1, [42, -42])
call pl3%set (2, [1, 2, 3, 4])
call pl1%match_replace (pl3, success)
call pl3%write (u)
write (u, "(1x,A,1x,L1,':',1x)", advance="no")  "=>", success
call pl1%write (u)
write (u, *)

write (u, *)

call pl2%init (2)
call pl2%set (1, 9)
call pl2%set (2, 42)
call pl2%write (u)
write (u, *)
call pl2%match_replace (pl3, success)
call pl3%write (u)
write (u, "(1x,A,1x,L1,':',1x)", advance="no")  "=>", success
call pl2%write (u)
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Test output end: pdg_arrays_5"

end subroutine pdg_arrays_5

```

13.3 Jets

The FastJet library is linked externally, if available. The wrapper code is also in a separate directory. Here, we define WHIZARD-specific procedures and tests.

```
<jets.f90>≡  
  <File header>  
  
  module jets  
  
    use fastjet !NODEP!  
  
    <Standard module head>  
  
    <Jets: public>  
  
    contains  
  
    <Jets: procedures>  
  
  end module jets
```

13.3.1 Re-exported symbols

We use this module as a proxy for the FastJet interface, therefore we re-export some symbols.

```
<Jets: public>≡  
  public :: fastjet_available  
  public :: fastjet_init  
  public :: jet_definition_t  
  public :: pseudojet_t  
  public :: pseudojet_vector_t  
  public :: cluster_sequence_t  
  public :: assignment (=)
```

The initialization routine prints the banner.

```
<Jets: procedures>≡  
  subroutine fastjet_init ()  
    call print_banner ()  
  end subroutine fastjet_init
```

The jet algorithm codes (actually, integers)

```
<Jets: public>+≡  
  public :: kt_algorithm  
  public :: cambridge_algorithm  
  public :: antikt_algorithm  
  public :: genkt_algorithm  
  public :: cambridge_for_passive_algorithm  
  public :: genkt_for_passive_algorithm  
  public :: ee_kt_algorithm  
  public :: ee_genkt_algorithm  
  public :: plugin_algorithm  
  public :: undefined_jet_algorithm
```

13.3.2 Unit tests

Test module, followed by the corresponding implementation module.

```
<jets.ut.f90>≡  
  <File header>
```

```
  module jets_ut  
    use unit_tests  
    use jets_uti
```

```
  <Standard module head>
```

```
  <Jets: public test>
```

```
  contains
```

```
  <Jets: test driver>
```

```
  end module jets_ut
```

```
<jets.uti.f90>≡  
  <File header>
```

```
  module jets_uti
```

```
  <Use kinds>  
    use fastjet !NODEP!
```

```
    use jets
```

```
  <Standard module head>
```

```
  <Jets: test declarations>
```

```
  contains
```

```
  <Jets: tests>
```

```
  end module jets_uti
```

API: driver for the unit tests below.

```
<Jets: public test>≡  
  public :: jets_test
```

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

This test is actually the minimal example from the FastJet manual, translated to Fortran.

Note that FastJet creates pseudojet vectors, which we mirror in the `pseudojet_vector_t`, but immediately assign to pseudojet arrays. Without automatic finalization available in the compilers, we should avoid this in actual code and rather introduce intermediate variables for those objects, which we can finalize explicitly.

```

<Jets: execute tests>≡
  call test (jets_1, "jets_1", &
    "basic FastJet functionality", &
    u, results)

<Jets: test declarations>≡
  public :: jets_1

<Jets: tests>≡
  subroutine jets_1 (u)
    integer, intent(in) :: u

    type(pseudojet_t), dimension(:), allocatable :: prt, jets, constituents
    type(jet_definition_t) :: jet_def
    type(cluster_sequence_t) :: cs

    integer, parameter :: dp = default
    integer :: i, j

    write (u, "(A)")  "* Test output: jets_1"
    write (u, "(A)")  "* Purpose: test basic FastJet functionality"
    write (u, "(A)")

    write (u, "(A)")  "* Print banner"
    call print_banner ()

    write (u, *)
    write (u, "(A)")  "* Prepare input particles"
    allocate (prt (3))
    call prt(1)%init ( 99._dp, 0.1_dp, 0._dp, 100._dp)
    call prt(2)%init (  4._dp,-0.1_dp, 0._dp,   5._dp)
    call prt(3)%init (-99._dp, 0._dp,  0._dp,  99._dp)

    write (u, *)
    write (u, "(A)")  "* Define jet algorithm"
    call jet_def%init (antikt_algorithm, 0.7_dp)

    write (u, *)
    write (u, "(A)")  "* Cluster particles according to jet algorithm"

    write (u, *)
    write (u, "(A,A)") "Clustering with ", jet_def%description ()
    call cs%init (pseudojet_vector (prt), jet_def)

    write (u, *)
    write (u, "(A)")  "* Sort output jets"
    jets = sorted_by_pt (cs%inclusive_jets ())

    write (u, *)

```

```

write (u, "(A)")  "* Print jet observables and constituents"
write (u, *)
write (u, "(4x,3(7x,A3))") "pt", "y", "phi"
do i = 1, size (jets)
  write (u, "(A,1x,I0,A,3(1x,F9.5))") &
    "jet", i, ":", jets(i)%perp (), jets(i)%rap (), jets(i)%phi ()
  constituents = jets(i)%constituents ()
  do j = 1, size (constituents)
    write (u, "(4x,A,1x,I0,A,F9.5)") &
      "constituent", j, "'s pt:", constituents(j)%perp ()
  end do
  do j = 1, size (constituents)
    call constituents(j)%final ()
  end do
end do

write (u, *)
write (u, "(A)")  "* Cleanup"

do i = 1, size (prt)
  call prt(i)%final ()
end do
do i = 1, size (jets)
  call jets(i)%final ()
end do
call jet_def%final ()
call cs%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: jets_1"

end subroutine jets_1

```

13.4 Subevents

The purpose of subevents is to store the relevant part of the physical event (either partonic or hadronic), and to hold particle selections and combinations which are constructed in cut or analysis expressions.

```
<subevents.f90>≡  
  <File header>  
  
  module subevents  
  
    use, intrinsic :: iso_c_binding !NODEP!  
  
    <Use kinds>  
    use io_units  
    use format_defs, only: FMT_14, FMT_19  
    use format_utils, only: pac_fmt  
    use physics_defs  
    use sorting  
    use c_particles  
    use lorentz  
    use pdg_arrays  
    use jets  
  
    <Standard module head>  
  
    <Subevents: public>  
  
    <Subevents: parameters>  
  
    <Subevents: types>  
  
    <Subevents: interfaces>  
  
    contains  
  
    <Subevents: procedures>  
  
  end module subevents
```

13.4.1 Particles

For the purpose of this module, a particle has a type which can indicate a beam, incoming, outgoing, or composite particle, flavor and helicity codes (integer, undefined for composite), four-momentum and invariant mass squared. (Other particles types are used in extended event types, but also defined here.) Furthermore, each particle has an allocatable array of ancestors – particle indices which indicate the building blocks of a composite particle. For an incoming/outgoing particle, the array contains only the index of the particle itself.

For incoming particles, the momentum is inverted before storing it in the particle object.

```
<Subevents: parameters>≡  
  integer, parameter, public :: PRT_UNDEFINED = 0
```

```

integer, parameter, public :: PRT_BEAM = -9
integer, parameter, public :: PRT_INCOMING = 1
integer, parameter, public :: PRT_OUTGOING = 2
integer, parameter, public :: PRT_COMPOSITE = 3
integer, parameter, public :: PRT_VIRTUAL = 4
integer, parameter, public :: PRT_RESONANT = 5
integer, parameter, public :: PRT_BEAM_REMNANT = 9

```

The type

We initialize only the type here and mark as unpolarized. The initializers below do the rest. The logicals `is_b_jet` and `is_c_jet` are true only if `prt_t` comes out of the `subevt_cluster` routine and fulfils the correct flavor content.

```

<Subevents: public>≡
  public :: prt_t

<Subevents: types>≡
  type :: prt_t
    private
    integer :: type = PRT_UNDEFINED
    integer :: pdg
    logical :: polarized = .false.
    logical :: colorized = .false.
    logical :: clustered = .false.
    logical :: is_b_jet = .false.
    logical :: is_c_jet = .false.
    integer :: h
    type(vector4_t) :: p
    real(default) :: p2
    integer, dimension(:), allocatable :: src
    integer, dimension(:), allocatable :: col
    integer, dimension(:), allocatable :: acl
  end type prt_t

```

Initializers. Polarization is set separately. Finalizers are not needed.

```

<Subevents: procedures>≡
  subroutine prt_init_beam (prt, pdg, p, p2, src)
    type(prt_t), intent(out) :: prt
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in) :: src
    prt%type = PRT_BEAM
    call prt_set (prt, pdg, - p, p2, src)
  end subroutine prt_init_beam

  subroutine prt_init_incoming (prt, pdg, p, p2, src)
    type(prt_t), intent(out) :: prt
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in) :: src
  end subroutine prt_init_incoming

```

```

    prt%type = PRT_INCOMING
    call prt_set (prt, pdg, - p, p2, src)
end subroutine prt_init_incoming

subroutine prt_init_outgoing (prt, pdg, p, p2, src)
    type(prt_t), intent(out) :: prt
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in) :: src
    prt%type = PRT_OUTGOING
    call prt_set (prt, pdg, p, p2, src)
end subroutine prt_init_outgoing

subroutine prt_init_composite (prt, p, src)
    type(prt_t), intent(out) :: prt
    type(vector4_t), intent(in) :: p
    integer, dimension(:), intent(in) :: src
    prt%type = PRT_COMPOSITE
    call prt_set (prt, 0, p, p**2, src)
end subroutine prt_init_composite

```

This version is for temporary particle objects, so the `src` array is not set.

```

<Subevents: public>+≡
    public :: prt_init_combine

<Subevents: procedures>+≡
    subroutine prt_init_combine (prt, prt1, prt2)
        type(prt_t), intent(out) :: prt
        type(prt_t), intent(in) :: prt1, prt2
        type(vector4_t) :: p
        integer, dimension(0) :: src
        prt%type = PRT_COMPOSITE
        p = prt1%p + prt2%p
        call prt_set (prt, 0, p, p**2, src)
    end subroutine prt_init_combine

```

Init from a pseudojet object.

```

<Subevents: procedures>+≡
    subroutine prt_init_pseudojet (prt, jet, src, pdg, is_b_jet, is_c_jet)
        type(prt_t), intent(out) :: prt
        type(pseudojet_t), intent(in) :: jet
        integer, dimension(:), intent(in) :: src
        integer, intent(in) :: pdg
        logical, intent(in) :: is_b_jet, is_c_jet
        type(vector4_t) :: p
        prt%type = PRT_COMPOSITE
        p = vector4_moving (jet%e(), &
            vector3_moving ([jet%px(), jet%py(), jet%pz()]))
        call prt_set (prt, pdg, p, p**2, src)
        prt%is_b_jet = is_b_jet
        prt%is_c_jet = is_c_jet
        prt%clustered = .true.
    end subroutine prt_init_pseudojet

```



```
end subroutine prt_init_pseudojet
```

Accessing contents

<Subevents: public>+≡

```
public :: prt_get_pdg
```

<Subevents: procedures>+≡

```
elemental function prt_get_pdg (prt) result (pdg)
  integer :: pdg
  type(prt_t), intent(in) :: prt
  pdg = prt%pdg
end function prt_get_pdg
```

<Subevents: public>+≡

```
public :: prt_get_momentum
```

<Subevents: procedures>+≡

```
elemental function prt_get_momentum (prt) result (p)
  type(vector4_t) :: p
  type(prt_t), intent(in) :: prt
  p = prt%p
end function prt_get_momentum
```

<Subevents: public>+≡

```
public :: prt_get_msq
```

<Subevents: procedures>+≡

```
elemental function prt_get_msq (prt) result (msq)
  real(default) :: msq
  type(prt_t), intent(in) :: prt
  msq = prt%p2
end function prt_get_msq
```

<Subevents: public>+≡

```
public :: prt_is_polarized
```

<Subevents: procedures>+≡

```
elemental function prt_is_polarized (prt) result (flag)
  logical :: flag
  type(prt_t), intent(in) :: prt
  flag = prt%polarized
end function prt_is_polarized
```

<Subevents: public>+≡

```
public :: prt_get_helicity
```

<Subevents: procedures>+≡

```
elemental function prt_get_helicity (prt) result (h)
  integer :: h
  type(prt_t), intent(in) :: prt
  h = prt%h
end function prt_get_helicity
```

```

<Subevents: public>+≡
    public :: prt_is_colorized

<Subevents: procedures>+≡
    elemental function prt_is_colorized (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt%colorized
    end function prt_is_colorized

<Subevents: public>+≡
    public :: prt_is_clustered

<Subevents: procedures>+≡
    elemental function prt_is_clustered (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt%clustered
    end function prt_is_clustered

<Subevents: public>+≡
    public :: prt_is_recombinable

<Subevents: procedures>+≡
    elemental function prt_is_recombinable (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt_is_parton (prt) .or. &
            abs(prt%pdg) == TOP_Q .or. &
            prt_is_lepton (prt) .or. &
            prt_is_photon (prt)
    end function prt_is_recombinable

<Subevents: public>+≡
    public :: prt_is_photon

<Subevents: procedures>+≡
    elemental function prt_is_photon (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt%pdg == PHOTON
    end function prt_is_photon

```

We do not take the top quark into account here.

```

<Subevents: public>+≡
    public :: prt_is_parton

<Subevents: procedures>+≡
    elemental function prt_is_parton (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = abs(prt%pdg) == DOWN_Q .or. &
            abs(prt%pdg) == UP_Q .or. &
            abs(prt%pdg) == STRANGE_Q .or. &
            abs(prt%pdg) == CHARM_Q .or. &

```

```

        abs(prt%pdg) == BOTTOM_Q .or. &
        prt%pdg == GLUON
    end function prt_is_parton

<Subevents: public>+≡
    public :: prt_is_lepton

<Subevents: procedures>+≡
    elemental function prt_is_lepton (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = abs(prt%pdg) == ELECTRON .or. &
               abs(prt%pdg) == MUON      .or. &
               abs(prt%pdg) == TAU
    end function prt_is_lepton

<Subevents: public>+≡
    public :: prt_is_b_jet

<Subevents: procedures>+≡
    elemental function prt_is_b_jet (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt%is_b_jet
    end function prt_is_b_jet

<Subevents: public>+≡
    public :: prt_is_c_jet

<Subevents: procedures>+≡
    elemental function prt_is_c_jet (prt) result (flag)
        logical :: flag
        type(prt_t), intent(in) :: prt
        flag = prt%is_c_jet
    end function prt_is_c_jet

```

The number of open color (anticolor) lines. We inspect the list of color (anticolor) lines and count the entries that do not appear in the list of anticolors (colors). (There is no check against duplicates; we assume that color line indices are unique.)

```

<Subevents: public>+≡
    public :: prt_get_n_col
    public :: prt_get_n_acl

<Subevents: procedures>+≡
    elemental function prt_get_n_col (prt) result (n)
        integer :: n
        type(prt_t), intent(in) :: prt
        integer, dimension(:), allocatable :: col, acl
        integer :: i
        n = 0
        if (prt%colorized) then
            do i = 1, size (prt%col)
                if (all (prt%col(i) /= prt%acl)) n = n + 1
            end do
        end if
    end function prt_get_n_col

```

```

        end do
    end if
end function prt_get_n_col

elemental function prt_get_n_acl (prt) result (n)
    integer :: n
    type(prt_t), intent(in) :: prt
    integer, dimension(:), allocatable :: col, acl
    integer :: i
    n = 0
    if (prt%colorized) then
        do i = 1, size (prt%acl)
            if (all (prt%acl(i) /= prt%col)) n = n + 1
        end do
    end if
end function prt_get_n_acl

```

Return the color and anticolor-flow line indices explicitly.

```

<Subevents: public>+≡
    public :: prt_get_color_indices

<Subevents: procedures>+≡
    subroutine prt_get_color_indices (prt, col, acl)
        type(prt_t), intent(in) :: prt
        integer, dimension(:), allocatable, intent(out) :: col, acl
        if (prt%colorized) then
            col = prt%col
            acl = prt%acl
        else
            col = [integer::]
            acl = [integer::]
        end if
    end subroutine prt_get_color_indices

```

Setting data

Set the PDG, momentum and momentum squared, and ancestors. If allocation-assignment is available, this can be simplified.

```

<Subevents: procedures>+≡
    subroutine prt_set (prt, pdg, p, p2, src)
        type(prt_t), intent(inout) :: prt
        integer, intent(in) :: pdg
        type(vector4_t), intent(in) :: p
        real(default), intent(in) :: p2
        integer, dimension(:), intent(in) :: src
        prt%pdg = pdg
        prt%p = p
        prt%p2 = p2
        if (allocated (prt%src)) then
            if (size (src) /= size (prt%src)) then
                deallocate (prt%src)
                allocate (prt%src (size (src)))
            end if
        else
            allocate (prt%src (size (src)))
        end if
    end subroutine prt_set

```

```

        end if
    else
        allocate (prt%src (size (src)))
    end if
    prt%src = src
end subroutine prt_set

```

Set the particle PDG code separately.

```

<Subevents: procedures>+≡
    elemental subroutine prt_set_pdg (prt, pdg)
        type(prt_t), intent(inout) :: prt
        integer, intent(in) :: pdg
        prt%pdg = pdg
    end subroutine prt_set_pdg

```

Set the momentum separately.

```

<Subevents: procedures>+≡
    elemental subroutine prt_set_p (prt, p)
        type(prt_t), intent(inout) :: prt
        type(vector4_t), intent(in) :: p
        prt%p = p
    end subroutine prt_set_p

```

Set the squared invariant mass separately.

```

<Subevents: procedures>+≡
    elemental subroutine prt_set_p2 (prt, p2)
        type(prt_t), intent(inout) :: prt
        real(default), intent(in) :: p2
        prt%p2 = p2
    end subroutine prt_set_p2

```

Set helicity (optional).

```

<Subevents: procedures>+≡
    subroutine prt_polarize (prt, h)
        type(prt_t), intent(inout) :: prt
        integer, intent(in) :: h
        prt%polarized = .true.
        prt%h = h
    end subroutine prt_polarize

```

Set color-flow indices (optional).

```

<Subevents: procedures>+≡
    subroutine prt_colorize (prt, col, acl)
        type(prt_t), intent(inout) :: prt
        integer, dimension(:), intent(in) :: col, acl
        prt%colorized = .true.
        prt%col = col
        prt%acl = acl
    end subroutine prt_colorize

```

Conversion

Transform a `prt_t` object into a `c_prt_t` object.

```
<Subevents: public>+≡
    public :: c_prt

<Subevents: interfaces>≡
    interface c_prt
        module procedure c_prt_from_prt
    end interface

<Subevents: procedures>+≡
    elemental function c_prt_from_prt (prt) result (c_prt)
        type(c_prt_t) :: c_prt
        type(prt_t), intent(in) :: prt
        c_prt = prt%p
        c_prt%type = prt%type
        c_prt%pdg = prt%pdg
        if (prt%polarized) then
            c_prt%polarized = 1
        else
            c_prt%polarized = 0
        end if
        c_prt%h = prt%h
    end function c_prt_from_prt
```

Output

```
<Subevents: public>+≡
    public :: prt_write

<Subevents: procedures>+≡
    subroutine prt_write (prt, unit, testflag)
        type(prt_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        logical :: pacified
        type(prt_t) :: tmp
        character(len=7) :: fmt
        integer :: u, i
        call pac_fmt (fmt, FMT_19, FMT_14, testflag)
        u = given_output_unit (unit); if (u < 0) return
        pacified = .false.; if (present (testflag)) pacified = testflag
        tmp = prt
        if (pacified) call pacify (tmp)
        write (u, "(1x,A)", advance="no") "prt("
        select case (prt%type)
            case (PRT_UNDEFINED); write (u, "('?'')", advance="no")
            case (PRT_BEAM); write (u, "('b:')", advance="no")
            case (PRT_INCOMING); write (u, "('i:')", advance="no")
            case (PRT_OUTGOING); write (u, "('o:')", advance="no")
            case (PRT_COMPOSITE); write (u, "('c:')", advance="no")
        end select
        select case (prt%type)
```

```

case (PRT_BEAM, PRT_INCOMING, PRT_OUTGOING)
  if (prt%polarized) then
    write (u, "(I0,'/',I0,'|')", advance="no") prt%pdg, prt%h
  else
    write (u, "(I0,'|')", advance="no") prt%pdg
  end if
end select
select case (prt%type)
case (PRT_BEAM, PRT_INCOMING, PRT_OUTGOING, PRT_COMPOSITE)
  if (prt%colorized) then
    write (u, "(*I0,:',',')", advance="no") prt%col
    write (u, "('/',)", advance="no")
    write (u, "(*I0,:',',')", advance="no") prt%acl
    write (u, "('/',)", advance="no")
  end if
end select
select case (prt%type)
case (PRT_BEAM, PRT_INCOMING, PRT_OUTGOING, PRT_COMPOSITE)
  write (u, "(" // FMT_14 // ",',';", " // FMT_14 // ",',';", " // &
    FMT_14 // ",',';", " // FMT_14 // ")", advance="no") tmp%p
  write (u, "('|', " // fmt // ")", advance="no") tmp%p2
end select
if (allocated (prt%src)) then
  write (u, "('|')", advance="no")
  do i = 1, size (prt%src)
    write (u, "(1x,I0)", advance="no") prt%src(i)
  end do
end if
if (prt%is_b_jet) then
  write (u, "('|b jet')", advance="no")
end if
if (prt%is_c_jet) then
  write (u, "('|c jet')", advance="no")
end if
write (u, "(A)" " ")
end subroutine prt_write

```

Tools

Two particles match if their `src` arrays are the same.

```

<Subevents: public>+≡
  public :: operator(.match.)

<Subevents: interfaces>+≡
  interface operator(.match.)
    module procedure prt_match
  end interface

<Subevents: procedures>+≡
  elemental function prt_match (prt1, prt2) result (match)
    logical :: match
    type(prt_t), intent(in) :: prt1, prt2
    if (size (prt1%src) == size (prt2%src)) then

```

```

        match = all (prt1%src == prt2%src)
    else
        match = .false.
    end if
end function prt_match

```

The combine operation makes a pseudoparticle whose momentum is the result of adding (the momenta of) the pair of input particles. We trace the particles from which a particle is built by storing a `src` array. Each particle entry in the `src` list contains a list of indices which indicates its building blocks. The indices refer to an original list of particles. Index lists are sorted, and they contain no element more than once.

We thus require that in a given pseudoparticle, each original particle occurs at most once.

The result is `intent(inout)`, so it will not be initialized when the subroutine is entered.

If the particles carry color, we recall that the combined particle is a composite which is understood as outgoing. If one of the arguments is an incoming particle, is color entries must be reversed.

```

<Subevents: procedures>+≡
subroutine prt_combine (prt, prt_in1, prt_in2, ok)
  type(prt_t), intent(inout) :: prt
  type(prt_t), intent(in) :: prt_in1, prt_in2
  logical :: ok
  integer, dimension(:), allocatable :: src
  integer, dimension(:), allocatable :: col1, ac11, col2, ac12
  call combine_index_lists (src, prt_in1%src, prt_in2%src)
  ok = allocated (src)
  if (ok) then
    call prt_init_composite (prt, prt_in1%p + prt_in2%p, src)
    if (prt_in1%colorized .or. prt_in2%colorized) then
      select case (prt_in1%type)
      case default
        call prt_get_color_indices (prt_in1, col1, ac11)
      case (PRT_BEAM, PRT_INCOMING)
        call prt_get_color_indices (prt_in1, ac11, col1)
      end select
      select case (prt_in2%type)
      case default
        call prt_get_color_indices (prt_in2, col2, ac12)
      case (PRT_BEAM, PRT_INCOMING)
        call prt_get_color_indices (prt_in2, ac12, col2)
      end select
      call prt_colorize (prt, [col1, col2], [ac11, ac12])
    end if
  end if
end subroutine prt_combine

```

This variant does not produce the combined particle, it just checks whether the combination is valid (no common `src` entry).

```

<Subevents: public>+≡
public :: are_disjoint

```



```

<Subevents: procedures>+≡
function are_disjoint (prt_in1, prt_in2) result (flag)
  logical :: flag
  type(prt_t), intent(in) :: prt_in1, prt_in2
  flag = index_lists_are_disjoint (prt_in1%src, prt_in2%src)
end function are_disjoint

```

src Lists with length > 1 are built by a combine operation which merges the lists in a sorted manner. If the result would have a duplicate entry, it is discarded, and the result is unallocated.

```

<Subevents: procedures>+≡
subroutine combine_index_lists (res, src1, src2)
  integer, dimension(:), intent(in) :: src1, src2
  integer, dimension(:), allocatable :: res
  integer :: i1, i2, i
  allocate (res (size (src1) + size (src2)))
  if (size (src1) == 0) then
    res = src2
    return
  else if (size (src2) == 0) then
    res = src1
    return
  end if
  i1 = 1
  i2 = 1
  LOOP: do i = 1, size (res)
    if (src1(i1) < src2(i2)) then
      res(i) = src1(i1); i1 = i1 + 1
      if (i1 > size (src1)) then
        res(i+1:) = src2(i2:)
        exit LOOP
      end if
    else if (src1(i1) > src2(i2)) then
      res(i) = src2(i2); i2 = i2 + 1
      if (i2 > size (src2)) then
        res(i+1:) = src1(i1:)
        exit LOOP
      end if
    else
      deallocate (res)
      exit LOOP
    end if
  end do LOOP
end subroutine combine_index_lists

```

This function is similar, but it does not actually merge the list, it just checks whether they are disjoint (no common src entry).

```

<Subevents: procedures>+≡
function index_lists_are_disjoint (src1, src2) result (flag)
  logical :: flag
  integer, dimension(:), intent(in) :: src1, src2
  integer :: i1, i2, i
  flag = .true.

```

```

i1 = 1
i2 = 1
LOOP: do i = 1, size (src1) + size (src2)
  if (src1(i1) < src2(i2)) then
    i1 = i1 + 1
    if (i1 > size (src1)) then
      exit LOOP
    end if
  else if (src1(i1) > src2(i2)) then
    i2 = i2 + 1
    if (i2 > size (src2)) then
      exit LOOP
    end if
  else
    flag = .false.
    exit LOOP
  end if
end do LOOP
end function index_lists_are_disjoint

```

13.4.2 subevents

Particles are collected in subevents. This type is implemented as a dynamically allocated array, which need not be completely filled. The value `n_active` determines the number of meaningful entries.

Type definition

```

<Subevents: public>+≡
  public :: subevt_t

<Subevents: types>+≡
  type :: subevt_t
  private
    integer :: n_active = 0
    type(prt_t), dimension(:), allocatable :: prt
  contains
    <Subevents: subevt: TBP>
  end type subevt_t

```

Initialize, allocating with size zero (default) or given size. The number of contained particles is set equal to the size.

```

<Subevents: public>+≡
  public :: subevt_init

<Subevents: procedures>+≡
  subroutine subevt_init (subevt, n_active)
    type(subevt_t), intent(out) :: subevt
    integer, intent(in), optional :: n_active
    if (present (n_active)) subevt%n_active = n_active
    allocate (subevt%prt (subevt%n_active))
  end subroutine subevt_init

```

(Re-)allocate the subevent with some given size. If the size is greater than the previous one, do a real reallocation. Otherwise, just reset the recorded size. Contents are untouched, but become invalid.

```

<Subevents: public>+≡
    public :: subevt_reset

<Subevents: procedures>+≡
    subroutine subevt_reset (subevt, n_active)
        type(subevt_t), intent(inout) :: subevt
        integer, intent(in) :: n_active
        subevt%n_active = n_active
        if (subevt%n_active > size (subevt%prt)) then
            deallocate (subevt%prt)
            allocate (subevt%prt (subevt%n_active))
        end if
    end subroutine subevt_reset

```

Output. No prefix for the headline 'subevt', because this will usually be printed appending to a previous line.

```

<Subevents: public>+≡
    public :: subevt_write

<Subevents: subevt: TBP>≡
    procedure :: write => subevt_write

<Subevents: procedures>+≡
    subroutine subevt_write (object, unit, prefix, pacified)
        class(subevt_t), intent(in) :: object
        integer, intent(in), optional :: unit
        character(*), intent(in), optional :: prefix
        logical, intent(in), optional :: pacified
        integer :: u, i
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1x,A)") "subevent:"
        do i = 1, object%n_active
            if (present (prefix)) write (u, "(A)", advance="no") prefix
            write (u, "(1x,I0)", advance="no") i
            call prt_write (object%prt(i), unit = unit, testflag = pacified)
        end do
    end subroutine subevt_write

```

Defined assignment: transfer only meaningful entries. This is a deep copy (as would be default assignment).

```

<Subevents: interfaces>+≡
    interface assignment(=)
        module procedure subevt_assign
    end interface

<Subevents: procedures>+≡
    subroutine subevt_assign (subevt, subevt_in)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: subevt_in
        if (.not. allocated (subevt%prt)) then

```

```

        call subevt_init (subevt, subevt_in%n_active)
    else
        call subevt_reset (subevt, subevt_in%n_active)
    end if
    subevt%prt(:subevt%n_active) = subevt_in%prt(:subevt%n_active)
end subroutine subevt_assign

```

Fill contents

Store incoming/outgoing particles which are completely defined.

<Subevents: public>+≡

```

    public :: subevt_set_beam
    public :: subevt_set_incoming
    public :: subevt_set_outgoing
    public :: subevt_set_composite

```

<Subevents: procedures>+≡

```

subroutine subevt_set_beam (subevt, i, pdg, p, p2, src)
    type(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in), optional :: src
    if (present (src)) then
        call prt_init_beam (subevt%prt(i), pdg, p, p2, src)
    else
        call prt_init_beam (subevt%prt(i), pdg, p, p2, [i])
    end if
end subroutine subevt_set_beam

subroutine subevt_set_incoming (subevt, i, pdg, p, p2, src)
    type(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in), optional :: src
    if (present (src)) then
        call prt_init_incoming (subevt%prt(i), pdg, p, p2, src)
    else
        call prt_init_incoming (subevt%prt(i), pdg, p, p2, [i])
    end if
end subroutine subevt_set_incoming

subroutine subevt_set_outgoing (subevt, i, pdg, p, p2, src)
    type(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    integer, intent(in) :: pdg
    type(vector4_t), intent(in) :: p
    real(default), intent(in) :: p2
    integer, dimension(:), intent(in), optional :: src
    if (present (src)) then

```

```

        call prt_init_outgoing (subevt%prt(i), pdg, p, p2, src)
    else
        call prt_init_outgoing (subevt%prt(i), pdg, p, p2, [i])
    end if
end subroutine subevt_set_outgoing

subroutine subevt_set_composite (subevt, i, p, src)
    type(subevt_t), intent(inout) :: subevt
    integer, intent(in) :: i
    type(vector4_t), intent(in) :: p
    integer, dimension(:), intent(in) :: src
    call prt_init_composite (subevt%prt(i), p, src)
end subroutine subevt_set_composite

```

Separately assign flavors, simultaneously for all incoming/outgoing particles.

```

<Subevents: public>+≡
    public :: subevt_set_pdg_beam
    public :: subevt_set_pdg_incoming
    public :: subevt_set_pdg_outgoing

<Subevents: procedures>+≡
    subroutine subevt_set_pdg_beam (subevt, pdg)
        type(subevt_t), intent(inout) :: subevt
        integer, dimension(:), intent(in) :: pdg
        integer :: i, j
        j = 1
        do i = 1, subevt%n_active
            if (subevt%prt(i)%type == PRT_BEAM) then
                call prt_set_pdg (subevt%prt(i), pdg(j))
                j = j + 1
                if (j > size (pdg)) exit
            end if
        end do
    end subroutine subevt_set_pdg_beam

    subroutine subevt_set_pdg_incoming (subevt, pdg)
        type(subevt_t), intent(inout) :: subevt
        integer, dimension(:), intent(in) :: pdg
        integer :: i, j
        j = 1
        do i = 1, subevt%n_active
            if (subevt%prt(i)%type == PRT_INCOMING) then
                call prt_set_pdg (subevt%prt(i), pdg(j))
                j = j + 1
                if (j > size (pdg)) exit
            end if
        end do
    end subroutine subevt_set_pdg_incoming

    subroutine subevt_set_pdg_outgoing (subevt, pdg)
        type(subevt_t), intent(inout) :: subevt
        integer, dimension(:), intent(in) :: pdg
        integer :: i, j
        j = 1

```

```

do i = 1, subvt%n_active
  if (subvt%prt(i)%type == PRT_OUTGOING) then
    call prt_set_pdg (subvt%prt(i), pdg(j))
    j = j + 1
    if (j > size (pdg)) exit
  end if
end do
end subroutine subvt_set_pdg_outgoing

```

Separately assign momenta, simultaneously for all incoming/outgoing particles.

(Subevents: public)+≡

```

public :: subvt_set_p_beam
public :: subvt_set_p_incoming
public :: subvt_set_p_outgoing

```

(Subevents: procedures)+≡

```

subroutine subvt_set_p_beam (subvt, p)
  type(subvt_t), intent(inout) :: subvt
  type(vector4_t), dimension(:), intent(in) :: p
  integer :: i, j
  j = 1
  do i = 1, subvt%n_active
    if (subvt%prt(i)%type == PRT_BEAM) then
      call prt_set_p (subvt%prt(i), p(j))
      j = j + 1
      if (j > size (p)) exit
    end if
  end do
end subroutine subvt_set_p_beam

subroutine subvt_set_p_incoming (subvt, p)
  type(subvt_t), intent(inout) :: subvt
  type(vector4_t), dimension(:), intent(in) :: p
  integer :: i, j
  j = 1
  do i = 1, subvt%n_active
    if (subvt%prt(i)%type == PRT_INCOMING) then
      call prt_set_p (subvt%prt(i), p(j))
      j = j + 1
      if (j > size (p)) exit
    end if
  end do
end subroutine subvt_set_p_incoming

subroutine subvt_set_p_outgoing (subvt, p)
  type(subvt_t), intent(inout) :: subvt
  type(vector4_t), dimension(:), intent(in) :: p
  integer :: i, j
  j = 1
  do i = 1, subvt%n_active
    if (subvt%prt(i)%type == PRT_OUTGOING) then
      call prt_set_p (subvt%prt(i), p(j))
      j = j + 1
      if (j > size (p)) exit
    end if
  end do
end subroutine subvt_set_p_outgoing

```

```

        end if
    end do
end subroutine subevt_set_p_outgoing

```

Separately assign the squared invariant mass, simultaneously for all incoming/outgoing particles.

<Subevents: public>+≡

```

    public :: subevt_set_p2_beam
    public :: subevt_set_p2_incoming
    public :: subevt_set_p2_outgoing

```

<Subevents: procedures>+≡

```

subroutine subevt_set_p2_beam (subevt, p2)
    type(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
        if (subevt%prt(i)%type == PRT_BEAM) then
            call prt_set_p2 (subevt%prt(i), p2(j))
            j = j + 1
            if (j > size (p2)) exit
        end if
    end do
end subroutine subevt_set_p2_beam

```

```

subroutine subevt_set_p2_incoming (subevt, p2)
    type(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
        if (subevt%prt(i)%type == PRT_INCOMING) then
            call prt_set_p2 (subevt%prt(i), p2(j))
            j = j + 1
            if (j > size (p2)) exit
        end if
    end do
end subroutine subevt_set_p2_incoming

```

```

subroutine subevt_set_p2_outgoing (subevt, p2)
    type(subevt_t), intent(inout) :: subevt
    real(default), dimension(:), intent(in) :: p2
    integer :: i, j
    j = 1
    do i = 1, subevt%n_active
        if (subevt%prt(i)%type == PRT_OUTGOING) then
            call prt_set_p2 (subevt%prt(i), p2(j))
            j = j + 1
            if (j > size (p2)) exit
        end if
    end do
end subroutine subevt_set_p2_outgoing

```

Set polarization for an entry

```
<Subevents: public>+≡  
  public :: subevt_polarize  
  
<Subevents: procedures>+≡  
  subroutine subevt_polarize (subevt, i, h)  
    type(subevt_t), intent(inout) :: subevt  
    integer, intent(in) :: i, h  
    call prt_polarize (subevt%prt(i), h)  
  end subroutine subevt_polarize
```

Set color-flow indices for an entry

```
<Subevents: public>+≡  
  public :: subevt_colorize  
  
<Subevents: procedures>+≡  
  subroutine subevt_colorize (subevt, i, col, acl)  
    type(subevt_t), intent(inout) :: subevt  
    integer, intent(in) :: i, col, acl  
    if (col > 0 .and. acl > 0) then  
      call prt_colorize (subevt%prt(i), [col], [acl])  
    else if (col > 0) then  
      call prt_colorize (subevt%prt(i), [col], [integer ::])  
    else if (acl > 0) then  
      call prt_colorize (subevt%prt(i), [integer ::], [acl])  
    else  
      call prt_colorize (subevt%prt(i), [integer ::], [integer ::])  
    end if  
  end subroutine subevt_colorize
```

Accessing contents

Return true if the subevent has entries.

```
<Subevents: public>+≡  
  public :: subevt_is_nonempty  
  
<Subevents: procedures>+≡  
  function subevt_is_nonempty (subevt) result (flag)  
    logical :: flag  
    type(subevt_t), intent(in) :: subevt  
    flag = subevt%n_active /= 0  
  end function subevt_is_nonempty
```

Return the number of entries

```
<Subevents: public>+≡  
  public :: subevt_get_length  
  
<Subevents: procedures>+≡  
  function subevt_get_length (subevt) result (length)  
    integer :: length  
    type(subevt_t), intent(in) :: subevt  
    length = subevt%n_active  
  end function subevt_get_length
```


Return a specific particle. The index is not checked for validity.

```

<Subevents: public>+≡
    public :: subevt_get_prt

<Subevents: procedures>+≡
    function subevt_get_prt (subevt, i) result (prt)
        type(prt_t) :: prt
        type(subevt_t), intent(in) :: subevt
        integer, intent(in) :: i
        prt = subevt%prt(i)
    end function subevt_get_prt

```

Return the partonic energy squared. We take the particles with flag PRT_INCOMING and compute their total invariant mass.

```

<Subevents: public>+≡
    public :: subevt_get_sqrts_hat

<Subevents: procedures>+≡
    function subevt_get_sqrts_hat (subevt) result (sqrts_hat)
        type(subevt_t), intent(in) :: subevt
        real(default) :: sqrts_hat
        type(vector4_t) :: p
        integer :: i
        do i = 1, subevt%n_active
            if (subevt%prt(i)%type == PRT_INCOMING) then
                p = p + prt_get_momentum (subevt%prt(i))
            end if
        end do
        sqrts_hat = p ** 1
    end function subevt_get_sqrts_hat

```

Return the number of incoming (outgoing) particles, respectively. Beam particles or composites are not counted.

```

<Subevents: public>+≡
    public :: subevt_get_n_in
    public :: subevt_get_n_out

<Subevents: procedures>+≡
    function subevt_get_n_in (subevt) result (n_in)
        type(subevt_t), intent(in) :: subevt
        integer :: n_in
        n_in = count (subevt%prt(:subevt%n_active)%type == PRT_INCOMING)
    end function subevt_get_n_in

    function subevt_get_n_out (subevt) result (n_out)
        type(subevt_t), intent(in) :: subevt
        integer :: n_out
        n_out = count (subevt%prt(:subevt%n_active)%type == PRT_OUTGOING)
    end function subevt_get_n_out

```

```

<Subevents: interfaces>+≡
    interface c_prt
        module procedure c_prt_from_subevt
    end interface

```

```

    module procedure c_prt_array_from_subevt
end interface

```

```

<Subevents: procedures>+≡
function c_prt_from_subevt (subevt, i) result (c_prt)
    type(c_prt_t) :: c_prt
    type(subevt_t), intent(in) :: subevt
    integer, intent(in) :: i
    c_prt = c_prt_from_prt (subevt%prt(i))
end function c_prt_from_subevt

function c_prt_array_from_subevt (subevt) result (c_prt_array)
    type(subevt_t), intent(in) :: subevt
    type(c_prt_t), dimension(subevt%n_active) :: c_prt_array
    c_prt_array = c_prt_from_prt (subevt%prt(1:subevt%n_active))
end function c_prt_array_from_subevt

```

Operations with subevents

The join operation joins two subevents. When appending the elements of the second list, we check for each particle whether it is already in the first list. If yes, it is discarded. The result list should be initialized already.

If a mask is present, it refers to the second subevent. Particles where the mask is not set are discarded.

```

<Subevents: public>+≡
    public :: subevt_join

<Subevents: procedures>+≡
subroutine subevt_join (subevt, pl1, pl2, mask2)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl1, pl2
    logical, dimension(:), intent(in), optional :: mask2
    integer :: n1, n2, i, n
    n1 = pl1%n_active
    n2 = pl2%n_active
    call subevt_reset (subevt, n1 + n2)
    subevt%prt(:n1) = pl1%prt(:n1)
    n = n1
    if (present (mask2)) then
        do i = 1, pl2%n_active
            if (mask2(i)) then
                if (disjoint (i)) then
                    n = n + 1
                    subevt%prt(n) = pl2%prt(i)
                end if
            end if
        end do
    else
        do i = 1, pl2%n_active
            if (disjoint (i)) then
                n = n + 1
                subevt%prt(n) = pl2%prt(i)
            end if
        end do
    end if
end subroutine subevt_join

```

```

        end if
    end do
end if
subevt%n_active = n
contains
function disjoint (i) result (flag)
    integer, intent(in) :: i
    logical :: flag
    integer :: j
    do j = 1, pl1%n_active
        if (.not. are_disjoint (pl1%prt(j), pl2%prt(i))) then
            flag = .false.
            return
        end if
    end do
    flag = .true.
end function disjoint
end subroutine subevt_join

```

The combine operation makes a subevent whose entries are the result of adding (the momenta of) each pair of particles in the input lists. We trace the particles from which a particle is built by storing a **src** array. Each particle entry in the **src** list contains a list of indices which indicates its building blocks. The indices refer to an original list of particles. Index lists are sorted, and they contain no element more than once.

We thus require that in a given pseudoparticle, each original particle occurs at most once.

```

<Subevents: public>+≡
    public :: subevt_combine

<Subevents: procedures>+≡
    subroutine subevt_combine (subevt, pl1, pl2, mask12)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl1, pl2
        logical, dimension(:,,:), intent(in), optional :: mask12
        integer :: n1, n2, i1, i2, n, j
        logical :: ok
        n1 = pl1%n_active
        n2 = pl2%n_active
        call subevt_reset (subevt, n1 * n2)
        n = 1
        do i1 = 1, n1
            do i2 = 1, n2
                if (present (mask12)) then
                    ok = mask12(i1,i2)
                else
                    ok = .true.
                end if
                if (ok) call prt_combine &
                    (subevt%prt(n), pl1%prt(i1), pl2%prt(i2), ok)
                if (ok) then
                    CHECK_DOUBLES: do j = 1, n - 1
                        if (subevt%prt(n) .match. subevt%prt(j)) then

```

```

        ok = .false.; exit CHECK_DOUBLES
    end if
end do CHECK_DOUBLES
if (ok) n = n + 1
end if
end do
end do
subevt%n_active = n - 1
end subroutine subevt_combine

```

The collect operation makes a single-entry subevent which results from combining (the momenta of) all particles in the input list. As above, the result does not contain an original particle more than once; this is checked for each particle when it is collected. Furthermore, each entry has a mask; where the mask is false, the entry is dropped.

(Thus, if the input particles are already composite, there is some chance that the result depends on the order of the input list and is not as expected. This situation should be avoided.)

```

<Subevents: public>+≡
    public :: subevt_collect

<Subevents: procedures>+≡
    subroutine subevt_collect (subevt, pl1, mask1)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl1
        logical, dimension(:), intent(in) :: mask1
        type(prt_t) :: prt
        integer :: i
        logical :: ok
        call subevt_reset (subevt, 1)
        subevt%n_active = 0
        do i = 1, pl1%n_active
            if (mask1(i)) then
                if (subevt%n_active == 0) then
                    subevt%n_active = 1
                    subevt%prt(1) = pl1%prt(i)
                else
                    call prt_combine (prt, subevt%prt(1), pl1%prt(i), ok)
                    if (ok) subevt%prt(1) = prt
                end if
            end if
        end do
    end subroutine subevt_collect

```

The cluster operation is similar to `collect`, but applies a jet algorithm. The result is a subevent consisting of jets and, possibly, unclustered extra particles. As above, the result does not contain an original particle more than once; this is checked for each particle when it is collected. Furthermore, each entry has a mask; where the mask is false, the entry is dropped.

The algorithm: first determine the (pseudo)particles that participate in the clustering. They should not overlap, and the mask entry must be set. We then cluster the particles, using the given jet definition. The result particles

are retrieved from the cluster sequence. We still have to determine the source indices for each jet: for each input particle, we get the jet index. Accumulating the source entries for all particles that are part of a given jet, we derive the jet source entries. Finally, we delete the C structures that have been constructed by FastJet and its interface.

```

<Subevents: public>+≡
    public :: subevt_cluster

<Subevents: procedures>+≡
    subroutine subevt_cluster (subevt, pl1, dcut, mask1, jet_def, &
        keep_jets, exclusive)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl1
        real(default), intent(in) :: dcut
        logical, dimension(:), intent(in) :: mask1
        type(jet_definition_t), intent(in) :: jet_def
        logical, intent(in) :: keep_jets, exclusive
        integer, dimension(:), allocatable :: map, jet_index
        type(pseudojet_t), dimension(:), allocatable :: jet_in, jet_out
        type(pseudojet_vector_t) :: jv_in, jv_out
        type(cluster_sequence_t) :: cs
        integer :: i, n_src, n_active
        call map_prt_index (pl1, mask1, n_src, map)
        n_active = count (map /= 0)
        allocate (jet_in (n_active))
        allocate (jet_index (n_active))
        do i = 1, n_active
            call jet_in(i)%init (prt_get_momentum (pl1%prt(map(i))))
        end do
        call jv_in%init (jet_in)
        call cs%init (jv_in, jet_def)
        if (exclusive) then
            jv_out = cs%exclusive_jets (dcut)
        else
            jv_out = cs%inclusive_jets ()
        end if
        call cs%assign_jet_indices (jv_out, jet_index)
        allocate (jet_out (jv_out%size ()))
        jet_out = jv_out
        call fill_pseudojet (subevt, pl1, jet_out, jet_index, n_src, map)
        do i = 1, size (jet_out)
            call jet_out(i)%final ()
        end do
        call jv_out%final ()
        call cs%final ()
        call jv_in%final ()
        do i = 1, size (jet_in)
            call jet_in(i)%final ()
        end do
contains
    ! Uniquely combine sources and add map those new indices to the old ones
    subroutine map_prt_index (pl1, mask1, n_src, map)
        type(subevt_t), intent(in) :: pl1
        logical, dimension(:), intent(in) :: mask1

```

```

integer, intent(out) :: n_src
integer, dimension(:), allocatable, intent(out) :: map
integer, dimension(:), allocatable :: src, src_tmp
integer :: i
allocate (src(0))
allocate (map (pl1%n_active), source = 0)
n_active = 0
do i = 1, pl1%n_active
  if (.not. mask1(i)) cycle
  call combine_index_lists (src_tmp, src, pl1%prt(i)%src)
  if (.not. allocated (src_tmp)) cycle
  call move_alloc (from=src_tmp, to=src)
  n_active = n_active + 1
  map(n_active) = i
end do
n_src = size (src)
end subroutine map_prt_index
! Retrieve source(s) of a jet and fill corresponding subevent
subroutine fill_pseudojet (subevt, pl1, jet_out, jet_index, n_src, map)
  type(subevt_t), intent(inout) :: subevt
  type(subevt_t), intent(in) :: pl1
  type(pseudojet_t), dimension(:), intent(in) :: jet_out
  integer, dimension(:), intent(in) :: jet_index
  integer, dimension(:), intent(in) :: map
  integer, intent(in) :: n_src
  integer, dimension(n_src) :: src_fill
  integer :: i, jet, k, combined_pdg, pdg, n_quarks, n_src_fill
  logical :: is_b, is_c
  call subevt_reset (subevt, size (jet_out))
  do jet = 1, size (jet_out)
    pdg = 0; src_fill = 0; n_src_fill = 0; combined_pdg = 0; n_quarks = 0
    is_b = .false.; is_c = .false.
    PARTICLE: do i = 1, size (jet_index)
      if (jet_index(i) /= jet) cycle PARTICLE
      associate (prt => pl1%prt(map(i)), n_src_prt => size(pl1%prt(map(i))%src))
        do k = 1, n_src_prt
          src_fill(n_src_fill + k) = prt%src(k)
        end do
        n_src_fill = n_src_fill + n_src_prt
        if (is_quark (prt%pdg)) then
          n_quarks = n_quarks + 1
          if (.not. is_b) then
            if (abs (prt%pdg) == 5) then
              is_b = .true.
              is_c = .false.
            else if (abs (prt%pdg) == 4) then
              is_c = .true.
            end if
          end if
          if (combined_pdg == 0) combined_pdg = prt%pdg
        end if
      end associate
    end do PARTICLE
    if (keep_jets .and. n_quarks == 1) pdg = combined_pdg
  end do
end subroutine fill_pseudojet

```

```

        call prt_init_pseudojet (subevt%prt(jet), jet_out(jet), &
            src_fill(:n_src_fill), pdg, is_b, is_c)
    end do
end subroutine fill_pseudojet
end subroutine subevt_cluster

```

Do recombination. The incoming subevent `pl` is left unchanged if it either does not contain photons at all, or consists just of a single photon and nothing else or the photon does have a larger $R > R_0$ distance to the nearest other particle or does not fulfill the `mask1` condition. Otherwise, the subevent is one entry shorter and contains a single recombined particle whose original flavor is kept depending on the setting `keep_flg`. When this subroutine is called, it is explicitly assumed that there is only one photon. For the moment, we take here the first photon from the subevent to possibly recombine and leave this open for generalization.

```

<Subevents: public>+≡
    public :: subevt_recombine

<Subevents: procedures>+≡
    subroutine subevt_recombine (subevt, pl, mask1, reco_r0, keep_flg)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        type(prt_t), dimension(:), allocatable :: prt_rec
        logical, dimension(:), intent(in) :: mask1
        logical, intent(in) :: keep_flg
        real(default), intent(in) :: reco_r0
        real(default), dimension(:), allocatable :: del_rlj
        integer, dimension(:), allocatable :: i_sortr
        type(prt_t) :: prt_gam, prt_comb
        logical :: recombine, ok
        integer :: i, n, i_gam, n_gam, n_rec, pdg_orig
        n = subevt_get_length (pl)
        n_gam = 0
        FIND_FIRST_PHOTON: do i = 1, n
            if (prt_is_photon (pl%prt (i))) then
                n_gam = n_gam + 1
                prt_gam = pl%prt (i)
                i_gam = i
                exit FIND_FIRST_PHOTON
            end if
        end do FIND_FIRST_PHOTON
        n_rec = n - n_gam
        if (n_gam == 0) then
            subevt = pl
        else
            if (n_rec > 0) then
                allocate (prt_rec (n_rec))
                do i = 1, n_rec
                    if (i == i_gam) cycle
                    if (i < i_gam) then
                        prt_rec(i) = pl%prt(i)
                    else
                        prt_rec(i) = pl%prt(i+n_gam)
                    end if
                end do
            end if
        end if
    end subroutine

```

```

end do
allocate (del_rij (n_rec), i_sortr (n_rec))
del_rij(1:n_rec) = eta_phi_distance(prt_get_momentum (prt_gam), &
    prt_get_momentum (prt_rec(1:n_rec)))
i_sortr = order (del_rij)
recombine = del_rij (i_sortr (1)) <= reco_r0 .and. mask1(i_gam)
if (recombine) then
    call subevt_reset (subevt, pl%n_active-n_gam)
    do i = 1, n_rec
        if (i == i_sortr(1)) then
            pdg_orig = prt_get_pdg (prt_rec(i_sortr (1)))
            call prt_combine (prt_comb, prt_gam, prt_rec(i_sortr (1)), ok)
            if (ok) then
                subevt%prt(i_sortr (1)) = prt_comb
                if (keep_flv) call prt_set_pdg &
                    (subevt%prt(i_sortr (1)), pdg_orig)
            end if
        else
            subevt%prt(i) = prt_rec(i)
        end if
    end do
else
    subevt = pl
end if
else
    subevt = pl
end if
end if
end subroutine subevt_recombine

```

Return a list of all particles for which the mask is true.

```

<Subevents: public>+≡
    public :: subevt_select

<Subevents: procedures>+≡
    subroutine subevt_select (subevt, pl, mask1)
        type(subevt_t), intent(inout) :: subevt
        type(subevt_t), intent(in) :: pl
        logical, dimension(:), intent(in) :: mask1
        integer :: i, n
        call subevt_reset (subevt, pl%n_active)
        n = 0
        do i = 1, pl%n_active
            if (mask1(i)) then
                n = n + 1
                subevt%prt(n) = pl%prt(i)
            end if
        end do
        subevt%n_active = n
    end subroutine subevt_select

```

Return a subevent which consists of the single particle with specified `index`. If `index` is negative, count from the end. If it is out of bounds, return an empty

list.

```
<Subevents: public>+≡
  public :: subevt_extract

<Subevents: procedures>+≡
  subroutine subevt_extract (subevt, pl, index)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl
    integer, intent(in) :: index
    if (index > 0) then
      if (index <= pl%n_active) then
        call subevt_reset (subevt, 1)
        subevt%prt(1) = pl%prt(index)
      else
        call subevt_reset (subevt, 0)
      end if
    else if (index < 0) then
      if (abs (index) <= pl%n_active) then
        call subevt_reset (subevt, 1)
        subevt%prt(1) = pl%prt(pl%n_active + 1 + index)
      else
        call subevt_reset (subevt, 0)
      end if
    else
      call subevt_reset (subevt, 0)
    end if
  end subroutine subevt_extract
```

Return the list of particles sorted according to increasing values of the provided integer or real array. If no array is given, sort by PDG value.

```
<Subevents: public>+≡
  public :: subevt_sort

<Subevents: interfaces>+≡
  interface subevt_sort
    module procedure subevt_sort_pdg
    module procedure subevt_sort_int
    module procedure subevt_sort_real
  end interface

<Subevents: procedures>+≡
  subroutine subevt_sort_pdg (subevt, pl)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl
    integer :: n
    n = subevt%n_active
    call subevt_sort_int (subevt, pl, abs (3 * subevt%prt(:n)%pdg - 1))
  end subroutine subevt_sort_pdg

  subroutine subevt_sort_int (subevt, pl, ival)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl
    integer, dimension(:), intent(in) :: ival
    call subevt_reset (subevt, pl%n_active)
```

```

    subevt%n_active = pl%n_active
    subevt%prt = pl%prt( order (ival) )
end subroutine subevt_sort_int

subroutine subevt_sort_real (subevt, pl, rval)
    type(subevt_t), intent(inout) :: subevt
    type(subevt_t), intent(in) :: pl
    real(default), dimension(:), intent(in) :: rval
    integer :: i
    integer, dimension(size(rval)) :: idx
    call subevt_reset (subevt, pl%n_active)
    subevt%n_active = pl%n_active
    if (allocated (subevt%prt)) deallocate (subevt%prt)
    allocate (subevt%prt (size(pl%prt)))
    idx = order (rval)
    do i = 1, size (idx)
        subevt%prt(i) = pl%prt (idx(i))
    end do
end subroutine subevt_sort_real

```

Return the list of particles which have any of the specified PDG codes (and optionally particle type: beam, incoming, outgoing).

```

<Subevents: public>+≡
    public :: subevt_select_pdg_code

<Subevents: procedures>+≡
    subroutine subevt_select_pdg_code (subevt, aval, subevt_in, prt_type)
        type(subevt_t), intent(inout) :: subevt
        type(pdg_array_t), intent(in) :: aval
        type(subevt_t), intent(in) :: subevt_in
        integer, intent(in), optional :: prt_type
        integer :: n_active, n_match
        logical, dimension(:), allocatable :: mask
        integer :: i, j
        n_active = subevt_in%n_active
        allocate (mask (n_active))
        forall (i = 1:n_active) &
            mask(i) = aval .match. subevt_in%prt(i)%pdg
        if (present (prt_type)) &
            mask = mask .and. subevt_in%prt(:n_active)%type == prt_type
        n_match = count (mask)
        call subevt_reset (subevt, n_match)
        j = 0
        do i = 1, n_active
            if (mask(i)) then
                j = j + 1
                subevt%prt(j) = subevt_in%prt(i)
            end if
        end do
    end subroutine subevt_select_pdg_code

```

13.4.3 Eliminate numerical noise

This is useful for testing purposes: set entries to zero that are smaller in absolute values than a given tolerance parameter.

Note: instead of setting the tolerance in terms of EPSILON (kind-dependent), we fix it to 10^{-16} , which is the typical value for double precision. The reason is that there are situations where intermediate representations (external libraries, files) are limited to double precision, even if the main program uses higher precision.

```
<Subevents: public>+≡
    public :: pacify

<Subevents: interfaces>+≡
    interface pacify
        module procedure pacify_prt
        module procedure pacify_subvt
    end interface pacify

<Subevents: procedures>+≡
    subroutine pacify_prt (prt)
        class(prt_t), intent(inout) :: prt
        real(default) :: e
        e = max (1E-10_default * energy (prt%p), 1E-13_default)
        call pacify (prt%p, e)
        call pacify (prt%p2, 1E3_default * e)
    end subroutine pacify_prt

    subroutine pacify_subvt (subvt)
        class(subvt_t), intent(inout) :: subvt
        integer :: i
        do i = 1, subvt%n_active
            call pacify (subvt%prt(i))
        end do
    end subroutine pacify_subvt
```

13.5 Analysis tools

This module defines structures useful for data analysis. These include observables, histograms, and plots.

Observables are quantities that are calculated and summed up event by event. At the end, one can compute the average and error.

Histograms have their bins in addition to the observable properties. Histograms are usually written out in tables and displayed graphically.

In plots, each record creates its own entry in a table. This can be used for scatter plots if called event by event, or for plotting dependencies on parameters if called once per integration run.

Graphs are container for histograms and plots, which carry their own graphics options.

The type layout is still somewhat obfuscated. This would become much simpler if type extension could be used.

```
<analysis.f90>≡  
  <File header>  
  
  module analysis  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use format_utils, only: quote_underscore, tex_format  
    use system_defs, only: TAB  
    use diagnostics  
    use os_interface  
    use ifiles  
  
    <Standard module head>  
  
    <Analysis: public>  
  
    <Analysis: parameters>  
  
    <Analysis: types>  
  
    <Analysis: interfaces>  
  
    <Analysis: variables>  
  
    contains  
  
    <Analysis: procedures>  
  
  end module analysis
```

13.5.1 Output formats

These formats share a common field width (alignment).

```
<Analysis: parameters>≡  
  character(*), parameter, public :: HISTOGRAM_HEAD_FORMAT = "1x,A15,3x"
```

```

character(*), parameter, public :: HISTOGRAM_INTG_FORMAT = "3x,I9,3x"
character(*), parameter, public :: HISTOGRAM_DATA_FORMAT = "ES19.12"

```

13.5.2 Graph options

These parameters are used for displaying data. They apply to a whole graph, which may contain more than one plot element.

The GAMELAN code chunks are part of both `graph_options` and `drawing_options`. The `drawing_options` copy is used in histograms and plots, also as graph elements. The `graph_options` copy is used for `graph` objects as a whole. Both copies are usually identical.

```

<Analysis: public>≡
    public :: graph_options_t

<Analysis: types>≡
    type :: graph_options_t
        private
        type(string_t) :: id
        type(string_t) :: title
        type(string_t) :: description
        type(string_t) :: x_label
        type(string_t) :: y_label
        integer :: width_mm = 130
        integer :: height_mm = 90
        logical :: x_log = .false.
        logical :: y_log = .false.
        real(default) :: x_min = 0
        real(default) :: x_max = 1
        real(default) :: y_min = 0
        real(default) :: y_max = 1
        logical :: x_min_set = .false.
        logical :: x_max_set = .false.
        logical :: y_min_set = .false.
        logical :: y_max_set = .false.
        type(string_t) :: gmlcode_bg
        type(string_t) :: gmlcode_fg
    end type graph_options_t

```

Initialize the record, all strings are empty. The limits are undefined.

```

<Analysis: public>+≡
    public :: graph_options_init

<Analysis: procedures>≡
    subroutine graph_options_init (graph_options)
        type(graph_options_t), intent(out) :: graph_options
        graph_options%id = ""
        graph_options%title = ""
        graph_options%description = ""
        graph_options%x_label = ""
        graph_options%y_label = ""
        graph_options%gmlcode_bg = ""
        graph_options%gmlcode_fg = ""
    end subroutine graph_options_init

```

```
end subroutine graph_options_init
```

Set individual options.

<Analysis: public>+≡

```
public :: graph_options_set
```

<Analysis: procedures>+≡

```
subroutine graph_options_set (graph_options, id, &
    title, description, x_label, y_label, width_mm, height_mm, &
    x_log, y_log, x_min, x_max, y_min, y_max, &
    gmlcode_bg, gmlcode_fg)
    type(graph_options_t), intent(inout) :: graph_options
    type(string_t), intent(in), optional :: id
    type(string_t), intent(in), optional :: title
    type(string_t), intent(in), optional :: description
    type(string_t), intent(in), optional :: x_label, y_label
    integer, intent(in), optional :: width_mm, height_mm
    logical, intent(in), optional :: x_log, y_log
    real(default), intent(in), optional :: x_min, x_max, y_min, y_max
    type(string_t), intent(in), optional :: gmlcode_bg, gmlcode_fg
    if (present (id)) graph_options%id = id
    if (present (title)) graph_options%title = title
    if (present (description)) graph_options%description = description
    if (present (x_label)) graph_options%x_label = x_label
    if (present (y_label)) graph_options%y_label = y_label
    if (present (width_mm)) graph_options%width_mm = width_mm
    if (present (height_mm)) graph_options%height_mm = height_mm
    if (present (x_log)) graph_options%x_log = x_log
    if (present (y_log)) graph_options%y_log = y_log
    if (present (x_min)) graph_options%x_min = x_min
    if (present (x_max)) graph_options%x_max = x_max
    if (present (y_min)) graph_options%y_min = y_min
    if (present (y_max)) graph_options%y_max = y_max
    if (present (x_min)) graph_options%x_min_set = .true.
    if (present (x_max)) graph_options%x_max_set = .true.
    if (present (y_min)) graph_options%y_min_set = .true.
    if (present (y_max)) graph_options%y_max_set = .true.
    if (present (gmlcode_bg)) graph_options%gmlcode_bg = gmlcode_bg
    if (present (gmlcode_fg)) graph_options%gmlcode_fg = gmlcode_fg
end subroutine graph_options_set
```

Write a simple account of all options.

<Analysis: public>+≡

```
public :: graph_options_write
```

<Analysis: procedures>+≡

```
subroutine graph_options_write (gro, unit)
    type(graph_options_t), intent(in) :: gro
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
1   format (A,1x,'"',A,'"')
2   format (A,1x,L1)
3   format (A,1x,ES19.12)
```

```

4  format (A,1x,I0)
5  format (A,1x,'[undefined]')
   write (u, 1) "title      =", char (gro%title)
   write (u, 1) "description =", char (gro%description)
   write (u, 1) "x_label    =", char (gro%x_label)
   write (u, 1) "y_label    =", char (gro%y_label)
   write (u, 2) "x_log      =", gro%x_log
   write (u, 2) "y_log      =", gro%y_log
   if (gro%x_min_set) then
       write (u, 3) "x_min      =", gro%x_min
   else
       write (u, 5) "x_min      ="
   end if
   if (gro%x_max_set) then
       write (u, 3) "x_max      =", gro%x_max
   else
       write (u, 5) "x_max      ="
   end if
   if (gro%y_min_set) then
       write (u, 3) "y_min      =", gro%y_min
   else
       write (u, 5) "y_min      ="
   end if
   if (gro%y_max_set) then
       write (u, 3) "y_max      =", gro%y_max
   else
       write (u, 5) "y_max      ="
   end if
   write (u, 4) "width_mm   =", gro%width_mm
   write (u, 4) "height_mm  =", gro%height_mm
   write (u, 1) "gmlcode_bg =", char (gro%gmlcode_bg)
   write (u, 1) "gmlcode_fg =", char (gro%gmlcode_fg)
end subroutine graph_options_write

```

Write a L^AT_EX header/footer for the analysis file.

(Analysis: procedures)+≡

```

subroutine graph_options_write_tex_header (gro, unit)
  type(graph_options_t), intent(in) :: gro
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  if (gro%title /= "") then
      write (u, "(A)")
      write (u, "(A)") "\section{" // char (gro%title) // "}"
  else
      write (u, "(A)") "\section{" // char (quote_underscore (gro%id)) // "}"
  end if
  if (gro%description /= "") then
      write (u, "(A)") char (gro%description)
      write (u, *)
      write (u, "(A)") "\vspace*{\baselineskip}"
  end if
  write (u, "(A)") "\vspace*{\baselineskip}"

```

```

write (u, "(A)") "\unitlength 1mm"
write (u, "(A,IO,',',IO,A)") &
"\begin{gmlgraph*}(", &
gro%width_mm, gro%height_mm, &
")[dat]"
end subroutine graph_options_write_tex_header

subroutine graph_options_write_tex_footer (gro, unit)
type(graph_options_t), intent(in) :: gro
integer, intent(in), optional :: unit
integer :: u, width, height
width = gro%width_mm - 10
height = gro%height_mm - 10
u = given_output_unit (unit)
write (u, "(A)") " \begin{gmlleps}""Whizard-Logo.eps"";"
write (u, "(A,IO,A,IO,A)") &
" \base := (", width, "\unitlength,", height, "\unitlength);"
write (u, "(A)") " \height := 9.6*\unitlength;"
write (u, "(A)") " \width := 11.2*\unitlength;"
write (u, "(A)") " \end{gmlleps};"
write (u, "(A)") "\end{gmlgraph*}"
end subroutine graph_options_write_tex_footer

```

Return the analysis object ID.

```

<Analysis: procedures>+≡
function graph_options_get_id (gro) result (id)
type(string_t) :: id
type(graph_options_t), intent(in) :: gro
id = gro%id
end function graph_options_get_id

```

Create an appropriate setup command (linear/log).

```

<Analysis: procedures>+≡
function graph_options_get_gml_setup (gro) result (cmd)
type(string_t) :: cmd
type(graph_options_t), intent(in) :: gro
type(string_t) :: x_str, y_str
if (gro%x_log) then
x_str = "log"
else
x_str = "linear"
end if
if (gro%y_log) then
y_str = "log"
else
y_str = "linear"
end if
cmd = "setup (" // x_str // ", " // y_str // ");"
end function graph_options_get_gml_setup

```

Return the labels in GAMELAN form.

```

<Analysis: procedures>+≡

```



```

function graph_options_get_gml_x_label (gro) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  cmd = 'label.bot (<' // '<' // gro%x_label // '>' // '>', out);'
end function graph_options_get_gml_x_label

function graph_options_get_gml_y_label (gro) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  cmd = 'label.ulft (<' // '<' // gro%y_label // '>' // '>', out);'
end function graph_options_get_gml_y_label

```

Create an appropriate `graphrange` statement for the given graph options. Where the graph options are not set, use the supplied arguments, if any, otherwise set the undefined value.

(*Analysis: procedures*) +=

```

function graph_options_get_gml_graphrange &
  (gro, x_min, x_max, y_min, y_max) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  real(default), intent(in), optional :: x_min, x_max, y_min, y_max
  type(string_t) :: x_min_str, x_max_str, y_min_str, y_max_str
  character(*), parameter :: fmt = "(ES15.8)"
  if (gro%x_min_set) then
    x_min_str = "#" // trim (adjustl (real2string (gro%x_min, fmt)))
  else if (present (x_min)) then
    x_min_str = "#" // trim (adjustl (real2string (x_min, fmt)))
  else
    x_min_str = "???"
  end if
  if (gro%x_max_set) then
    x_max_str = "#" // trim (adjustl (real2string (gro%x_max, fmt)))
  else if (present (x_max)) then
    x_max_str = "#" // trim (adjustl (real2string (x_max, fmt)))
  else
    x_max_str = "???"
  end if
  if (gro%y_min_set) then
    y_min_str = "#" // trim (adjustl (real2string (gro%y_min, fmt)))
  else if (present (y_min)) then
    y_min_str = "#" // trim (adjustl (real2string (y_min, fmt)))
  else
    y_min_str = "???"
  end if
  if (gro%y_max_set) then
    y_max_str = "#" // trim (adjustl (real2string (gro%y_max, fmt)))
  else if (present (y_max)) then
    y_max_str = "#" // trim (adjustl (real2string (y_max, fmt)))
  else
    y_max_str = "???"
  end if
  cmd = "graphrange (" // x_min_str // ", " // y_min_str // " ), " &
    // "(" // x_max_str // ", " // y_max_str // " );"

```

```
end function graph_options_get_gml_graphrange
```

Get extra GAMELAN code to be executed before and after the usual drawing commands.

```
<Analysis: procedures>+≡
function graph_options_get_gml_bg_command (gro) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  cmd = gro%gmlcode_bg
end function graph_options_get_gml_bg_command

function graph_options_get_gml_fg_command (gro) result (cmd)
  type(string_t) :: cmd
  type(graph_options_t), intent(in) :: gro
  cmd = gro%gmlcode_fg
end function graph_options_get_gml_fg_command
```

Append the header for generic data output in ifile format. We print only labels, not graphics parameters.

```
<Analysis: procedures>+≡
subroutine graph_options_get_header (pl, header, comment)
  type(graph_options_t), intent(in) :: pl
  type(ifile_t), intent(inout) :: header
  type(string_t), intent(in), optional :: comment
  type(string_t) :: c
  if (present (comment)) then
    c = comment
  else
    c = ""
  end if
  call ifile_append (header, &
    c // "ID: " // pl%id)
  call ifile_append (header, &
    c // "title: " // pl%title)
  call ifile_append (header, &
    c // "description: " // pl%description)
  call ifile_append (header, &
    c // "x axis label: " // pl%x_label)
  call ifile_append (header, &
    c // "y axis label: " // pl%y_label)
end subroutine graph_options_get_header
```

13.5.3 Drawing options

These options apply to an individual graph element (histogram or plot).

```
<Analysis: public>+≡
public :: drawing_options_t

<Analysis: types>+≡
type :: drawing_options_t
  type(string_t) :: dataset
  logical :: with_hbars = .false.
```

```

        logical :: with_base = .false.
        logical :: piecewise = .false.
        logical :: fill = .false.
        logical :: draw = .false.
        logical :: err = .false.
        logical :: symbols = .false.
        type(string_t) :: fill_options
        type(string_t) :: draw_options
        type(string_t) :: err_options
        type(string_t) :: symbol
        type(string_t) :: gmlcode_bg
        type(string_t) :: gmlcode_fg
    end type drawing_options_t

```

Write a simple account of all options.

<Analysis: public>+≡

```
public :: drawing_options_write
```

<Analysis: procedures>+≡

```

subroutine drawing_options_write (dro, unit)
    type(drawing_options_t), intent(in) :: dro
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
1   format (A,1x,'"',A,'"')
2   format (A,1x,L1)
    write (u, 2) "with_hbars =", dro%with_hbars
    write (u, 2) "with_base  =", dro%with_base
    write (u, 2) "piecewise  =", dro%piecewise
    write (u, 2) "fill       =", dro%fill
    write (u, 2) "draw       =", dro%draw
    write (u, 2) "err        =", dro%err
    write (u, 2) "symbols    =", dro%symbols
    write (u, 1) "fill_options=", char (dro%fill_options)
    write (u, 1) "draw_options=", char (dro%draw_options)
    write (u, 1) "err_options =", char (dro%err_options)
    write (u, 1) "symbol     =", char (dro%symbol)
    write (u, 1) "gmlcode_bg  =", char (dro%gmlcode_bg)
    write (u, 1) "gmlcode_fg  =", char (dro%gmlcode_fg)
end subroutine drawing_options_write

```

Init with empty strings and default options, appropriate for either histogram or plot.

<Analysis: public>+≡

```
public :: drawing_options_init_histogram
public :: drawing_options_init_plot
```

<Analysis: procedures>+≡

```

subroutine drawing_options_init_histogram (dro)
    type(drawing_options_t), intent(out) :: dro
    dro%dataset = "dat"
    dro%with_hbars = .true.
    dro%with_base = .true.
    dro%piecewise = .true.

```

```

    dro%fill = .true.
    dro%draw = .true.
    dro%fill_options = "withcolor col.default"
    dro%draw_options = ""
    dro%err_options = ""
    dro%symbol = "fshape(circle scaled 1mm())"
    dro%gmlcode_bg = ""
    dro%gmlcode_fg = ""
end subroutine drawing_options_init_histogram

```

```

subroutine drawing_options_init_plot (dro)
  type(drawing_options_t), intent(out) :: dro
  dro%dataset = "dat"
  dro%draw = .true.
  dro%fill_options = "withcolor col.default"
  dro%draw_options = ""
  dro%err_options = ""
  dro%symbol = "fshape(circle scaled 1mm())"
  dro%gmlcode_bg = ""
  dro%gmlcode_fg = ""
end subroutine drawing_options_init_plot

```

Set individual options.

<Analysis: public>+≡

```

  public :: drawing_options_set

```

<Analysis: procedures>+≡

```

subroutine drawing_options_set (dro, dataset, &
  with_hbars, with_base, piecewise, fill, draw, err, symbols, &
  fill_options, draw_options, err_options, symbol, &
  gmlcode_bg, gmlcode_fg)
  type(drawing_options_t), intent(inout) :: dro
  type(string_t), intent(in), optional :: dataset
  logical, intent(in), optional :: with_hbars, with_base, piecewise
  logical, intent(in), optional :: fill, draw, err, symbols
  type(string_t), intent(in), optional :: fill_options, draw_options
  type(string_t), intent(in), optional :: err_options, symbol
  type(string_t), intent(in), optional :: gmlcode_bg, gmlcode_fg
  if (present (dataset)) dro%dataset = dataset
  if (present (with_hbars)) dro%with_hbars = with_hbars
  if (present (with_base)) dro%with_base = with_base
  if (present (piecewise)) dro%piecewise = piecewise
  if (present (fill)) dro%fill = fill
  if (present (draw)) dro%draw = draw
  if (present (err)) dro%err = err
  if (present (symbols)) dro%symbols = symbols
  if (present (fill_options)) dro%fill_options = fill_options
  if (present (draw_options)) dro%draw_options = draw_options
  if (present (err_options)) dro%err_options = err_options
  if (present (symbol)) dro%symbol = symbol
  if (present (gmlcode_bg)) dro%gmlcode_bg = gmlcode_bg
  if (present (gmlcode_fg)) dro%gmlcode_fg = gmlcode_fg
end subroutine drawing_options_set

```

There are separate commands for drawing the curve and for drawing errors. The symbols are applied to the latter. First of all, we may have to compute a baseline:

```

<Analysis: procedures>+≡
function drawing_options_get_calc_command (dro) result (cmd)
  type(string_t) :: cmd
  type(drawing_options_t), intent(in) :: dro
  if (dro%with_base) then
    cmd = "calculate " // dro%dataset // ".base (" // dro%dataset // ") " &
      // "(x, #0);"
  else
    cmd = ""
  end if
end function drawing_options_get_calc_command

```

Return the drawing command.

```

<Analysis: procedures>+≡
function drawing_options_get_draw_command (dro) result (cmd)
  type(string_t) :: cmd
  type(drawing_options_t), intent(in) :: dro
  if (dro%fill) then
    cmd = "fill"
  else if (dro%draw) then
    cmd = "draw"
  else
    cmd = ""
  end if
  if (dro%fill .or. dro%draw) then
    if (dro%piecewise) cmd = cmd // " piecewise"
    if (dro%draw .and. dro%with_base) cmd = cmd // " cyclic"
    cmd = cmd // " from (" // dro%dataset
    if (dro%with_base) then
      if (dro%piecewise) then
        cmd = cmd // ", " // dro%dataset // ".base\" ! "
      else
        cmd = cmd // " ~ " // dro%dataset // ".base\" ! "
      end if
    end if
    cmd = cmd // ")"
    if (dro%fill) then
      cmd = cmd // " " // dro%fill_options
      if (dro%draw) cmd = cmd // " outlined"
    end if
    if (dro%draw) cmd = cmd // " " // dro%draw_options
    cmd = cmd // ";"
  end if
end function drawing_options_get_draw_command

```

The error command draws error bars, if any.

```

<Analysis: procedures>+≡
function drawing_options_get_err_command (dro) result (cmd)
  type(string_t) :: cmd
  type(drawing_options_t), intent(in) :: dro

```

```

if (dro%err) then
  cmd = "draw piecewise " &
    // "from (" // dro%dataset // ".err)" &
    // " " // dro%err_options // ";"
else
  cmd = ""
end if
end function drawing_options_get_err_command

```

The symbol command draws symbols, if any.

```

<Analysis: procedures>+≡
function drawing_options_get_symb_command (dro) result (cmd)
  type(string_t) :: cmd
  type(drawing_options_t), intent(in) :: dro
  if (dro%symbols) then
    cmd = "phantom" &
      // " from (" // dro%dataset // ")" &
      // " withsymbol (" // dro%symbol // ");"
  else
    cmd = ""
  end if
end function drawing_options_get_symb_command

```

Get extra GAMELAN code to be executed before and after the usual drawing commands.

```

<Analysis: procedures>+≡
function drawing_options_get_gml_bg_command (dro) result (cmd)
  type(string_t) :: cmd
  type(drawing_options_t), intent(in) :: dro
  cmd = dro%gmlcode_bg
end function drawing_options_get_gml_bg_command

function drawing_options_get_gml_fg_command (dro) result (cmd)
  type(string_t) :: cmd
  type(drawing_options_t), intent(in) :: dro
  cmd = dro%gmlcode_fg
end function drawing_options_get_gml_fg_command

```

13.5.4 Observables

The observable type holds the accumulated observable values and weight sums which are necessary for proper averaging.

```

<Analysis: types>+≡
type :: observable_t
  private
  real(default) :: sum_values = 0
  real(default) :: sum_squared_values = 0
  real(default) :: sum_weights = 0
  real(default) :: sum_squared_weights = 0
  integer :: count = 0
  type(string_t) :: obs_label

```

```

        type(string_t) :: obs_unit
        type(graph_options_t) :: graph_options
    end type observable_t

```

Initialize with defined properties

<Analysis: procedures>+≡

```

subroutine observable_init (obs, obs_label, obs_unit, graph_options)
    type(observable_t), intent(out) :: obs
    type(string_t), intent(in), optional :: obs_label, obs_unit
    type(graph_options_t), intent(in), optional :: graph_options
    if (present (obs_label)) then
        obs%obs_label = obs_label
    else
        obs%obs_label = ""
    end if
    if (present (obs_unit)) then
        obs%obs_unit = obs_unit
    else
        obs%obs_unit = ""
    end if
    if (present (graph_options)) then
        obs%graph_options = graph_options
    else
        call graph_options_init (obs%graph_options)
    end if
end subroutine observable_init

```

Reset all numeric entries.

<Analysis: procedures>+≡

```

subroutine observable_clear (obs)
    type(observable_t), intent(inout) :: obs
    obs%sum_values = 0
    obs%sum_squared_values = 0
    obs%sum_weights = 0
    obs%sum_squared_weights = 0
    obs%count = 0
end subroutine observable_clear

```

Record a value. Always successful for observables.

<Analysis: interfaces>≡

```

interface observable_record_value
    module procedure observable_record_value_unweighted
    module procedure observable_record_value_weighted
end interface

```

<Analysis: procedures>+≡

```

subroutine observable_record_value_unweighted (obs, value, success)
    type(observable_t), intent(inout) :: obs
    real(default), intent(in) :: value
    logical, intent(out), optional :: success
    obs%sum_values = obs%sum_values + value
    obs%sum_squared_values = obs%sum_squared_values + value**2

```

```

    obs%sum_weights = obs%sum_weights + 1
    obs%sum_squared_weights = obs%sum_squared_weights + 1
    obs%count = obs%count + 1
    if (present (success)) success = .true.
end subroutine observable_record_value_unweighted

subroutine observable_record_value_weighted (obs, value, weight, success)
    type(observable_t), intent(inout) :: obs
    real(default), intent(in) :: value, weight
    logical, intent(out), optional :: success
    obs%sum_values = obs%sum_values + value * weight
    obs%sum_squared_values = obs%sum_squared_values + value**2 * weight
    obs%sum_weights = obs%sum_weights + weight
    obs%sum_squared_weights = obs%sum_squared_weights + weight**2
    obs%count = obs%count + 1
    if (present (success)) success = .true.
end subroutine observable_record_value_weighted

```

Here are the statistics formulas:

1. Unweighted case: Given a sample of n values x_i , the average is

$$\langle x \rangle = \frac{\sum x_i}{n} \quad (13.4)$$

and the error estimate

$$\Delta x = \sqrt{\frac{1}{n-1} \langle \sum (x_i - \langle x \rangle)^2 \rangle} \quad (13.5)$$

$$= \sqrt{\frac{1}{n-1} \left(\frac{\sum x_i^2}{n} - \frac{(\sum x_i)^2}{n^2} \right)} \quad (13.6)$$

2. Weighted case: Instead of weight 1, each event comes with weight w_i .

$$\langle x \rangle = \frac{\sum x_i w_i}{\sum w_i} \quad (13.7)$$

and

$$\Delta x = \sqrt{\frac{1}{n-1} \left(\frac{\sum x_i^2 w_i}{\sum w_i} - \frac{(\sum x_i w_i)^2}{(\sum w_i)^2} \right)} \quad (13.8)$$

For $w_i = 1$, this specializes to the previous formula.

<Analysis: procedures>+≡

```

function observable_get_n_entries (obs) result (n)
    integer :: n
    type(observable_t), intent(in) :: obs
    n = obs%count
end function observable_get_n_entries

function observable_get_average (obs) result (avg)
    real(default) :: avg
    type(observable_t), intent(in) :: obs

```



```

    if (obs%sum_weights /= 0) then
        avg = obs%sum_values / obs%sum_weights
    else
        avg = 0
    end if
end function observable_get_average

function observable_get_error (obs) result (err)
    real(default) :: err
    type(observable_t), intent(in) :: obs
    real(default) :: var, n
    if (obs%sum_weights /= 0) then
        select case (obs%count)
            case (0:1)
                err = 0
            case default
                n = obs%count
                var = obs%sum_squared_values / obs%sum_weights &
                    - (obs%sum_values / obs%sum_weights) ** 2
                err = sqrt (max (var, 0._default) / (n - 1))
        end select
    else
        err = 0
    end if
end function observable_get_error

```

Write label and/or physical unit to a string.

<Analysis: procedures>+≡

```

function observable_get_label (obs, wl, wu) result (string)
    type(string_t) :: string
    type(observable_t), intent(in) :: obs
    logical, intent(in) :: wl, wu
    type(string_t) :: obs_label, obs_unit
    if (wl) then
        if (obs%obs_label /= "") then
            obs_label = obs%obs_label
        else
            obs_label = "\textrm{Observable}"
        end if
    else
        obs_label = ""
    end if
    if (wu) then
        if (obs%obs_unit /= "") then
            if (wl) then
                obs_unit = "\;[" // obs%obs_unit // "]"
            else
                obs_unit = obs%obs_unit
            end if
        else
            obs_unit = ""
        end if
    else

```

```

        obs_unit = ""
    end if
    string = obs_label // obs_unit
end function observable_get_label

```

13.5.5 Output

(Analysis: procedures)+≡

```

subroutine observable_write (obs, unit)
    type(observable_t), intent(in) :: obs
    integer, intent(in), optional :: unit
    real(default) :: avg, err, relerr
    integer :: n
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    avg = observable_get_average (obs)
    err = observable_get_error (obs)
    if (avg /= 0) then
        relerr = err / abs (avg)
    else
        relerr = 0
    end if
    n = observable_get_n_entries (obs)
    if (obs%graph_options%title /= "") then
        write (u, "(A,1x,3A)") &
            "title          =", "'", char (obs%graph_options%title), "'"
    end if
    if (obs%graph_options%description /= "") then
        write (u, "(A,1x,3A)") &
            "description =", "'", char (obs%graph_options%description), "'"
    end if
    write (u, "(A,1x," // HISTOGRAM_DATA_FORMAT // ") ", advance = "no") &
        "average          =", avg
    call write_unit ()
    write (u, "(A,1x," // HISTOGRAM_DATA_FORMAT // ") ", advance = "no") &
        "error[abs]       =", err
    call write_unit ()
    write (u, "(A,1x," // HISTOGRAM_DATA_FORMAT // ")") &
        "error[rel]      =", relerr
    write (u, "(A,1x,I0)") &
        "n_entries        =", n
contains
    subroutine write_unit ()
        if (obs%obs_unit /= "") then
            write (u, "(1x,A)") char (obs%obs_unit)
        else
            write (u, *)
        end if
    end subroutine write_unit
end subroutine observable_write

```

L^AT_EX output.

<Analysis: procedures>+≡

```

subroutine observable_write_driver (obs, unit, write_heading)
  type(observable_t), intent(in) :: obs
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: write_heading
  real(default) :: avg, err
  integer :: n_digits
  logical :: heading
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  heading = .true.; if (present (write_heading)) heading = write_heading
  avg = observable_get_average (obs)
  err = observable_get_error (obs)
  if (avg /= 0 .and. err /= 0) then
    n_digits = max (2, 2 - int (log10 (abs (err / real (avg, default)))))
  else if (avg /= 0) then
    n_digits = 100
  else
    n_digits = 1
  end if
  if (heading) then
    write (u, "(A)")
    if (obs%graph_options%title /= "") then
      write (u, "(A)") "\section{" // char (obs%graph_options%title) &
        // "}"
    else
      write (u, "(A)") "\section{Observable}"
    end if
    if (obs%graph_options%description /= "") then
      write (u, "(A)") char (obs%graph_options%description)
      write (u, *)
    end if
    write (u, "(A)") "\begin{flushleft}"
  end if
  write (u, "(A)", advance="no") " $\langle$ " ! $ sign
  write (u, "(A)", advance="no") char (observable_get_label (obs, wl=.true., wu=.false.))
  write (u, "(A)", advance="no") " \rangle = "
  write (u, "(A)", advance="no") char (tex_format (avg, n_digits))
  write (u, "(A)", advance="no") "\pm"
  write (u, "(A)", advance="no") char (tex_format (err, 2))
  write (u, "(A)", advance="no") "\;{"
  write (u, "(A)", advance="no") char (observable_get_label (obs, wl=.false., wu=.true.))
  write (u, "(A)") "}"
  write (u, "(A)", advance="no") " \quad[n_{\text{entries}}] = "
  write (u, "(IO)", advance="no") observable_get_n_entries (obs)
  write (u, "(A)") "]"$ " ! $ fool Emacs' noweb mode
  if (heading) then
    write (u, "(A)") "\end{flushleft}"
  end if
end subroutine observable_write_driver

```

13.5.6 Histograms

Bins

<Analysis: types>+≡

```
type :: bin_t
  private
    real(default) :: midpoint = 0
    real(default) :: width = 0
    real(default) :: sum_weights = 0
    real(default) :: sum_squared_weights = 0
    real(default) :: sum_excess_weights = 0
    integer :: count = 0
end type bin_t
```

<Analysis: procedures>+≡

```
subroutine bin_init (bin, midpoint, width)
  type(bin_t), intent(out) :: bin
  real(default), intent(in) :: midpoint, width
  bin%midpoint = midpoint
  bin%width = width
end subroutine bin_init
```

<Analysis: procedures>+≡

```
elemental subroutine bin_clear (bin)
  type(bin_t), intent(inout) :: bin
  bin%sum_weights = 0
  bin%sum_squared_weights = 0
  bin%sum_excess_weights = 0
  bin%count = 0
end subroutine bin_clear
```

<Analysis: procedures>+≡

```
subroutine bin_record_value (bin, normalize, weight, excess)
  type(bin_t), intent(inout) :: bin
  logical, intent(in) :: normalize
  real(default), intent(in) :: weight
  real(default), intent(in), optional :: excess
  real(default) :: w, e
  if (normalize) then
    if (bin%width /= 0) then
      w = weight / bin%width
      if (present (excess)) e = excess / bin%width
    else
      w = 0
      if (present (excess)) e = 0
    end if
  else
    w = weight
    if (present (excess)) e = excess
  end if
  bin%sum_weights = bin%sum_weights + w
  bin%sum_squared_weights = bin%sum_squared_weights + w ** 2
  if (present (excess)) &
```

```

        bin%sum_excess_weights = bin%sum_excess_weights + abs (e)
    bin%count = bin%count + 1
end subroutine bin_record_value

```

<Analysis: procedures>+≡

```

function bin_get_midpoint (bin) result (x)
    real(default) :: x
    type(bin_t), intent(in) :: bin
    x = bin%midpoint
end function bin_get_midpoint

function bin_get_width (bin) result (w)
    real(default) :: w
    type(bin_t), intent(in) :: bin
    w = bin%width
end function bin_get_width

function bin_get_n_entries (bin) result (n)
    integer :: n
    type(bin_t), intent(in) :: bin
    n = bin%count
end function bin_get_n_entries

function bin_get_sum (bin) result (s)
    real(default) :: s
    type(bin_t), intent(in) :: bin
    s = bin%sum_weights
end function bin_get_sum

function bin_get_error (bin) result (err)
    real(default) :: err
    type(bin_t), intent(in) :: bin
    err = sqrt (bin%sum_squared_weights)
end function bin_get_error

function bin_get_excess (bin) result (excess)
    real(default) :: excess
    type(bin_t), intent(in) :: bin
    excess = bin%sum_excess_weights
end function bin_get_excess

```

<Analysis: procedures>+≡

```

subroutine bin_write_header (unit)
    integer, intent(in), optional :: unit
    character(120) :: buffer
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (buffer, "(A,4(1x," //HISTOGRAM_HEAD_FORMAT // " ),2x,A)") &
        "#", "bin midpoint", "value", "error", &
        "excess", "n"
    write (u, "(A)") trim (buffer)
end subroutine bin_write_header

```

```

subroutine bin_write (bin, unit)
  type(bin_t), intent(in) :: bin
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,4(1x," // HISTOGRAM_DATA_FORMAT // "),2x,IO)") &
    bin_get_midpoint (bin), &
    bin_get_sum (bin), &
    bin_get_error (bin), &
    bin_get_excess (bin), &
    bin_get_n_entries (bin)
end subroutine bin_write

```

Histograms

(Analysis: types)+≡

```

type :: histogram_t
  private
  real(default) :: lower_bound = 0
  real(default) :: upper_bound = 0
  real(default) :: width = 0
  integer :: n_bins = 0
  logical :: normalize_bins = .false.
  type(observable_t) :: obs
  type(observable_t) :: obs_within_bounds
  type(bin_t) :: underflow
  type(bin_t), dimension(:), allocatable :: bin
  type(bin_t) :: overflow
  type(graph_options_t) :: graph_options
  type(drawing_options_t) :: drawing_options
end type histogram_t

```

Initializer/finalizer

Initialize a histogram. We may provide either the bin width or the number of bins. A finalizer is not needed, since the histogram contains no pointer (sub)components.

(Analysis: interfaces)+≡

```

interface histogram_init
  module procedure histogram_init_n_bins
  module procedure histogram_init_bin_width
end interface

```

(Analysis: procedures)+≡

```

subroutine histogram_init_n_bins (h, id, &
  lower_bound, upper_bound, n_bins, normalize_bins, &
  obs_label, obs_unit, graph_options, drawing_options)
  type(histogram_t), intent(out) :: h
  type(string_t), intent(in) :: id
  real(default), intent(in) :: lower_bound, upper_bound

```

```

integer, intent(in) :: n_bins
logical, intent(in) :: normalize_bins
type(string_t), intent(in), optional :: obs_label, obs_unit
type(graph_options_t), intent(in), optional :: graph_options
type(drawing_options_t), intent(in), optional :: drawing_options
real(default) :: bin_width
integer :: i
call observable_init (h%obs_within_bounds, obs_label, obs_unit)
call observable_init (h%obs, obs_label, obs_unit)
h%lower_bound = lower_bound
h%upper_bound = upper_bound
h%n_bins = max (n_bins, 1)
h%width = h%upper_bound - h%lower_bound
h%normalize_bins = normalize_bins
bin_width = h%width / h%n_bins
allocate (h%bin (h%n_bins))
call bin_init (h%underflow, h%lower_bound, 0._default)
do i = 1, h%n_bins
    call bin_init (h%bin(i), &
        h%lower_bound - bin_width/2 + i * bin_width, bin_width)
end do
call bin_init (h%overflow, h%upper_bound, 0._default)
if (present (graph_options)) then
    h%graph_options = graph_options
else
    call graph_options_init (h%graph_options)
end if
call graph_options_set (h%graph_options, id = id)
if (present (drawing_options)) then
    h%drawing_options = drawing_options
else
    call drawing_options_init_histogram (h%drawing_options)
end if
end subroutine histogram_init_n_bins

subroutine histogram_init_bin_width (h, id, &
    lower_bound, upper_bound, bin_width, normalize_bins, &
    obs_label, obs_unit, graph_options, drawing_options)
type(histogram_t), intent(out) :: h
type(string_t), intent(in) :: id
real(default), intent(in) :: lower_bound, upper_bound, bin_width
logical, intent(in) :: normalize_bins
type(string_t), intent(in), optional :: obs_label, obs_unit
type(graph_options_t), intent(in), optional :: graph_options
type(drawing_options_t), intent(in), optional :: drawing_options
integer :: n_bins
if (bin_width /= 0) then
    n_bins = nint ((upper_bound - lower_bound) / bin_width)
else
    n_bins = 1
end if
call histogram_init_n_bins (h, id, &
    lower_bound, upper_bound, n_bins, normalize_bins, &
    obs_label, obs_unit, graph_options, drawing_options)

```

```
end subroutine histogram_init_bin_width
```

Initialize a histogram by copying another one.

Since `h` has no pointer (sub)components, intrinsic assignment is sufficient. Optionally, we replace the drawing options.

<Analysis: procedures>+≡

```
subroutine histogram_init_histogram (h, h_in, drawing_options)
  type(histogram_t), intent(out) :: h
  type(histogram_t), intent(in)  :: h_in
  type(drawing_options_t), intent(in), optional :: drawing_options
  h = h_in
  if (present (drawing_options)) then
    h%drawing_options = drawing_options
  end if
end subroutine histogram_init_histogram
```

Fill histograms

Clear the histogram contents, but do not modify the structure.

<Analysis: procedures>+≡

```
subroutine histogram_clear (h)
  type(histogram_t), intent(inout) :: h
  call observable_clear (h%obs)
  call observable_clear (h%obs_within_bounds)
  call bin_clear (h%underflow)
  if (allocated (h%bin)) call bin_clear (h%bin)
  call bin_clear (h%overflow)
end subroutine histogram_clear
```

Record a value. Successful if the value is within bounds, otherwise it is recorded as under-/overflow. Optionally, we may provide an excess weight that could be returned by the unweighting procedure.

<Analysis: procedures>+≡

```
subroutine histogram_record_value_unweighted (h, value, excess, success)
  type(histogram_t), intent(inout) :: h
  real(default), intent(in) :: value
  real(default), intent(in), optional :: excess
  logical, intent(out), optional :: success
  integer :: i_bin
  call observable_record_value (h%obs, value)
  if (h%width /= 0) then
    i_bin = floor (((value - h%lower_bound) / h%width) * h%n_bins) + 1
  else
    i_bin = 0
  end if
  if (i_bin <= 0) then
    call bin_record_value (h%underflow, .false., 1._default, excess)
    if (present (success)) success = .false.
  else if (i_bin <= h%n_bins) then
    call observable_record_value (h%obs_within_bounds, value)
    call bin_record_value &
```



```

        (h%bin(i_bin), h%normalize_bins, 1._default, excess)
    if (present (success)) success = .true.
else
    call bin_record_value (h%overflow, .false., 1._default, excess)
    if (present (success)) success = .false.
end if
end subroutine histogram_record_value_unweighted

```

Weighted events: analogous, but no excess weight.

<Analysis: procedures>+≡

```

subroutine histogram_record_value_weighted (h, value, weight, success)
    type(histogram_t), intent(inout) :: h
    real(default), intent(in) :: value, weight
    logical, intent(out), optional :: success
    integer :: i_bin
    call observable_record_value (h%obs, value, weight)
    if (h%width /= 0) then
        i_bin = floor (((value - h%lower_bound) / h%width) * h%n_bins) + 1
    else
        i_bin = 0
    end if
    if (i_bin <= 0) then
        call bin_record_value (h%underflow, .false., weight)
        if (present (success)) success = .false.
    else if (i_bin <= h%n_bins) then
        call observable_record_value (h%obs_within_bounds, value, weight)
        call bin_record_value (h%bin(i_bin), h%normalize_bins, weight)
        if (present (success)) success = .true.
    else
        call bin_record_value (h%overflow, .false., weight)
        if (present (success)) success = .false.
    end if
end subroutine histogram_record_value_weighted

```

Access contents

Inherited from the observable component (all-over average etc.)

<Analysis: procedures>+≡

```

function histogram_get_n_entries (h) result (n)
    integer :: n
    type(histogram_t), intent(in) :: h
    n = observable_get_n_entries (h%obs)
end function histogram_get_n_entries

function histogram_get_average (h) result (avg)
    real(default) :: avg
    type(histogram_t), intent(in) :: h
    avg = observable_get_average (h%obs)
end function histogram_get_average

function histogram_get_error (h) result (err)
    real(default) :: err

```

```

    type(histogram_t), intent(in) :: h
    err = observable_get_error (h%obs)
end function histogram_get_error

```

Analogous, but applied only to events within bounds.

```

<Analysis: procedures>+≡
function histogram_get_n_entries_within_bounds (h) result (n)
    integer :: n
    type(histogram_t), intent(in) :: h
    n = observable_get_n_entries (h%obs_within_bounds)
end function histogram_get_n_entries_within_bounds

function histogram_get_average_within_bounds (h) result (avg)
    real(default) :: avg
    type(histogram_t), intent(in) :: h
    avg = observable_get_average (h%obs_within_bounds)
end function histogram_get_average_within_bounds

function histogram_get_error_within_bounds (h) result (err)
    real(default) :: err
    type(histogram_t), intent(in) :: h
    err = observable_get_error (h%obs_within_bounds)
end function histogram_get_error_within_bounds

```

Get the number of bins

```

<Analysis: procedures>+≡
function histogram_get_n_bins (h) result (n)
    type(histogram_t), intent(in) :: h
    integer :: n
    n = h%n_bins
end function histogram_get_n_bins

```

Check bins. If the index is zero or above the limit, return the results for underflow or overflow, respectively.

```

<Analysis: procedures>+≡
function histogram_get_n_entries_for_bin (h, i) result (n)
    integer :: n
    type(histogram_t), intent(in) :: h
    integer, intent(in) :: i
    if (i <= 0) then
        n = bin_get_n_entries (h%underflow)
    else if (i <= h%n_bins) then
        n = bin_get_n_entries (h%bin(i))
    else
        n = bin_get_n_entries (h%overflow)
    end if
end function histogram_get_n_entries_for_bin

function histogram_get_sum_for_bin (h, i) result (avg)
    real(default) :: avg
    type(histogram_t), intent(in) :: h
    integer, intent(in) :: i

```

```

    if (i <= 0) then
        avg = bin_get_sum (h%underflow)
    else if (i <= h%n_bins) then
        avg = bin_get_sum (h%bin(i))
    else
        avg = bin_get_sum (h%overflow)
    end if
end function histogram_get_sum_for_bin

function histogram_get_error_for_bin (h, i) result (err)
    real(default) :: err
    type(histogram_t), intent(in) :: h
    integer, intent(in) :: i
    if (i <= 0) then
        err = bin_get_error (h%underflow)
    else if (i <= h%n_bins) then
        err = bin_get_error (h%bin(i))
    else
        err = bin_get_error (h%overflow)
    end if
end function histogram_get_error_for_bin

function histogram_get_excess_for_bin (h, i) result (err)
    real(default) :: err
    type(histogram_t), intent(in) :: h
    integer, intent(in) :: i
    if (i <= 0) then
        err = bin_get_excess (h%underflow)
    else if (i <= h%n_bins) then
        err = bin_get_excess (h%bin(i))
    else
        err = bin_get_excess (h%overflow)
    end if
end function histogram_get_excess_for_bin

```

Return a pointer to the graph options.

<Analysis: procedures>+≡

```

function histogram_get_graph_options_ptr (h) result (ptr)
    type(graph_options_t), pointer :: ptr
    type(histogram_t), intent(in), target :: h
    ptr => h%graph_options
end function histogram_get_graph_options_ptr

```

Return a pointer to the drawing options.

<Analysis: procedures>+≡

```

function histogram_get_drawing_options_ptr (h) result (ptr)
    type(drawing_options_t), pointer :: ptr
    type(histogram_t), intent(in), target :: h
    ptr => h%drawing_options
end function histogram_get_drawing_options_ptr

```

Output

(Analysis: procedures)+≡

```
subroutine histogram_write (h, unit)
  type(histogram_t), intent(in) :: h
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  call bin_write_header (u)
  if (allocated (h%bin)) then
    do i = 1, h%n_bins
      call bin_write (h%bin(i), u)
    end do
  end if
  write (u, "(A)")
  write (u, "(A,1x,A)" ) "#", "Underflow:"
  call bin_write (h%underflow, u)
  write (u, "(A)")
  write (u, "(A,1x,A)" ) "#", "Overflow:"
  call bin_write (h%overflow, u)
  write (u, "(A)")
  write (u, "(A,1x,A)" ) "#", "Summary: data within bounds"
  call observable_write (h%obs_within_bounds, u)
  write (u, "(A)")
  write (u, "(A,1x,A)" ) "#", "Summary: all data"
  call observable_write (h%obs, u)
  write (u, "(A)")
end subroutine histogram_write
```

Write the GAMELAN reader for histogram contents.

(Analysis: procedures)+≡

```
subroutine histogram_write_gml_reader (h, filename, unit)
  type(histogram_t), intent(in) :: h
  type(string_t), intent(in) :: filename
  integer, intent(in), optional :: unit
  character(*), parameter :: fmt = "(ES15.8)"
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(2x,A)" ) 'fromfile "' // char (filename) // '":'
  write (u, "(4x,A)" ) 'key "# Histogram:";'
  write (u, "(4x,A)" ) 'dx := #' &
    // real2char (h%width / h%n_bins / 2, fmt) // ';'
  write (u, "(4x,A)" ) 'for i withinblock:'
  write (u, "(6x,A)" ) 'get x, y, y.d, y.n, y.e;'
  if (h%drawing_options%with_hbars) then
    write (u, "(6x,A)" ) 'plot (' // char (h%drawing_options%dataset) &
      // ') (x,y) hbar dx;'
  else
    write (u, "(6x,A)" ) 'plot (' // char (h%drawing_options%dataset) &
      // ') (x,y);'
  end if
  if (h%drawing_options%err) then
    write (u, "(6x,A)" ) 'plot (' // char (h%drawing_options%dataset) &
      // '.err) ' &
```

```

// '(x,y) vbar y.d;'
end if
!!! Future excess options for plots
! write (u, "(6x,A)") 'if show_excess: ' // &
!           & 'plot(dat.e)(x, y plus y.e) hbar dx; fi'
write (u, "(4x,A)") 'endfor'
write (u, "(2x,A)") 'endfrom'
end subroutine histogram_write_gml_reader

```

LaTeX and GAMELAN output.

(Analysis: procedures)+≡

```

subroutine histogram_write_gml_driver (h, filename, unit)
  type(histogram_t), intent(in) :: h
  type(string_t), intent(in) :: filename
  integer, intent(in), optional :: unit
  type(string_t) :: calc_cmd, bg_cmd, draw_cmd, err_cmd, symb_cmd, fg_cmd
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  call graph_options_write_tex_header (h%graph_options, unit)
  write (u, "(2x,A)") char (graph_options_get_gml_setup (h%graph_options))
  write (u, "(2x,A)") char (graph_options_get_gml_graphrange &
    (h%graph_options, x_min=h%lower_bound, x_max=h%upper_bound))
  call histogram_write_gml_reader (h, filename, unit)
  calc_cmd = drawing_options_get_calc_command (h%drawing_options)
  if (calc_cmd /= "") write (u, "(2x,A)") char (calc_cmd)
  bg_cmd = drawing_options_get_gml_bg_command (h%drawing_options)
  if (bg_cmd /= "") write (u, "(2x,A)") char (bg_cmd)
  draw_cmd = drawing_options_get_draw_command (h%drawing_options)
  if (draw_cmd /= "") write (u, "(2x,A)") char (draw_cmd)
  err_cmd = drawing_options_get_err_command (h%drawing_options)
  if (err_cmd /= "") write (u, "(2x,A)") char (err_cmd)
  symb_cmd = drawing_options_get_symb_command (h%drawing_options)
  if (symb_cmd /= "") write (u, "(2x,A)") char (symb_cmd)
  fg_cmd = drawing_options_get_gml_fg_command (h%drawing_options)
  if (fg_cmd /= "") write (u, "(2x,A)") char (fg_cmd)
  write (u, "(2x,A)") char (graph_options_get_gml_x_label (h%graph_options))
  write (u, "(2x,A)") char (graph_options_get_gml_y_label (h%graph_options))
  call graph_options_write_tex_footer (h%graph_options, unit)
  write (u, "(A)") "\vspace*{2\baselineskip}"
  write (u, "(A)") "\begin{flushleft}"
  write (u, "(A)") "\textbf{Data within bounds:} \\"
  call observable_write_driver (h%obs_within_bounds, unit, &
    write_heading=.false.)
  write (u, "(A)") "\\[0.5\baselineskip]"
  write (u, "(A)") "\textbf{All data:} \\"
  call observable_write_driver (h%obs, unit, write_heading=.false.)
  write (u, "(A)") "\end{flushleft}"
end subroutine histogram_write_gml_driver

```

Return the header for generic data output as an ifile.

(Analysis: procedures)+≡

```

subroutine histogram_get_header (h, header, comment)
  type(histogram_t), intent(in) :: h

```

```

type(ifile_t), intent(inout) :: header
type(string_t), intent(in), optional :: comment
type(string_t) :: c
if (present (comment)) then
    c = comment
else
    c = ""
end if
call ifile_append (header, c // "WHIZARD histogram data")
call graph_options_get_header (h%graph_options, header, comment)
call ifile_append (header, &
    c // "range: " // real2string (h%lower_bound) &
    // " - " // real2string (h%upper_bound))
call ifile_append (header, &
    c // "counts total: " &
    // int2char (histogram_get_n_entries_within_bounds (h)))
call ifile_append (header, &
    c // "total average: " &
    // real2string (histogram_get_average_within_bounds (h)) // " +- " &
    // real2string (histogram_get_error_within_bounds (h)))
end subroutine histogram_get_header

```

13.5.7 Plots

Points

(Analysis: types)+≡

```

type :: point_t
private
    real(default) :: x = 0
    real(default) :: y = 0
    real(default) :: yerr = 0
    real(default) :: xerr = 0
    type(point_t), pointer :: next => null ()
end type point_t

```

(Analysis: interfaces)+≡

```

interface point_init
    module procedure point_init_contents
    module procedure point_init_point
end interface

```

(Analysis: procedures)+≡

```

subroutine point_init_contents (point, x, y, yerr, xerr)
    type(point_t), intent(out) :: point
    real(default), intent(in) :: x, y
    real(default), intent(in), optional :: yerr, xerr
    point%x = x
    point%y = y
    if (present (yerr)) point%yerr = yerr
    if (present (xerr)) point%xerr = xerr
end subroutine point_init_contents

```

```

subroutine point_init_point (point, point_in)
  type(point_t), intent(out) :: point
  type(point_t), intent(in) :: point_in
  point%x = point_in%x
  point%y = point_in%y
  point%yerr = point_in%yerr
  point%xerr = point_in%xerr
end subroutine point_init_point

```

<Analysis: procedures>+≡

```

function point_get_x (point) result (x)
  real(default) :: x
  type(point_t), intent(in) :: point
  x = point%x
end function point_get_x

function point_get_y (point) result (y)
  real(default) :: y
  type(point_t), intent(in) :: point
  y = point%y
end function point_get_y

function point_get_xerr (point) result (xerr)
  real(default) :: xerr
  type(point_t), intent(in) :: point
  xerr = point%xerr
end function point_get_xerr

function point_get_yerr (point) result (yerr)
  real(default) :: yerr
  type(point_t), intent(in) :: point
  yerr = point%yerr
end function point_get_yerr

```

<Analysis: procedures>+≡

```

subroutine point_write_header (unit)
  integer, intent(in) :: unit
  character(120) :: buffer
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (buffer, "(A,4(1x," // HISTOGRAM_HEAD_FORMAT // "))" ) &
    "#", "x", "y", "yerr", "xerr"
  write (u, "(A)") trim (buffer)
end subroutine point_write_header

subroutine point_write (point, unit)
  type(point_t), intent(in) :: point
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,4(1x," // HISTOGRAM_DATA_FORMAT // "))" ) &
    point_get_x (point), &
    point_get_y (point), &

```

```

        point_get_yerr (point), &
        point_get_xerr (point)
    end subroutine point_write

```

Plots

<Analysis: types>+≡

```

    type :: plot_t
    private
    type(point_t), pointer :: first => null ()
    type(point_t), pointer :: last => null ()
    integer :: count = 0
    type(graph_options_t) :: graph_options
    type(drawing_options_t) :: drawing_options
end type plot_t

```

Initializer/finalizer

Initialize a plot. We provide the lower and upper bound in the x direction.

<Analysis: interfaces>+≡

```

    interface plot_init
    module procedure plot_init_empty
    module procedure plot_init_plot
    end interface

```

<Analysis: procedures>+≡

```

subroutine plot_init_empty (p, id, graph_options, drawing_options)
    type(plot_t), intent(out) :: p
    type(string_t), intent(in) :: id
    type(graph_options_t), intent(in), optional :: graph_options
    type(drawing_options_t), intent(in), optional :: drawing_options
    if (present (graph_options)) then
        p%graph_options = graph_options
    else
        call graph_options_init (p%graph_options)
    end if
    call graph_options_set (p%graph_options, id = id)
    if (present (drawing_options)) then
        p%drawing_options = drawing_options
    else
        call drawing_options_init_plot (p%drawing_options)
    end if
end subroutine plot_init_empty

```

Initialize a plot by copying another one, optionally merging in a new set of drawing options.

Since p has pointer (sub)components, we have to explicitly deep-copy the original.

<Analysis: procedures>+≡

```

subroutine plot_init_plot (p, p_in, drawing_options)
    type(plot_t), intent(out) :: p

```



```

type(plot_t), intent(in) :: p_in
type(drawing_options_t), intent(in), optional :: drawing_options
type(point_t), pointer :: current, new
current => p_in%first
do while (associated (current))
    allocate (new)
    call point_init (new, current)
    if (associated (p%last)) then
        p%last%next => new
    else
        p%first => new
    end if
    p%last => new
    current => current%next
end do
p%count = p_in%count
p%graph_options = p_in%graph_options
if (present (drawing_options)) then
    p%drawing_options = drawing_options
else
    p%drawing_options = p_in%drawing_options
end if
end subroutine plot_init_plot

```

Finalize the plot by deallocating the list of points.

⟨Analysis: procedures⟩+≡

```

subroutine plot_final (plot)
    type(plot_t), intent(inout) :: plot
    type(point_t), pointer :: current
    do while (associated (plot%first))
        current => plot%first
        plot%first => current%next
        deallocate (current)
    end do
    plot%last => null ()
end subroutine plot_final

```

Fill plots

Clear the plot contents, but do not modify the structure.

⟨Analysis: procedures⟩+≡

```

subroutine plot_clear (plot)
    type(plot_t), intent(inout) :: plot
    plot%count = 0
    call plot_final (plot)
end subroutine plot_clear

```

Record a value. Successful if the value is within bounds, otherwise it is recorded as under-/overflow.

⟨Analysis: procedures⟩+≡

```

subroutine plot_record_value (plot, x, y, yerr, xerr, success)

```

```

type(plot_t), intent(inout) :: plot
real(default), intent(in) :: x, y
real(default), intent(in), optional :: yerr, xerr
logical, intent(out), optional :: success
type(point_t), pointer :: point
plot%count = plot%count + 1
allocate (point)
call point_init (point, x, y, yerr, xerr)
if (associated (plot%first)) then
    plot%last%next => point
else
    plot%first => point
end if
plot%last => point
if (present (success)) success = .true.
end subroutine plot_record_value

```

Access contents

The number of points.

<Analysis: procedures>+≡

```

function plot_get_n_entries (plot) result (n)
    integer :: n
    type(plot_t), intent(in) :: plot
    n = plot%count
end function plot_get_n_entries

```

Return a pointer to the graph options.

<Analysis: procedures>+≡

```

function plot_get_graph_options_ptr (p) result (ptr)
    type(graph_options_t), pointer :: ptr
    type(plot_t), intent(in), target :: p
    ptr => p%graph_options
end function plot_get_graph_options_ptr

```

Return a pointer to the drawing options.

<Analysis: procedures>+≡

```

function plot_get_drawing_options_ptr (p) result (ptr)
    type(drawing_options_t), pointer :: ptr
    type(plot_t), intent(in), target :: p
    ptr => p%drawing_options
end function plot_get_drawing_options_ptr

```

Output

This output format is used by the GAMELAN driver below.

<Analysis: procedures>+≡

```

subroutine plot_write (plot, unit)
    type(plot_t), intent(in) :: plot
    integer, intent(in), optional :: unit

```

```

type(point_t), pointer :: point
integer :: u
u = given_output_unit (unit); if (u < 0) return
call point_write_header (u)
point => plot%first
do while (associated (point))
    call point_write (point, unit)
    point => point%next
end do
write (u, *)
write (u, "(A,1x,A)" ) "#", "Summary:"
write (u, "(A,1x,I0)" ) &
    "n_entries =", plot_get_n_entries (plot)
write (u, *)
end subroutine plot_write

```

Write the GAMELAN reader for plot contents.

<Analysis: procedures>+≡

```

subroutine plot_write_gml_reader (p, filename, unit)
type(plot_t), intent(in) :: p
type(string_t), intent(in) :: filename
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit); if (u < 0) return
write (u, "(2x,A)" ) 'fromfile ' // char (filename) // ':"'
write (u, "(4x,A)" ) 'key "# Plot:";'
write (u, "(4x,A)" ) 'for i withinblock:'
write (u, "(6x,A)" ) 'get x, y, y.err, x.err;'
write (u, "(6x,A)" ) 'plot (' // char (p%drawing_options%dataset) &
    // ') (x,y);'
if (p%drawing_options%err) then
    write (u, "(6x,A)" ) 'plot (' // char (p%drawing_options%dataset) &
        // '.err) (x,y) vbar y.err hbar x.err;'
end if
write (u, "(4x,A)" ) 'endfor'
write (u, "(2x,A)" ) 'endfrom'
end subroutine plot_write_gml_reader

```

L^AT_EX and GAMELAN output. Analogous to histogram output.

<Analysis: procedures>+≡

```

subroutine plot_write_gml_driver (p, filename, unit)
type(plot_t), intent(in) :: p
type(string_t), intent(in) :: filename
integer, intent(in), optional :: unit
type(string_t) :: calc_cmd, bg_cmd, draw_cmd, err_cmd, symb_cmd, fg_cmd
integer :: u
u = given_output_unit (unit); if (u < 0) return
call graph_options_write_tex_header (p%graph_options, unit)
write (u, "(2x,A)" ) &
    char (graph_options_get_gml_setup (p%graph_options))
write (u, "(2x,A)" ) &
    char (graph_options_get_gml_graphrange (p%graph_options))
call plot_write_gml_reader (p, filename, unit)

```

```

calc_cmd = drawing_options_get_calc_command (p%drawing_options)
if (calc_cmd /= "") write (u, "(2x,A)") char (calc_cmd)
bg_cmd = drawing_options_get_gml_bg_command (p%drawing_options)
if (bg_cmd /= "") write (u, "(2x,A)") char (bg_cmd)
draw_cmd = drawing_options_get_draw_command (p%drawing_options)
if (draw_cmd /= "") write (u, "(2x,A)") char (draw_cmd)
err_cmd = drawing_options_get_err_command (p%drawing_options)
if (err_cmd /= "") write (u, "(2x,A)") char (err_cmd)
symb_cmd = drawing_options_get_symb_command (p%drawing_options)
if (symb_cmd /= "") write (u, "(2x,A)") char (symb_cmd)
fg_cmd = drawing_options_get_gml_fg_command (p%drawing_options)
if (fg_cmd /= "") write (u, "(2x,A)") char (fg_cmd)
write (u, "(2x,A)") char (graph_options_get_gml_x_label (p%graph_options))
write (u, "(2x,A)") char (graph_options_get_gml_y_label (p%graph_options))
call graph_options_write_tex_footer (p%graph_options, unit)
end subroutine plot_write_gml_driver

```

Append header for generic data output in ifile format.

```

<Analysis: procedures>+≡
subroutine plot_get_header (plot, header, comment)
  type(plot_t), intent(in) :: plot
  type(ifile_t), intent(inout) :: header
  type(string_t), intent(in), optional :: comment
  type(string_t) :: c
  if (present (comment)) then
    c = comment
  else
    c = ""
  end if
  call ifile_append (header, c // "WHIZARD plot data")
  call graph_options_get_header (plot%graph_options, header, comment)
  call ifile_append (header, &
    c // "number of points: " &
    // int2char (plot_get_n_entries (plot)))
end subroutine plot_get_header

```

13.5.8 Graphs

A graph is a container for several graph elements. Each graph element is either a plot or a histogram. There is an appropriate base type below (the `analysis_object_t`), but to avoid recursion, we define a separate base type here. Note that there is no actual recursion: a graph is an analysis object, but a graph cannot contain graphs.

(If we could use type extension, the implementation would be much more transparent.)

Graph elements

Graph elements cannot be filled by the `record` command directly. The contents are always copied from elementary histograms or plots.

```

<Analysis: types>+≡

```

```

type :: graph_element_t
private
integer :: type = AN_UNDEFINED
type(histogram_t), pointer :: h => null ()
type(plot_t), pointer :: p => null ()
end type graph_element_t

```

<Analysis: procedures>+≡

```

subroutine graph_element_final (el)
type(graph_element_t), intent(inout) :: el
select case (el%type)
case (AN_HISTOGRAM)
deallocate (el%h)
case (AN_PLOT)
call plot_final (el%p)
deallocate (el%p)
end select
el%type = AN_UNDEFINED
end subroutine graph_element_final

```

Return the number of entries in the graph element:

<Analysis: procedures>+≡

```

function graph_element_get_n_entries (el) result (n)
integer :: n
type(graph_element_t), intent(in) :: el
select case (el%type)
case (AN_HISTOGRAM); n = histogram_get_n_entries (el%h)
case (AN_PLOT);      n = plot_get_n_entries (el%p)
case default;        n = 0
end select
end function graph_element_get_n_entries

```

Return a pointer to the graph / drawing options.

<Analysis: procedures>+≡

```

function graph_element_get_graph_options_ptr (el) result (ptr)
type(graph_options_t), pointer :: ptr
type(graph_element_t), intent(in) :: el
select case (el%type)
case (AN_HISTOGRAM); ptr => histogram_get_graph_options_ptr (el%h)
case (AN_PLOT);      ptr => plot_get_graph_options_ptr (el%p)
case default;        ptr => null ()
end select
end function graph_element_get_graph_options_ptr

function graph_element_get_drawing_options_ptr (el) result (ptr)
type(drawing_options_t), pointer :: ptr
type(graph_element_t), intent(in) :: el
select case (el%type)
case (AN_HISTOGRAM); ptr => histogram_get_drawing_options_ptr (el%h)
case (AN_PLOT);      ptr => plot_get_drawing_options_ptr (el%p)
case default;        ptr => null ()
end select

```

```
end function graph_element_get_drawing_options_ptr
```

Output, simple wrapper for the plot/histogram writer.

(Analysis: procedures)+≡

```
subroutine graph_element_write (el, unit)
  type(graph_element_t), intent(in) :: el
  integer, intent(in), optional :: unit
  type(graph_options_t), pointer :: gro
  type(string_t) :: id
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  gro => graph_element_get_graph_options_ptr (el)
  id = graph_options_get_id (gro)
  write (u, "(A,A)" ' #', repeat ("-", 78)
  select case (el%type)
  case (AN_HISTOGRAM)
    write (u, "(A)", advance="no") "# Histogram: "
    write (u, "(1x,A)" char (id)
    call histogram_write (el%h, unit)
  case (AN_PLOT)
    write (u, "(A)", advance="no") "# Plot: "
    write (u, "(1x,A)" char (id)
    call plot_write (el%p, unit)
  end select
end subroutine graph_element_write
```

(Analysis: procedures)+≡

```
subroutine graph_element_write_gml_reader (el, filename, unit)
  type(graph_element_t), intent(in) :: el
  type(string_t), intent(in) :: filename
  integer, intent(in), optional :: unit
  select case (el%type)
  case (AN_HISTOGRAM); call histogram_write_gml_reader (el%h, filename, unit)
  case (AN_PLOT);      call plot_write_gml_reader (el%p, filename, unit)
  end select
end subroutine graph_element_write_gml_reader
```

The graph type

The actual graph type contains its own `graph_options`, which override the individual settings. The `drawing_options` are set in the graph elements. This distinction motivates the separation of the two types.

(Analysis: types)+≡

```
type :: graph_t
  private
  type(graph_element_t), dimension(:), allocatable :: el
  type(graph_options_t) :: graph_options
end type graph_t
```

Initializer/finalizer

The graph is created with a definite number of elements. The elements are filled one by one, optionally with modified drawing options.

(Analysis: procedures)+≡

```
subroutine graph_init (g, id, n_elements, graph_options)
  type(graph_t), intent(out) :: g
  type(string_t), intent(in) :: id
  integer, intent(in) :: n_elements
  type(graph_options_t), intent(in), optional :: graph_options
  allocate (g%el (n_elements))
  if (present (graph_options)) then
    g%graph_options = graph_options
  else
    call graph_options_init (g%graph_options)
  end if
  call graph_options_set (g%graph_options, id = id)
end subroutine graph_init
```

(Analysis: procedures)+≡

```
subroutine graph_insert_histogram (g, i, h, drawing_options)
  type(graph_t), intent(inout), target :: g
  integer, intent(in) :: i
  type(histogram_t), intent(in) :: h
  type(drawing_options_t), intent(in), optional :: drawing_options
  type(graph_options_t), pointer :: gro
  type(drawing_options_t), pointer :: dro
  type(string_t) :: id
  g%el(i)%type = AN_HISTOGRAM
  allocate (g%el(i)%h)
  call histogram_init_histogram (g%el(i)%h, h, drawing_options)
  gro => histogram_get_graph_options_ptr (g%el(i)%h)
  dro => histogram_get_drawing_options_ptr (g%el(i)%h)
  id = graph_options_get_id (gro)
  call drawing_options_set (dro, dataset = "dat." // id)
end subroutine graph_insert_histogram
```

(Analysis: procedures)+≡

```
subroutine graph_insert_plot (g, i, p, drawing_options)
  type(graph_t), intent(inout) :: g
  integer, intent(in) :: i
  type(plot_t), intent(in) :: p
  type(drawing_options_t), intent(in), optional :: drawing_options
  type(graph_options_t), pointer :: gro
  type(drawing_options_t), pointer :: dro
  type(string_t) :: id
  g%el(i)%type = AN_PLOT
  allocate (g%el(i)%p)
  call plot_init_plot (g%el(i)%p, p, drawing_options)
  gro => plot_get_graph_options_ptr (g%el(i)%p)
  dro => plot_get_drawing_options_ptr (g%el(i)%p)
  id = graph_options_get_id (gro)
  call drawing_options_set (dro, dataset = "dat." // id)
```

```
end subroutine graph_insert_plot
```

Finalizer.

```
<Analysis: procedures>+≡
subroutine graph_final (g)
  type(graph_t), intent(inout) :: g
  integer :: i
  do i = 1, size (g%el)
    call graph_element_final (g%el(i))
  end do
  deallocate (g%el)
end subroutine graph_final
```

Access contents

The number of elements.

```
<Analysis: procedures>+≡
function graph_get_n_elements (graph) result (n)
  integer :: n
  type(graph_t), intent(in) :: graph
  n = size (graph%el)
end function graph_get_n_elements
```

Retrieve a pointer to the drawing options of an element, so they can be modified. (The `target` attribute is not actually needed because the components are pointers.)

```
<Analysis: procedures>+≡
function graph_get_drawing_options_ptr (g, i) result (ptr)
  type(drawing_options_t), pointer :: ptr
  type(graph_t), intent(in), target :: g
  integer, intent(in) :: i
  ptr => graph_element_get_drawing_options_ptr (g%el(i))
end function graph_get_drawing_options_ptr
```

Output

The default output format just writes histogram and plot data.

```
<Analysis: procedures>+≡
subroutine graph_write (graph, unit)
  type(graph_t), intent(in) :: graph
  integer, intent(in), optional :: unit
  integer :: i
  do i = 1, size (graph%el)
    call graph_element_write (graph%el(i), unit)
  end do
end subroutine graph_write
```


The GAMELAN driver is not a simple wrapper, but it writes the plot/histogram contents embedded the complete graph. First, data are read in, global background commands next, then individual elements, then global foreground commands.

<Analysis: procedures>+≡

```
subroutine graph_write_gml_driver (g, filename, unit)
  type(graph_t), intent(in) :: g
  type(string_t), intent(in) :: filename
  type(string_t) :: calc_cmd, bg_cmd, draw_cmd, err_cmd, symb_cmd, fg_cmd
  integer, intent(in), optional :: unit
  type(drawing_options_t), pointer :: dro
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  call graph_options_write_tex_header (g%graph_options, unit)
  write (u, "(2x,A)") &
    char (graph_options_get_gml_setup (g%graph_options))
  write (u, "(2x,A)") &
    char (graph_options_get_gml_graphrange (g%graph_options))
  do i = 1, size (g%el)
    call graph_element_write_gml_reader (g%el(i), filename, unit)
    calc_cmd = drawing_options_get_calc_command &
      (graph_element_get_drawing_options_ptr (g%el(i)))
    if (calc_cmd /= "") write (u, "(2x,A)") char (calc_cmd)
  end do
  bg_cmd = graph_options_get_gml_bg_command (g%graph_options)
  if (bg_cmd /= "") write (u, "(2x,A)") char (bg_cmd)
  do i = 1, size (g%el)
    dro => graph_element_get_drawing_options_ptr (g%el(i))
    bg_cmd = drawing_options_get_gml_bg_command (dro)
    if (bg_cmd /= "") write (u, "(2x,A)") char (bg_cmd)
    draw_cmd = drawing_options_get_draw_command (dro)
    if (draw_cmd /= "") write (u, "(2x,A)") char (draw_cmd)
    err_cmd = drawing_options_get_err_command (dro)
    if (err_cmd /= "") write (u, "(2x,A)") char (err_cmd)
    symb_cmd = drawing_options_get_symb_command (dro)
    if (symb_cmd /= "") write (u, "(2x,A)") char (symb_cmd)
    fg_cmd = drawing_options_get_gml_fg_command (dro)
    if (fg_cmd /= "") write (u, "(2x,A)") char (fg_cmd)
  end do
  fg_cmd = graph_options_get_gml_fg_command (g%graph_options)
  if (fg_cmd /= "") write (u, "(2x,A)") char (fg_cmd)
  write (u, "(2x,A)") char (graph_options_get_gml_x_label (g%graph_options))
  write (u, "(2x,A)") char (graph_options_get_gml_y_label (g%graph_options))
  call graph_options_write_tex_footer (g%graph_options, unit)
end subroutine graph_write_gml_driver
```

Append header for generic data output in ifile format.

<Analysis: procedures>+≡

```
subroutine graph_get_header (graph, header, comment)
  type(graph_t), intent(in) :: graph
  type(ifile_t), intent(inout) :: header
  type(string_t), intent(in), optional :: comment
  type(string_t) :: c
```

```

    if (present (comment)) then
        c = comment
    else
        c = ""
    end if
    call ifile_append (header, c // "WHIZARD graph data")
    call graph_options_get_header (graph%graph_options, header, comment)
    call ifile_append (header, &
        c // "number of graph elements: " &
        // int2char (graph_get_n_elements (graph)))
end subroutine graph_get_header

```

13.5.9 Analysis objects

This data structure holds all observables, histograms and such that are currently active. We have one global store; individual items are identified by their ID strings.

(This should rather be coded by type extension.)

```

<Analysis: parameters>+≡
    integer, parameter :: AN_UNDEFINED = 0
    integer, parameter :: AN_OBSERVABLE = 1
    integer, parameter :: AN_HISTOGRAM = 2
    integer, parameter :: AN_PLOT = 3
    integer, parameter :: AN_GRAPH = 4

<Analysis: public>+≡
    public :: AN_UNDEFINED, AN_HISTOGRAM, AN_OBSERVABLE, AN_PLOT, AN_GRAPH

<Analysis: types>+≡
    type :: analysis_object_t
    private
        type(string_t) :: id
        integer :: type = AN_UNDEFINED
        type(observable_t), pointer :: obs => null ()
        type(histogram_t), pointer :: h => null ()
        type(plot_t), pointer :: p => null ()
        type(graph_t), pointer :: g => null ()
        type(analysis_object_t), pointer :: next => null ()
    end type analysis_object_t

```

Initializer/finalizer

Allocate with the correct type but do not fill initial values.

```

<Analysis: procedures>+≡
    subroutine analysis_object_init (obj, id, type)
        type(analysis_object_t), intent(out) :: obj
        type(string_t), intent(in) :: id
        integer, intent(in) :: type
        obj%id = id
        obj%type = type
        select case (obj%type)

```

```

        case (AN_OBSERVABLE); allocate (obj%obs)
        case (AN_HISTOGRAM);   allocate (obj%h)
        case (AN_PLOT);        allocate (obj%p)
        case (AN_GRAPH);       allocate (obj%g)
    end select
end subroutine analysis_object_init

```

<Analysis: procedures>+≡

```

subroutine analysis_object_final (obj)
    type(analysis_object_t), intent(inout) :: obj
    select case (obj%type)
    case (AN_OBSERVABLE)
        deallocate (obj%obs)
    case (AN_HISTOGRAM)
        deallocate (obj%h)
    case (AN_PLOT)
        call plot_final (obj%p)
        deallocate (obj%p)
    case (AN_GRAPH)
        call graph_final (obj%g)
        deallocate (obj%g)
    end select
    obj%type = AN_UNDEFINED
end subroutine analysis_object_final

```

Clear the analysis object, i.e., reset it to its initial state. Not applicable to graphs, which are always combinations of other existing objects.

<Analysis: procedures>+≡

```

subroutine analysis_object_clear (obj)
    type(analysis_object_t), intent(inout) :: obj
    select case (obj%type)
    case (AN_OBSERVABLE)
        call observable_clear (obj%obs)
    case (AN_HISTOGRAM)
        call histogram_clear (obj%h)
    case (AN_PLOT)
        call plot_clear (obj%p)
    end select
end subroutine analysis_object_clear

```

Fill with data

Record data. The effect depends on the type of analysis object.

<Analysis: procedures>+≡

```

subroutine analysis_object_record_data (obj, &
    x, y, yerr, xerr, weight, excess, success)
    type(analysis_object_t), intent(inout) :: obj
    real(default), intent(in) :: x
    real(default), intent(in), optional :: y, yerr, xerr, weight, excess
    logical, intent(out), optional :: success
    select case (obj%type)

```

```

case (AN_OBSERVABLE)
  if (present (weight)) then
    call observable_record_value_weighted (obj%obs, x, weight, success)
  else
    call observable_record_value_unweighted (obj%obs, x, success)
  end if
case (AN_HISTOGRAM)
  if (present (weight)) then
    call histogram_record_value_weighted (obj%h, x, weight, success)
  else
    call histogram_record_value_unweighted (obj%h, x, excess, success)
  end if
case (AN_PLOT)
  if (present (y)) then
    call plot_record_value (obj%p, x, y, yerr, xerr, success)
  else
    if (present (success)) success = .false.
  end if
case default
  if (present (success)) success = .false.
end select
end subroutine analysis_object_record_data

```

Explicitly set the pointer to the next object in the list.

```

<Analysis: procedures>+≡
subroutine analysis_object_set_next_ptr (obj, next)
  type(analysis_object_t), intent(inout) :: obj
  type(analysis_object_t), pointer :: next
  obj%next => next
end subroutine analysis_object_set_next_ptr

```

Access contents

Return a pointer to the next object in the list.

```

<Analysis: procedures>+≡
function analysis_object_get_next_ptr (obj) result (next)
  type(analysis_object_t), pointer :: next
  type(analysis_object_t), intent(in) :: obj
  next => obj%next
end function analysis_object_get_next_ptr

```

Return data as appropriate for the object type.

```

<Analysis: procedures>+≡
function analysis_object_get_n_elements (obj) result (n)
  integer :: n
  type(analysis_object_t), intent(in) :: obj
  select case (obj%type)
  case (AN_HISTOGRAM)
    n = 1
  case (AN_PLOT)
    n = 1

```

```

    case (AN_GRAPH)
        n = graph_get_n_elements (obj%g)
    case default
        n = 0
    end select
end function analysis_object_get_n_elements

function analysis_object_get_n_entries (obj, within_bounds) result (n)
    integer :: n
    type(analysis_object_t), intent(in) :: obj
    logical, intent(in), optional :: within_bounds
    logical :: wb
    select case (obj%type)
    case (AN_OBSERVABLE)
        n = observable_get_n_entries (obj%obs)
    case (AN_HISTOGRAM)
        wb = .false.; if (present (within_bounds)) wb = within_bounds
        if (wb) then
            n = histogram_get_n_entries_within_bounds (obj%h)
        else
            n = histogram_get_n_entries (obj%h)
        end if
    case (AN_PLOT)
        n = plot_get_n_entries (obj%p)
    case default
        n = 0
    end select
end function analysis_object_get_n_entries

function analysis_object_get_average (obj, within_bounds) result (avg)
    real(default) :: avg
    type(analysis_object_t), intent(in) :: obj
    logical, intent(in), optional :: within_bounds
    logical :: wb
    select case (obj%type)
    case (AN_OBSERVABLE)
        avg = observable_get_average (obj%obs)
    case (AN_HISTOGRAM)
        wb = .false.; if (present (within_bounds)) wb = within_bounds
        if (wb) then
            avg = histogram_get_average_within_bounds (obj%h)
        else
            avg = histogram_get_average (obj%h)
        end if
    case default
        avg = 0
    end select
end function analysis_object_get_average

function analysis_object_get_error (obj, within_bounds) result (err)
    real(default) :: err
    type(analysis_object_t), intent(in) :: obj
    logical, intent(in), optional :: within_bounds
    logical :: wb

```

```

select case (obj%type)
case (AN_OBSERVABLE)
    err = observable_get_error (obj%obs)
case (AN_HISTOGRAM)
    wb = .false.; if (present (within_bounds)) wb = within_bounds
    if (wb) then
        err = histogram_get_error_within_bounds (obj%h)
    else
        err = histogram_get_error (obj%h)
    end if
case default
    err = 0
end select
end function analysis_object_get_error

```

Return pointers to the actual contents:

(Analysis: procedures)+≡

```

function analysis_object_get_observable_ptr (obj) result (obs)
    type(observable_t), pointer :: obs
    type(analysis_object_t), intent(in) :: obj
    select case (obj%type)
    case (AN_OBSERVABLE); obs => obj%obs
    case default;         obs => null ()
    end select
end function analysis_object_get_observable_ptr

function analysis_object_get_histogram_ptr (obj) result (h)
    type(histogram_t), pointer :: h
    type(analysis_object_t), intent(in) :: obj
    select case (obj%type)
    case (AN_HISTOGRAM); h => obj%h
    case default;       h => null ()
    end select
end function analysis_object_get_histogram_ptr

function analysis_object_get_plot_ptr (obj) result (plot)
    type(plot_t), pointer :: plot
    type(analysis_object_t), intent(in) :: obj
    select case (obj%type)
    case (AN_PLOT); plot => obj%p
    case default;   plot => null ()
    end select
end function analysis_object_get_plot_ptr

function analysis_object_get_graph_ptr (obj) result (g)
    type(graph_t), pointer :: g
    type(analysis_object_t), intent(in) :: obj
    select case (obj%type)
    case (AN_GRAPH); g => obj%g
    case default;    g => null ()
    end select
end function analysis_object_get_graph_ptr

```

Return true if the object has a graphical representation:

```

<Analysis: procedures>+≡
function analysis_object_has_plot (obj) result (flag)
  logical :: flag
  type(analysis_object_t), intent(in) :: obj
  select case (obj%type)
    case (AN_HISTOGRAM); flag = .true.
    case (AN_PLOT);      flag = .true.
    case (AN_GRAPH);     flag = .true.
    case default;        flag = .false.
  end select
end function analysis_object_has_plot

```

Output

```

<Analysis: procedures>+≡
subroutine analysis_object_write (obj, unit, verbose)
  type(analysis_object_t), intent(in) :: obj
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  logical :: verb
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  verb = .false.; if (present (verbose)) verb = verbose
  write (u, "(A)") repeat ("#", 79)
  select case (obj%type)
    case (AN_OBSERVABLE)
      write (u, "(A)", advance="no")  "# Observable:"
    case (AN_HISTOGRAM)
      write (u, "(A)", advance="no")  "# Histogram: "
    case (AN_PLOT)
      write (u, "(A)", advance="no")  "# Plot: "
    case (AN_GRAPH)
      write (u, "(A)", advance="no")  "# Graph: "
    case default
      write (u, "(A)") "# [undefined analysis object]"
      return
  end select
  write (u, "(1x,A)") char (obj%id)
  select case (obj%type)
    case (AN_OBSERVABLE)
      call observable_write (obj%obs, unit)
    case (AN_HISTOGRAM)
      if (verb) then
        call graph_options_write (obj%h%graph_options, unit)
        write (u, *)
        call drawing_options_write (obj%h%drawing_options, unit)
        write (u, *)
      end if
      call histogram_write (obj%h, unit)
    case (AN_PLOT)
      if (verb) then
        call graph_options_write (obj%p%graph_options, unit)

```

```

        write (u, *)
        call drawing_options_write (obj%p%drawing_options, unit)
        write (u, *)
    end if
    call plot_write (obj%p, unit)
case (AN_GRAPH)
    call graph_write (obj%g, unit)
end select
end subroutine analysis_object_write

```

Write the object part of the L^AT_EX driver file.

<Analysis: procedures>+≡

```

subroutine analysis_object_write_driver (obj, filename, unit)
    type(analysis_object_t), intent(in) :: obj
    type(string_t), intent(in) :: filename
    integer, intent(in), optional :: unit
    select case (obj%type)
    case (AN_OBSERVABLE)
        call observable_write_driver (obj%obs, unit)
    case (AN_HISTOGRAM)
        call histogram_write_gml_driver (obj%h, filename, unit)
    case (AN_PLOT)
        call plot_write_gml_driver (obj%p, filename, unit)
    case (AN_GRAPH)
        call graph_write_gml_driver (obj%g, filename, unit)
    end select
end subroutine analysis_object_write_driver

```

Return a data header for external formats, in ifile form.

<Analysis: procedures>+≡

```

subroutine analysis_object_get_header (obj, header, comment)
    type(analysis_object_t), intent(in) :: obj
    type(ifile_t), intent(inout) :: header
    type(string_t), intent(in), optional :: comment
    select case (obj%type)
    case (AN_HISTOGRAM)
        call histogram_get_header (obj%h, header, comment)
    case (AN_PLOT)
        call plot_get_header (obj%p, header, comment)
    end select
end subroutine analysis_object_get_header

```

13.5.10 Analysis object iterator

Analysis objects are containers which have iterable data structures: histograms/bins and plots/points. If they are to be treated on a common basis, it is useful to have an iterator which hides the implementation details.

The iterator is used only for elementary analysis objects that contain plot data: histograms or plots. It is invalid for meta-objects (graphs) and non-graphical objects (observables).

<Analysis: public>+≡


```

public :: analysis_iterator_t
<Analysis: types>+≡
type :: analysis_iterator_t
  private
  integer :: type = AN_UNDEFINED
  type(analysis_object_t), pointer :: object => null ()
  integer :: index = 1
  type(point_t), pointer :: point => null ()
end type

```

The initializer places the iterator at the beginning of the analysis object.

```

<Analysis: procedures>+≡
subroutine analysis_iterator_init (iterator, object)
  type(analysis_iterator_t), intent(out) :: iterator
  type(analysis_object_t), intent(in), target :: object
  iterator%object => object
  if (associated (iterator%object)) then
    iterator%type = iterator%object%type
    select case (iterator%type)
    case (AN_PLOT)
      iterator%point => iterator%object%p%first
    end select
  end if
end subroutine analysis_iterator_init

```

The iterator is valid as long as it points to an existing entry. An iterator for a data object without array data (observable) is always invalid.

```

<Analysis: public>+≡
public :: analysis_iterator_is_valid
<Analysis: procedures>+≡
function analysis_iterator_is_valid (iterator) result (valid)
  logical :: valid
  type(analysis_iterator_t), intent(in) :: iterator
  if (associated (iterator%object)) then
    select case (iterator%type)
    case (AN_HISTOGRAM)
      valid = iterator%index <= histogram_get_n_bins (iterator%object%h)
    case (AN_PLOT)
      valid = associated (iterator%point)
    case default
      valid = .false.
    end select
  else
    valid = .false.
  end if
end function analysis_iterator_is_valid

```

Advance the iterator.

```

<Analysis: public>+≡
public :: analysis_iterator_advance

```

```

<Analysis: procedures>+≡
subroutine analysis_iterator_advance (iterator)
  type(analysis_iterator_t), intent(inout) :: iterator
  if (associated (iterator%object)) then
    select case (iterator%type)
    case (AN_PLOT)
      iterator%point => iterator%point%next
    end select
    iterator%index = iterator%index + 1
  end if
end subroutine analysis_iterator_advance

```

Retrieve the object type:

```

<Analysis: public>+≡
public :: analysis_iterator_get_type

<Analysis: procedures>+≡
function analysis_iterator_get_type (iterator) result (type)
  integer :: type
  type(analysis_iterator_t), intent(in) :: iterator
  type = iterator%type
end function analysis_iterator_get_type

```

Use the iterator to retrieve data. We implement a common routine which takes the data descriptors as optional arguments. Data which do not occur in the selected type trigger to an error condition.

The iterator must point to a valid entry.

```

<Analysis: public>+≡
public :: analysis_iterator_get_data

<Analysis: procedures>+≡
subroutine analysis_iterator_get_data (iterator, &
  x, y, yerr, xerr, width, excess, index, n_total)
  type(analysis_iterator_t), intent(in) :: iterator
  real(default), intent(out), optional :: x, y, yerr, xerr, width, excess
  integer, intent(out), optional :: index, n_total
  select case (iterator%type)
  case (AN_HISTOGRAM)
    if (present (x)) &
      x = bin_get_midpoint (iterator%object%h%bin(iterator%index))
    if (present (y)) &
      y = bin_get_sum (iterator%object%h%bin(iterator%index))
    if (present (yerr)) &
      yerr = bin_get_error (iterator%object%h%bin(iterator%index))
    if (present (xerr)) &
      call invalid ("histogram", "xerr")
    if (present (width)) &
      width = bin_get_width (iterator%object%h%bin(iterator%index))
    if (present (excess)) &
      excess = bin_get_excess (iterator%object%h%bin(iterator%index))
    if (present (index)) &
      index = iterator%index
    if (present (n_total)) &
      n_total = histogram_get_n_bins (iterator%object%h)
  end select
end subroutine analysis_iterator_get_data

```

```

case (AN_PLOT)
  if (present (x)) &
    x = point_get_x (iterator%point)
  if (present (y)) &
    y = point_get_y (iterator%point)
  if (present (yerr)) &
    yerr = point_get_yerr (iterator%point)
  if (present (xerr)) &
    xerr = point_get_xerr (iterator%point)
  if (present (width)) &
    call invalid ("plot", "width")
  if (present (excess)) &
    call invalid ("plot", "excess")
  if (present (index)) &
    index = iterator%index
  if (present (n_total)) &
    n_total = plot_get_n_entries (iterator%object%p)
case default
  call msg_bug ("analysis_iterator_get_data: called " &
    // "for unsupported analysis object type")
end select
contains
  subroutine invalid (typestr, objstr)
    character(*), intent(in) :: typestr, objstr
    call msg_bug ("analysis_iterator_get_data: attempt to get '" &
      // objstr // "' for type '" // typestr // "'")
  end subroutine invalid
end subroutine analysis_iterator_get_data

```

13.5.11 Analysis store

This data structure holds all observables, histograms and such that are currently active. We have one global store; individual items are identified by their ID strings and types.

```

<Analysis: variables>≡
  type(analysis_store_t), save :: analysis_store

<Analysis: types>+≡
  type :: analysis_store_t
  private
    type(analysis_object_t), pointer :: first => null ()
    type(analysis_object_t), pointer :: last => null ()
  end type analysis_store_t

```

Delete the analysis store

```

<Analysis: public>+≡
  public :: analysis_final

<Analysis: procedures>+≡
  subroutine analysis_final ()
    type(analysis_object_t), pointer :: current

```

```

do while (associated (analysis_store%first))
  current => analysis_store%first
  analysis_store%first => current%next
  call analysis_object_final (current)
end do
analysis_store%last => null ()
end subroutine analysis_final

```

Append a new analysis object

```

<Analysis: procedures>+≡
subroutine analysis_store_append_object (id, type)
  type(string_t), intent(in) :: id
  integer, intent(in) :: type
  type(analysis_object_t), pointer :: obj
  allocate (obj)
  call analysis_object_init (obj, id, type)
  if (associated (analysis_store%last)) then
    analysis_store%last%next => obj
  else
    analysis_store%first => obj
  end if
  analysis_store%last => obj
end subroutine analysis_store_append_object

```

Return a pointer to the analysis object with given ID.

```

<Analysis: procedures>+≡
function analysis_store_get_object_ptr (id) result (obj)
  type(string_t), intent(in) :: id
  type(analysis_object_t), pointer :: obj
  obj => analysis_store%first
  do while (associated (obj))
    if (obj%id == id) return
    obj => obj%next
  end do
end function analysis_store_get_object_ptr

```

Initialize an analysis object: either reset it if present, or append a new entry.

```

<Analysis: procedures>+≡
subroutine analysis_store_init_object (id, type, obj)
  type(string_t), intent(in) :: id
  integer, intent(in) :: type
  type(analysis_object_t), pointer :: obj, next
  obj => analysis_store_get_object_ptr (id)
  if (associated (obj)) then
    next => analysis_object_get_next_ptr (obj)
    call analysis_object_final (obj)
    call analysis_object_init (obj, id, type)
    call analysis_object_set_next_ptr (obj, next)
  else
    call analysis_store_append_object (id, type)
    obj => analysis_store%last
  end if
end subroutine

```

```
end subroutine analysis_store_init_object
```

Get the type of a analysis object

<Analysis: public>+≡

```
public :: analysis_store_get_object_type
```

<Analysis: procedures>+≡

```
function analysis_store_get_object_type (id) result (type)
  type(string_t), intent(in) :: id
  integer :: type
  type(analysis_object_t), pointer :: object
  object => analysis_store_get_object_ptr (id)
  if (associated (object)) then
    type = object%type
  else
    type = AN_UNDEFINED
  end if
end function analysis_store_get_object_type
```

Return the number of objects in the store.

<Analysis: procedures>+≡

```
function analysis_store_get_n_objects () result (n)
  integer :: n
  type(analysis_object_t), pointer :: current
  n = 0
  current => analysis_store%first
  do while (associated (current))
    n = n + 1
    current => current%next
  end do
end function analysis_store_get_n_objects
```

Allocate an array and fill it with all existing IDs.

<Analysis: public>+≡

```
public :: analysis_store_get_ids
```

<Analysis: procedures>+≡

```
subroutine analysis_store_get_ids (id)
  type(string_t), dimension(:), allocatable, intent(out) :: id
  type(analysis_object_t), pointer :: current
  integer :: i
  allocate (id (analysis_store_get_n_objects()))
  i = 0
  current => analysis_store%first
  do while (associated (current))
    i = i + 1
    id(i) = current%id
    current => current%next
  end do
end subroutine analysis_store_get_ids
```

13.5.12 L^AT_EX driver file

Write a driver file for all objects in the store.

```

<Analysis: procedures>+≡
subroutine analysis_store_write_driver_all (filename_data, unit)
  type(string_t), intent(in) :: filename_data
  integer, intent(in), optional :: unit
  type(analysis_object_t), pointer :: obj
  call analysis_store_write_driver_header (unit)
  obj => analysis_store%first
  do while (associated (obj))
    call analysis_object_write_driver (obj, filename_data, unit)
    obj => obj%next
  end do
  call analysis_store_write_driver_footer (unit)
end subroutine analysis_store_write_driver_all

```

Write a driver file for an array of objects.

```

<Analysis: procedures>+≡
subroutine analysis_store_write_driver_obj (filename_data, id, unit)
  type(string_t), intent(in) :: filename_data
  type(string_t), dimension(:), intent(in) :: id
  integer, intent(in), optional :: unit
  type(analysis_object_t), pointer :: obj
  integer :: i
  call analysis_store_write_driver_header (unit)
  do i = 1, size (id)
    obj => analysis_store_get_object_ptr (id(i))
    if (associated (obj)) &
      call analysis_object_write_driver (obj, filename_data, unit)
  end do
  call analysis_store_write_driver_footer (unit)
end subroutine analysis_store_write_driver_obj

```

The beginning of the driver file.

```

<Analysis: procedures>+≡
subroutine analysis_store_write_driver_header (unit)
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, '(A)') "\documentclass[12pt]{article}"
  write (u, *)
  write (u, '(A)') "\usepackage{gamelan}"
  write (u, '(A)') "\usepackage{amsmath}"
  write (u, '(A)') "\usepackage{ifpdf}"
  write (u, '(A)') "\ifpdf"
  write (u, '(A)') "  \DeclareGraphicsRule{*}{mps}{*}{"
  write (u, '(A)') "\else"
  write (u, '(A)') "  \DeclareGraphicsRule{*}{eps}{*}{"
  write (u, '(A)') "\fi"
  write (u, *)
  write (u, '(A)') "\begin{document}"
  write (u, '(A)') "\begin{gmlfile}"

```

```

write (u, *)
write (u, '(A)') "\begin{gmlcode}"
write (u, '(A)') " color col.default, col.excess;"
write (u, '(A)') " col.default = 0.9white;"
write (u, '(A)') " col.excess = red;"
write (u, '(A)') " boolean show_excess;"
!!! Future excess options for plots
! if (mcs(1)%plot_excess .and. mcs(1)%unweighted) then
!   write (u, '(A)') " show_excess = true;"
! else
write (u, '(A)') " show_excess = false;"
! end if
write (u, '(A)') "\end{gmlcode}"
write (u, *)
end subroutine analysis_store_write_driver_header

```

The end of the driver file.

```

<Analysis: procedures>+≡
subroutine analysis_store_write_driver_footer (unit)
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit); if (u < 0) return
write(u, *)
write(u, '(A)') "\end{gmlfile}"
write(u, '(A)') "\end{document}"
end subroutine analysis_store_write_driver_footer

```

13.5.13 API

Creating new objects

The specific versions below:

```

<Analysis: public>+≡
public :: analysis_init_observable

<Analysis: procedures>+≡
subroutine analysis_init_observable (id, obs_label, obs_unit, graph_options)
type(string_t), intent(in) :: id
type(string_t), intent(in), optional :: obs_label, obs_unit
type(graph_options_t), intent(in), optional :: graph_options
type(analysis_object_t), pointer :: obj
type(observable_t), pointer :: obs
call analysis_store_init_object (id, AN_OBSERVABLE, obj)
obs => analysis_object_get_observable_ptr (obj)
call observable_init (obs, obs_label, obs_unit, graph_options)
end subroutine analysis_init_observable

<Analysis: public>+≡
public :: analysis_init_histogram

<Analysis: interfaces>+≡
interface analysis_init_histogram
module procedure analysis_init_histogram_n_bins

```

```

    module procedure analysis_init_histogram_bin_width
end interface

```

<Analysis: procedures>+≡

```

subroutine analysis_init_histogram_n_bins &
    (id, lower_bound, upper_bound, n_bins, normalize_bins, &
     obs_label, obs_unit, graph_options, drawing_options)
type(string_t), intent(in) :: id
real(default), intent(in) :: lower_bound, upper_bound
integer, intent(in) :: n_bins
logical, intent(in) :: normalize_bins
type(string_t), intent(in), optional :: obs_label, obs_unit
type(graph_options_t), intent(in), optional :: graph_options
type(drawing_options_t), intent(in), optional :: drawing_options
type(analysis_object_t), pointer :: obj
type(histogram_t), pointer :: h
call analysis_store_init_object (id, AN_HISTOGRAM, obj)
h => analysis_object_get_histogram_ptr (obj)
call histogram_init (h, id, &
    lower_bound, upper_bound, n_bins, normalize_bins, &
    obs_label, obs_unit, graph_options, drawing_options)
end subroutine analysis_init_histogram_n_bins

```

```

subroutine analysis_init_histogram_bin_width &
    (id, lower_bound, upper_bound, bin_width, normalize_bins, &
     obs_label, obs_unit, graph_options, drawing_options)
type(string_t), intent(in) :: id
real(default), intent(in) :: lower_bound, upper_bound, bin_width
logical, intent(in) :: normalize_bins
type(string_t), intent(in), optional :: obs_label, obs_unit
type(graph_options_t), intent(in), optional :: graph_options
type(drawing_options_t), intent(in), optional :: drawing_options
type(analysis_object_t), pointer :: obj
type(histogram_t), pointer :: h
call analysis_store_init_object (id, AN_HISTOGRAM, obj)
h => analysis_object_get_histogram_ptr (obj)
call histogram_init (h, id, &
    lower_bound, upper_bound, bin_width, normalize_bins, &
    obs_label, obs_unit, graph_options, drawing_options)
end subroutine analysis_init_histogram_bin_width

```

<Analysis: public>+≡

```

public :: analysis_init_plot

```

<Analysis: procedures>+≡

```

subroutine analysis_init_plot (id, graph_options, drawing_options)
type(string_t), intent(in) :: id
type(graph_options_t), intent(in), optional :: graph_options
type(drawing_options_t), intent(in), optional :: drawing_options
type(analysis_object_t), pointer :: obj
type(plot_t), pointer :: plot
call analysis_store_init_object (id, AN_PLOT, obj)
plot => analysis_object_get_plot_ptr (obj)
call plot_init (plot, id, graph_options, drawing_options)

```



```

end subroutine analysis_init_plot

<Analysis: public>+≡
public :: analysis_init_graph

<Analysis: procedures>+≡
subroutine analysis_init_graph (id, n_elements, graph_options)
  type(string_t), intent(in) :: id
  integer, intent(in) :: n_elements
  type(graph_options_t), intent(in), optional :: graph_options
  type(analysis_object_t), pointer :: obj
  type(graph_t), pointer :: graph
  call analysis_store_init_object (id, AN_GRAPH, obj)
  graph => analysis_object_get_graph_ptr (obj)
  call graph_init (graph, id, n_elements, graph_options)
end subroutine analysis_init_graph

```

Recording data

This procedure resets an object or the whole store to its initial state.

```

<Analysis: public>+≡
public :: analysis_clear

<Analysis: interfaces>+≡
interface analysis_clear
  module procedure analysis_store_clear_obj
  module procedure analysis_store_clear_all
end interface

<Analysis: procedures>+≡
subroutine analysis_store_clear_obj (id)
  type(string_t), intent(in) :: id
  type(analysis_object_t), pointer :: obj
  obj => analysis_store_get_object_ptr (id)
  if (associated (obj)) then
    call analysis_object_clear (obj)
  end if
end subroutine analysis_store_clear_obj

subroutine analysis_store_clear_all ()
  type(analysis_object_t), pointer :: obj
  obj => analysis_store%first
  do while (associated (obj))
    call analysis_object_clear (obj)
    obj => obj%next
  end do
end subroutine analysis_store_clear_all

```

There is one generic recording function whose behavior depends on the type of analysis object.

```

<Analysis: public>+≡
public :: analysis_record_data

```

<Analysis: procedures>+≡

```

subroutine analysis_record_data (id, x, y, yerr, xerr, &
    weight, excess, success, exist)
    type(string_t), intent(in) :: id
    real(default), intent(in) :: x
    real(default), intent(in), optional :: y, yerr, xerr, weight, excess
    logical, intent(out), optional :: success, exist
    type(analysis_object_t), pointer :: obj
    obj => analysis_store_get_object_ptr (id)
    if (associated (obj)) then
        call analysis_object_record_data (obj, x, y, yerr, xerr, &
            weight, excess, success)
        if (present (exist)) exist = .true.
    else
        if (present (success)) success = .false.
        if (present (exist)) exist = .false.
    end if
end subroutine analysis_record_data

```

Build a graph

This routine sets up the array of graph elements by copying the graph elements given as input. The object must exist and already be initialized as a graph.

<Analysis: public>+≡

```

public :: analysis_fill_graph

```

<Analysis: procedures>+≡

```

subroutine analysis_fill_graph (id, i, id_in, drawing_options)
    type(string_t), intent(in) :: id
    integer, intent(in) :: i
    type(string_t), intent(in) :: id_in
    type(drawing_options_t), intent(in), optional :: drawing_options
    type(analysis_object_t), pointer :: obj
    type(graph_t), pointer :: g
    type(histogram_t), pointer :: h
    type(plot_t), pointer :: p
    obj => analysis_store_get_object_ptr (id)
    g => analysis_object_get_graph_ptr (obj)
    obj => analysis_store_get_object_ptr (id_in)
    if (associated (obj)) then
        select case (obj%type)
        case (AN_HISTOGRAM)
            h => analysis_object_get_histogram_ptr (obj)
            call graph_insert_histogram (g, i, h, drawing_options)
        case (AN_PLOT)
            p => analysis_object_get_plot_ptr (obj)
            call graph_insert_plot (g, i, p, drawing_options)
        case default
            call msg_error ("Graph '" // char (id) // "': Element '" &
                // char (id_in) // "' is neither histogram nor plot.")
        end select
    else
        call msg_error ("Graph '" // char (id) // "': Element '" &

```

```

        // char (id_in) // '' is undefined.")
    end if
end subroutine analysis_fill_graph

```

Retrieve generic results

Check if a named object exists.

```

<Analysis: public>+≡
    public :: analysis_exists

<Analysis: procedures>+≡
    function analysis_exists (id) result (flag)
        type(string_t), intent(in) :: id
        logical :: flag
        type(analysis_object_t), pointer :: obj
        flag = .true.
        obj => analysis_store%first
        do while (associated (obj))
            if (obj%id == id) return
            obj => obj%next
        end do
        flag = .false.
    end function analysis_exists

```

The following functions should work for all kinds of analysis object:

```

<Analysis: public>+≡
    public :: analysis_get_n_elements
    public :: analysis_get_n_entries
    public :: analysis_get_average
    public :: analysis_get_error

<Analysis: procedures>+≡
    function analysis_get_n_elements (id) result (n)
        integer :: n
        type(string_t), intent(in) :: id
        type(analysis_object_t), pointer :: obj
        obj => analysis_store_get_object_ptr (id)
        if (associated (obj)) then
            n = analysis_object_get_n_elements (obj)
        else
            n = 0
        end if
    end function analysis_get_n_elements

    function analysis_get_n_entries (id, within_bounds) result (n)
        integer :: n
        type(string_t), intent(in) :: id
        logical, intent(in), optional :: within_bounds
        type(analysis_object_t), pointer :: obj
        obj => analysis_store_get_object_ptr (id)
        if (associated (obj)) then
            n = analysis_object_get_n_entries (obj, within_bounds)
        else

```

```

        n = 0
    end if
end function analysis_get_n_entries

function analysis_get_average (id, within_bounds) result (avg)
    real(default) :: avg
    type(string_t), intent(in) :: id
    type(analysis_object_t), pointer :: obj
    logical, intent(in), optional :: within_bounds
    obj => analysis_store_get_object_ptr (id)
    if (associated (obj)) then
        avg = analysis_object_get_average (obj, within_bounds)
    else
        avg = 0
    end if
end function analysis_get_average

function analysis_get_error (id, within_bounds) result (err)
    real(default) :: err
    type(string_t), intent(in) :: id
    type(analysis_object_t), pointer :: obj
    logical, intent(in), optional :: within_bounds
    obj => analysis_store_get_object_ptr (id)
    if (associated (obj)) then
        err = analysis_object_get_error (obj, within_bounds)
    else
        err = 0
    end if
end function analysis_get_error

```

Return true if any analysis object is graphical

```

<Analysis: public>+≡
    public :: analysis_has_plots

<Analysis: interfaces>+≡
    interface analysis_has_plots
        module procedure analysis_has_plots_any
        module procedure analysis_has_plots_obj
    end interface

<Analysis: procedures>+≡
    function analysis_has_plots_any () result (flag)
        logical :: flag
        type(analysis_object_t), pointer :: obj
        flag = .false.
        obj => analysis_store%first
        do while (associated (obj))
            flag = analysis_object_has_plot (obj)
            if (flag) return
        end do
    end function analysis_has_plots_any

    function analysis_has_plots_obj (id) result (flag)
        logical :: flag

```

```

type(string_t), dimension(:), intent(in) :: id
type(analysis_object_t), pointer :: obj
integer :: i
flag = .false.
do i = 1, size (id)
  obj => analysis_store_get_object_ptr (id(i))
  if (associated (obj)) then
    flag = analysis_object_has_plot (obj)
    if (flag) return
  end if
end do
end function analysis_has_plots_obj

```

Iterators

Initialize an iterator for the given object. If the object does not exist or has wrong type, the iterator will be invalid.

```

<Analysis: public>+≡
public :: analysis_init_iterator

<Analysis: procedures>+≡
subroutine analysis_init_iterator (id, iterator)
  type(string_t), intent(in) :: id
  type(analysis_iterator_t), intent(out) :: iterator
  type(analysis_object_t), pointer :: obj
  obj => analysis_store_get_object_ptr (id)
  if (associated (obj)) call analysis_iterator_init (iterator, obj)
end subroutine analysis_init_iterator

```

Output

```

<Analysis: public>+≡
public :: analysis_write

<Analysis: interfaces>+≡
interface analysis_write
  module procedure analysis_write_object
  module procedure analysis_write_all
end interface

<Analysis: procedures>+≡
subroutine analysis_write_object (id, unit, verbose)
  type(string_t), intent(in) :: id
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  type(analysis_object_t), pointer :: obj
  obj => analysis_store_get_object_ptr (id)
  if (associated (obj)) then
    call analysis_object_write (obj, unit, verbose)
  else
    call msg_error ("Analysis object '" // char (id) // "' not found")
  end if
end if

```

```

end subroutine analysis_write_object

subroutine analysis_write_all (unit, verbose)
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  type(analysis_object_t), pointer :: obj
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  obj => analysis_store%first
  do while (associated (obj))
    call analysis_object_write (obj, unit, verbose)
    obj => obj%next
  end do
end subroutine analysis_write_all

<Analysis: public>+≡
public :: analysis_write_driver

<Analysis: procedures>+≡
subroutine analysis_write_driver (filename_data, id, unit)
  type(string_t), intent(in) :: filename_data
  type(string_t), dimension(:), intent(in), optional :: id
  integer, intent(in), optional :: unit
  if (present (id)) then
    call analysis_store_write_driver_obj (filename_data, id, unit)
  else
    call analysis_store_write_driver_all (filename_data, unit)
  end if
end subroutine analysis_write_driver

<Analysis: public>+≡
public :: analysis_compile_tex

<Analysis: procedures>+≡
subroutine analysis_compile_tex (file, has_gmlcode, os_data)
  type(string_t), intent(in) :: file
  logical, intent(in) :: has_gmlcode
  type(os_data_t), intent(in) :: os_data
  integer :: status
  if (os_data%event_analysis_ps) then
    call os_system_call ("make compile " // os_data%makeflags // " -f " // &
      char (file) // "_ana.makefile", status)
    if (status /= 0) then
      call msg_error ("Unable to compile analysis output file")
    end if
  else
    call msg_warning ("Skipping results display because " &
      // "latex/mpost/dvips is not available")
  end if
end subroutine analysis_compile_tex

```

Write header for generic data output to an ifile.

```

<Analysis: public>+≡
public :: analysis_get_header

```

```

<Analysis: procedures>+≡
subroutine analysis_get_header (id, header, comment)
  type(string_t), intent(in) :: id
  type(ifile_t), intent(inout) :: header
  type(string_t), intent(in), optional :: comment
  type(analysis_object_t), pointer :: object
  object => analysis_store_get_object_ptr (id)
  if (associated (object)) then
    call analysis_object_get_header (object, header, comment)
  end if
end subroutine analysis_get_header

```

Write a makefile in order to do the compile steps.

```

<Analysis: public>+≡
public :: analysis_write_makefile

<Analysis: procedures>+≡
subroutine analysis_write_makefile (filename, unit, has_gmlcode, os_data)
  type(string_t), intent(in) :: filename
  integer, intent(in) :: unit
  logical, intent(in) :: has_gmlcode
  type(os_data_t), intent(in) :: os_data
  write (unit, "(3A)")  "# WHIZARD: Makefile for analysis '", &
    char (filename), "'"
  write (unit, "(A)")  "# Automatically generated file, do not edit"
  write (unit, "(A)")  ""
  write (unit, "(A)")  "# LaTeX setup"
  write (unit, "(A)")  "LATEX = " // char (os_data%latex)
  write (unit, "(A)")  "MPOST = " // char (os_data%mpost)
  write (unit, "(A)")  "GML = " // char (os_data%gml)
  write (unit, "(A)")  "DVIPS = " // char (os_data%dvips)
  write (unit, "(A)")  "PS2PDF = " // char (os_data%ps2pdf)
  write (unit, "(A)")  'TEX_FLAGS = "$$TEXINPUTS:' // &
    char(os_data%whizard_texpath) // ' "'
  write (unit, "(A)")  'MP_FLAGS = "$$MPINPUTS:' // &
    char(os_data%whizard_texpath) // ' "'
  write (unit, "(A)")  ""
  write (unit, "(5A)")  "TEX_SOURCES = ", char (filename), ".tex"
  if (os_data%event_analysis_pdf) then
    write (unit, "(5A)")  "TEX_OBJECTS = ", char (filename), ".pdf"
  else
    write (unit, "(5A)")  "TEX_OBJECTS = ", char (filename), ".ps"
  end if
  if (os_data%event_analysis_ps) then
    if (os_data%event_analysis_pdf) then
      write (unit, "(5A)")  char (filename), ".pdf: ", &
        char (filename), ".tex"
    else
      write (unit, "(5A)")  char (filename), ".ps: ", &
        char (filename), ".tex"
    end if
  end if
  write (unit, "(5A)")  TAB, "-TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
    char (filename) // ".tex"
  if (has_gmlcode) then

```

```

        write (unit, "(5A)") TAB, "$(GML) " // char (filename)
        write (unit, "(5A)") TAB, "TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
            char (filename) // ".tex"
    end if
    write (unit, "(5A)") TAB, "$(DVIPS) -o " // char (filename) // ".ps " // &
        char (filename) // ".dvi"
    if (os_data%event_analysis_pdf) then
        write (unit, "(5A)") TAB, "$(PS2PDF) " // char (filename) // ".ps"
    end if
end if
write (unit, "(A)")
write (unit, "(A)") "compile: $(TEX_OBJECTS)"
write (unit, "(A)") ".PHONY: compile"
write (unit, "(A)")
write (unit, "(5A)") "CLEAN_OBJECTS = ", char (filename), ".aux"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".log"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".dvi"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".out"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".[1-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".[1-9][0-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".[1-9][0-9][0-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".t[1-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".t[1-9][0-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".t[1-9][0-9][0-9]"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".ltp"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".mp"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".mpx"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".dvi"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".ps"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (filename), ".pdf"
write (unit, "(A)")
write (unit, "(A)") "# Generic cleanup targets"
write (unit, "(A)") "clean-objects:"
write (unit, "(A)") TAB // "rm -f $(CLEAN_OBJECTS)"
write (unit, "(A)") ""
write (unit, "(A)") "clean: clean-objects"
write (unit, "(A)") ".PHONY: clean"
end subroutine analysis_write_makefile

```

13.5.14 Unit tests

Test module, followed by the corresponding implementation module.

<analysis_ut.f90>≡

<File header>

```

module analysis_ut
    use unit_tests
    use analysis_uti

```

<Standard module head>

<Analysis: public test>


```

contains

  <Analysis: test driver>

end module analysis_ut

<analysis_util.f90>≡
  <File header>

  module analysis_util

    <Use kinds>
    <Use strings>
    use format_defs, only: FMT_19

    use analysis

    <Standard module head>

    <Analysis: test declarations>

contains

  <Analysis: tests>

end module analysis_util
API: driver for the unit tests below.
<Analysis: public test>≡
  public :: analysis_test
<Analysis: test driver>≡
  subroutine analysis_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Analysis: execute tests>
  end subroutine analysis_test

<Analysis: execute tests>≡
  call test (analysis_1, "analysis_1", &
    "check elementary analysis building blocks", &
    u, results)
<Analysis: test declarations>≡
  public :: analysis_1
<Analysis: tests>≡
  subroutine analysis_1 (u)
    integer, intent(in) :: u
    type(string_t) :: id1, id2, id3, id4
    integer :: i
    id1 = "foo"
    id2 = "bar"
    id3 = "hist"
    id4 = "plot"

```

```

write (u, "(A)")  "* Test output: Analysis"
write (u, "(A)")  "* Purpose: test the analysis routines"
write (u, "(A)")

call analysis_init_observable (id1)
call analysis_init_observable (id2)
call analysis_init_histogram &
    (id3, 0.5_default, 5.5_default, 1._default, normalize_bins=.false.)
call analysis_init_plot (id4)
do i = 1, 3
    write (u, "(A,1x," // FMT_19 // ")") "data = ", real(i,default)
    call analysis_record_data (id1, real(i,default))
    call analysis_record_data (id2, real(i,default), &
        weight=real(i,default))
    call analysis_record_data (id3, real(i,default))
    call analysis_record_data (id4, real(i,default), real(i,default)**2)
end do
write (u, "(A,10(1x,I5))") "n_entries = ", &
    analysis_get_n_entries (id1), &
    analysis_get_n_entries (id2), &
    analysis_get_n_entries (id3), &
    analysis_get_n_entries (id3, within_bounds = .true.), &
    analysis_get_n_entries (id4), &
    analysis_get_n_entries (id4, within_bounds = .true.)
write (u, "(A,10(1x," // FMT_19 // ")") "average = ", &
    analysis_get_average (id1), &
    analysis_get_average (id2), &
    analysis_get_average (id3), &
    analysis_get_average (id3, within_bounds = .true.)
write (u, "(A,10(1x," // FMT_19 // ")") "error = ", &
    analysis_get_error (id1), &
    analysis_get_error (id2), &
    analysis_get_error (id3), &
    analysis_get_error (id3, within_bounds = .true.)

write (u, "(A)")
write (u, "(A)") "* Clear analysis #2"
write (u, "(A)")

call analysis_clear (id2)
do i = 4, 6
    print *, "data = ", real(i,default)
    call analysis_record_data (id1, real(i,default))
    call analysis_record_data (id2, real(i,default), &
        weight=real(i,default))
    call analysis_record_data (id3, real(i,default))
    call analysis_record_data (id4, real(i,default), real(i,default)**2)
end do
write (u, "(A,10(1x,I5))") "n_entries = ", &
    analysis_get_n_entries (id1), &
    analysis_get_n_entries (id2), &
    analysis_get_n_entries (id3), &
    analysis_get_n_entries (id3, within_bounds = .true.), &

```

```

        analysis_get_n_entries (id4), &
        analysis_get_n_entries (id4, within_bounds = .true.)
write (u, "(A,10(1x," // FMT_19 // "))") "average  = ", &
        analysis_get_average (id1), &
        analysis_get_average (id2), &
        analysis_get_average (id3), &
        analysis_get_average (id3, within_bounds = .true.)
write (u, "(A,10(1x," // FMT_19 // "))") "error    = ", &
        analysis_get_error (id1), &
        analysis_get_error (id2), &
        analysis_get_error (id3), &
        analysis_get_error (id3, within_bounds = .true.)
write (u, "(A)")
call analysis_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call analysis_clear ()
call analysis_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: analysis_1"
end subroutine analysis_1

```

Chapter 14

Matrix Element Handling

In this chapter, we support internal and external matrix elements: initialization, automatic generation where necessary, and numerical evaluation. We provide the interface for code generation and linking. Matrix-element code is organized in processes and process libraries.

process_constants A record of static process properties, for easy transfer between various WHIZARD modules.

prclib_interfaces This module deals with matrix-element code which is accessible via external libraries (Fortran libraries or generic C-compatible libraries) and must either be generated by the program or provided by the user explicitly.

The module defines and uses an abstract type `prc_writer_t` and two abstract extensions, one for a Fortran module and one for a C-compatible library. The implementation provides the specific methods for writing the appropriate parts in external matrix element code.

prc_core_def This module defines the abstract types `prc_core_def_t` and `prc_driver_t`. The implementation of the former provides the configuration for processes of a certain class, while the latter accesses the corresponding matrix element, in particular those generated by the appropriate `prc_writer_t` object.

process_libraries This module combines the functionality of the previous module with the means for holding processes definitions (the internal counterpart of appropriate declarations in the user interface), for handling matrix elements which do not need external code, and for accessing the matrix elements by the procedures for matrix-element evaluation, integration and event generation.

prclib_stacks Collect process libraries.

test_me This module provides a test implementation for the abstract types in the `prc_core_def` module. The implementation is intended for self-tests of several later modules. The implementation is internal, i.e., no external code has is generated.

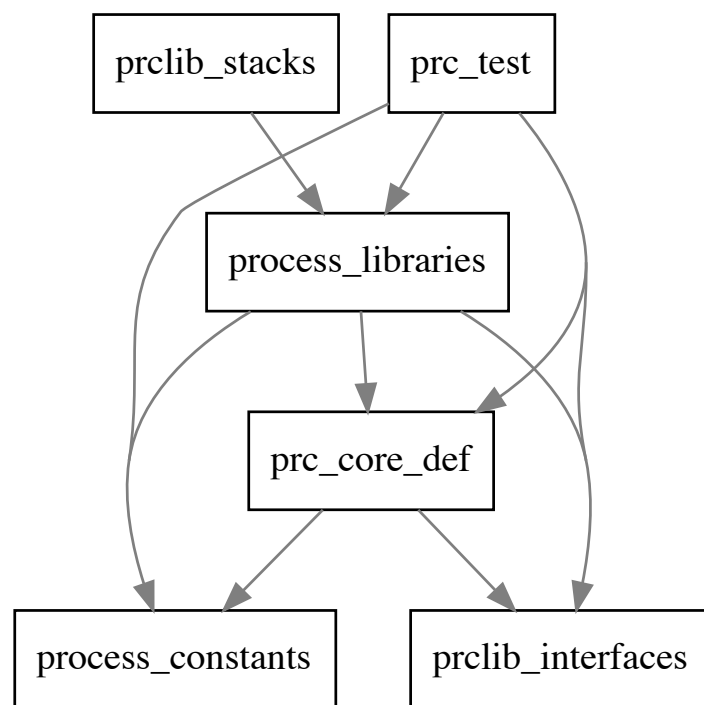


Figure 14.1: Module dependencies in `src/matrix_elements`.

All data structures which are specific for a particular way of generating code or evaluating matrix element are kept abstract and thus generic. Later modules such as `prc_omega` provide implementations, in the form of type extensions for the various abstract types.

14.1 Process data block

We define a simple transparent type that contains universal constant process data. We will reference objects of this type for the phase-space setup, for interfacing with process libraries, for implementing matrix-element generation, and in the master process-handling module.

```

<process_constants.f90>≡
  <File header>

  module process_constants

    <Use kinds>
    <Use strings>

    use io_units, only: given_output_unit, free_unit
    use format_utils, only: write_integer_array
    use md5, only: md5sum

    use pdg_arrays

    <Standard module head>

    <Process Constants: public>

    <Process Constants: types>

    contains

    <Process Constants: procedures>

  end module process_constants

```

The data type is just a block of public objects, only elementary types, no type-bound procedures.

```

<Process Constants: public>≡
  public :: process_constants_t

<Process Constants: types>≡
  type :: process_constants_t
    type(string_t) :: id
    type(string_t) :: model_name
    character(32) :: md5sum = ""
    logical :: openmp_supported = .false.
    integer :: n_in = 0
    integer :: n_out = 0
    integer :: n_flv = 0
    integer :: n_hel = 0
    integer :: n_col = 0
    integer :: n_cin = 0
    integer :: n_cf = 0
    integer, dimension(:,:), allocatable :: flv_state
    integer, dimension(:,:), allocatable :: hel_state
    integer, dimension(:,:), allocatable :: col_state
    logical, dimension(:,:), allocatable :: ghost_flag
    complex(default), dimension(:), allocatable :: color_factors

```

```

        integer, dimension(:,:), allocatable :: cf_index
        integer, dimension(:), allocatable :: eqv_flv_index
        integer, dimension(:), allocatable :: eqv_hel_index
contains
<Process Constants: process constants: TBP>
end type process_constants_t

<Process Constants: process constants: TBP>≡
    procedure :: get_n_tot => process_constants_get_n_tot

<Process Constants: procedures>≡
    elemental function process_constants_get_n_tot (prc_const) result (n_tot)
        integer :: n_tot
        class(process_constants_t), intent(in) :: prc_const
        n_tot = prc_const%n_in + prc_const%n_out
    end function process_constants_get_n_tot

<Process Constants: process constants: TBP>+≡
    procedure :: get_flv_state => process_constants_get_flv_state

<Process Constants: procedures>+≡
    subroutine process_constants_get_flv_state (prc_const, flv_state)
        class(process_constants_t), intent(in) :: prc_const
        integer, dimension(:,:), allocatable, intent(out) :: flv_state
        allocate (flv_state (size (prc_const%flv_state, 1), &
            size (prc_const%flv_state, 2)))
        flv_state = prc_const%flv_state
    end subroutine process_constants_get_flv_state

<Process Constants: process constants: TBP>+≡
    procedure :: get_n_flv => process_constants_get_n_flv

<Process Constants: procedures>+≡
    function process_constants_get_n_flv (data) result (n_flv)
        integer :: n_flv
        class(process_constants_t), intent(in) :: data
        n_flv = data%n_flv
    end function process_constants_get_n_flv

<Process Constants: process constants: TBP>+≡
    procedure :: get_n_hel => process_constants_get_n_hel

<Process Constants: procedures>+≡
    function process_constants_get_n_hel (data) result (n_hel)
        integer :: n_hel
        class(process_constants_t), intent(in) :: data
        n_hel = data%n_hel
    end function process_constants_get_n_hel

<Process Constants: process constants: TBP>+≡
    procedure :: get_hel_state => process_constants_get_hel_state

```



```

(Process Constants: procedures)+≡
  subroutine process_constants_get_hel_state (prc_const, hel_state)
    class(process_constants_t), intent(in) :: prc_const
    integer, dimension(:,:), allocatable, intent(out) :: hel_state
    allocate (hel_state (size (prc_const%hel_state, 1), &
      size (prc_const%hel_state, 2)))
    hel_state = prc_const%hel_state
  end subroutine process_constants_get_hel_state

(Process Constants: process constants: TBP)+≡
  procedure :: get_col_state => process_constants_get_col_state

(Process Constants: procedures)+≡
  subroutine process_constants_get_col_state (prc_const, col_state)
    class(process_constants_t), intent(in) :: prc_const
    integer, dimension(:,:), allocatable, intent(out) :: col_state
    allocate (col_state (size (prc_const%col_state, 1), &
      size (prc_const%col_state, 2), size (prc_const%col_state, 3)))
    col_state = prc_const%col_state
  end subroutine process_constants_get_col_state

(Process Constants: process constants: TBP)+≡
  procedure :: get_ghost_flag => process_constants_get_ghost_flag

(Process Constants: procedures)+≡
  subroutine process_constants_get_ghost_flag (prc_const, ghost_flag)
    class(process_constants_t), intent(in) :: prc_const
    logical, dimension(:,:), allocatable, intent(out) :: ghost_flag
    allocate (ghost_flag (size (prc_const%ghost_flag, 1), &
      size (prc_const%ghost_flag, 2)))
    ghost_flag = prc_const%ghost_flag
  end subroutine process_constants_get_ghost_flag

(Process Constants: process constants: TBP)+≡
  procedure :: get_color_factors => process_constants_get_color_factors

(Process Constants: procedures)+≡
  subroutine process_constants_get_color_factors (prc_const, col_facts)
    class(process_constants_t), intent(in) :: prc_const
    complex(default), dimension(:), allocatable, intent(out) :: col_facts
    allocate (col_facts (size (prc_const%color_factors)))
    col_facts = prc_const%color_factors
  end subroutine process_constants_get_color_factors

(Process Constants: process constants: TBP)+≡
  procedure :: get_cf_index => process_constants_get_cf_index

(Process Constants: procedures)+≡
  subroutine process_constants_get_cf_index (prc_const, cf_index)
    class(process_constants_t), intent(in) :: prc_const
    integer, intent(out), dimension(:), allocatable :: cf_index
    allocate (cf_index (size (prc_const%cf_index, 1), &
      size (prc_const%cf_index, 2)))
    cf_index = prc_const%cf_index

```

```

end subroutine process_constants_get_cf_index

<Process Constants: process constants: TBP>+≡
  procedure :: set_flv_state => process_constants_set_flv_state

<Process Constants: procedures>+≡
  subroutine process_constants_set_flv_state (prc_const, flv_state)
    class(process_constants_t), intent(inout) :: prc_const
    integer, intent(in), dimension(:,:), allocatable :: flv_state
    if (allocated (prc_const%flv_state)) deallocate (prc_const%flv_state)
    allocate (prc_const%flv_state (size (flv_state, 1), &
      size (flv_state, 2)))
    prc_const%flv_state = flv_state
    prc_const%n_flv = size (flv_state, 2)
  end subroutine process_constants_set_flv_state

<Process Constants: process constants: TBP>+≡
  procedure :: set_col_state => process_constants_set_col_state

<Process Constants: procedures>+≡
  subroutine process_constants_set_col_state (prc_const, col_state)
    class(process_constants_t), intent(inout) :: prc_const
    integer, intent(in), dimension(:,:,:), allocatable :: col_state
    allocate (prc_const%col_state (size (col_state, 1), &
      size (col_state, 2), size (col_state, 3)))
    prc_const%col_state = col_state
  end subroutine process_constants_set_col_state

<Process Constants: process constants: TBP>+≡
  procedure :: set_cf_index => process_constants_set_cf_index

<Process Constants: procedures>+≡
  subroutine process_constants_set_cf_index (prc_const, cf_index)
    class(process_constants_t), intent(inout) :: prc_const
    integer, dimension(:,:), intent(in), allocatable :: cf_index
    allocate (prc_const%cf_index (size (cf_index, 1), &
      size (cf_index, 2)))
    prc_const%cf_index = cf_index
  end subroutine process_constants_set_cf_index

<Process Constants: process constants: TBP>+≡
  procedure :: set_color_factors => process_constants_set_color_factors

<Process Constants: procedures>+≡
  subroutine process_constants_set_color_factors (prc_const, color_factors)
    class(process_constants_t), intent(inout) :: prc_const
    complex(default), dimension(:), intent(in), allocatable :: color_factors
    allocate (prc_const%color_factors (size (color_factors)))
    prc_const%color_factors = color_factors
  end subroutine process_constants_set_color_factors

<Process Constants: process constants: TBP>+≡
  procedure :: set_ghost_flag => process_constants_set_ghost_flag

```

```

(Process Constants: procedures)+≡
subroutine process_constants_set_ghost_flag (prc_const, ghost_flag)
  class(process_constants_t), intent(inout) :: prc_const
  logical, dimension(:,:), allocatable, intent(in) :: ghost_flag
  allocate (prc_const%ghost_flag (size (ghost_flag, 1), &
    size (ghost_flag, 2)))
  prc_const%ghost_flag = ghost_flag
end subroutine process_constants_set_ghost_flag

(Process Constants: process constants: TBP)+≡
procedure :: get_pdg_in => process_constants_get_pdg_in

(Process Constants: procedures)+≡
function process_constants_get_pdg_in (prc_const) result (pdg_in)
  type(pdg_array_t), dimension(:), allocatable :: pdg_in
  class(process_constants_t), intent(in) :: prc_const
  type(pdg_array_t) :: pdg_tmp
  integer :: i
  allocate (pdg_in (prc_const%n_in))
  do i = 1, prc_const%n_in
    pdg_tmp = prc_const%flv_state(i,:)
    pdg_in(i) = sort_abs (pdg_tmp, unique = .true.)
  end do
end function process_constants_get_pdg_in

(Process Constants: process constants: TBP)+≡
procedure :: compute_md5sum => process_constants_compute_md5sum

(Process Constants: procedures)+≡
subroutine process_constants_compute_md5sum (prc_const, include_id)
  class(process_constants_t), intent(inout) :: prc_const
  logical, intent(in) :: include_id
  integer :: unit
  unit = prc_const%fill_unit_for_md5sum (include_id)
  rewind (unit)
  prc_const%md5sum = md5sum (unit)
  close (unit)
end subroutine process_constants_compute_md5sum

(Process Constants: process constants: TBP)+≡
procedure :: fill_unit_for_md5sum => process_constants_fill_unit_for_md5sum

(Process Constants: procedures)+≡
function process_constants_fill_unit_for_md5sum (prc_const, include_id) result (unit)
  integer :: unit
  class(process_constants_t), intent(in) :: prc_const
  logical, intent(in) :: include_id
  integer :: i, j, k
  unit = free_unit ()
  open (unit, status="scratch", action="readwrite")
  if (include_id) write (unit, '(A)') char (prc_const%id)
  write (unit, '(A)') char (prc_const%model_name)
  write (unit, '(L1)') prc_const%openmp_supported
  write (unit, '(I0)') prc_const%n_in
  write (unit, '(I0)') prc_const%n_out

```

```

write (unit, '(I0)') prc_const%n_flv
write (unit, '(I0)') prc_const%n_hel
write (unit, '(I0)') prc_const%n_col
write (unit, '(I0)') prc_const%n_cin
write (unit, '(I0)') prc_const%n_cf
do i = 1, size (prc_const%flv_state, dim=1)
  do j = 1, size (prc_const%flv_state, dim=2)
    write (unit, '(I0)') prc_const%flv_state (i, j)
  end do
end do
do i = 1, size (prc_const%hel_state, dim=1)
  do j = 1, size (prc_const%hel_state, dim=2)
    write (unit, '(I0)') prc_const%hel_state (i, j)
  end do
end do
do i = 1, size (prc_const%col_state, dim=1)
  do j = 1, size (prc_const%col_state, dim=2)
    do k = 1, size (prc_const%col_state, dim=3)
      write (unit, '(I0)') prc_const%col_state (i, j, k)
    end do
  end do
end do
do i = 1, size (prc_const%ghost_flag, dim=1)
  do j = 1, size (prc_const%ghost_flag, dim=2)
    write (unit, '(I1)') prc_const%ghost_flag (i, j)
  end do
end do
do i = 1, size (prc_const%color_factors)
  write (unit, '(F0.0,F0.0)') real (prc_const%color_factors(i)), &
    aimag (prc_const%color_factors(i))
end do
do i = 1, size (prc_const%cf_index, dim=1)
  do j = 1, size (prc_const%cf_index, dim=2)
    write (unit, '(I0)') prc_const%cf_index(i, j)
  end do
end do
end function process_constants_fill_unit_for_md5sum

```

(Process Constants: process constants: TBP)+≡

```
procedure :: write => process_constants_write
```

(Process Constants: procedures)+≡

```

subroutine process_constants_write (prc_const, unit)
  class(process_constants_t), intent(in) :: prc_const
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A,A)") "Process data of id: ", char (prc_const%id)
  write (u, "(1x,A,A)") "Associated model: ", char (prc_const%model_name)
  write (u, "(1x,A,I0)") "n_in: ", prc_const%n_in
  write (u, "(1x,A,I0)") "n_out: ", prc_const%n_out
  write (u, "(1x,A,I0)") "n_flv: ", prc_const%n_flv
  write (u, "(1x,A,I0)") "n_hel: ", prc_const%n_hel
  write (u, "(1x,A,I0)") "n_col: ", prc_const%n_col

```

```

write (u, "(1x,A,I0)") "n_cin: ", prc_const%n_cin
write (u, "(1x,A,I0)") "n_cf: ", prc_const%n_cf
write (u, "(1x,A)") "Flavors: "
do i = 1, prc_const%n_flv
  write (u, "(1x,A,I0)") "i_flv: ", i
  call write_integer_array (prc_const%flv_state (:,i))
end do
end subroutine process_constants_write

```

14.2 Process library interface

The module `prclib_interfaces` handles external matrix-element code.

14.2.1 Overview

The top-level data structure is the `prclib_driver_t` data type. The associated type-bound procedures deal with the generation of external code, compilation and linking, and accessing the active external library.

An object of type `prclib_driver_t` consists of the following parts:

1. Metadata that identify name and status of the library driver, etc.
2. An array of process records (`prclib_driver_record_t`), one for each external matrix element.
3. A record of type `dlaccess_t` which handles the operating-system part of linking a dynamically loadable library.
4. A collection of procedure pointers which have a counterpart in the external library interface. Given the unique identifier of a matrix element, the procedures retrieve generic matrix-element information such as the particle content and helicity combination tables. There is also a procedure which returns pointers to the more specific procedures that a matrix element provides, called *features*.

The process records of type `prclib_driver_record_t` handle the individual matrix elements. Each record identifies a process by name (`id`), names the physics model to be loaded for this process, lists the features that the associated matrix-element code provides, and holds a `writer` object which handles all operations that depend on the process type. The numbering of process records is identical to the numbering of matrix-element codes in the external library.

The writer object is of abstract type `prc_writer_t`. The module defines two basic, also abstract, extensions: `prc_writer_f_module_t` and `prc_writer_c_lib_t`. The first version is for matrix-element code that is available in form of Fortran modules. The writer contains type-bound procedures which create appropriate `use` directives and C-compatible wrapper functions for the given set of Fortran modules and their features. The second version is for matrix-element code that is available in form of a C-compatible library (this includes Fortran libraries with proper C bindings). The writer needs not write wrapper function, but explicit interface blocks for the matrix-element features.

Each matrix-element variant is encoded in an appropriate extension of `prc_writer_t`. For instance, O’MEGA matrix elements provide an implementation `omega_writer_t` which extends `prc_writer_f_module_t`.

14.2.2 Workflow

We expect that the functionality provided by this module is called in the following order:

1. The caller initializes the `prclib_driver_t` object and fills the array of `prclib_record_t` entries with the appropriate process data and process-specific writer objects.
2. It calls the `generate_makefile` method to set up an appropriate makefile in the current directory. The makefile will handle source generation, compilation and linking both for the individual matrix elements (unless this has to be done manually) and for the common external driver code which interfaces those matrix element.
3. The `generate_driver_code` writes the common driver as source code to file.
4. The methods `make_source`, `make_compile`, and `make_link` individually perform the corresponding steps in building the library. Wherever possible, they simply use the generated makefile. By calling `make`, we make sure that we can avoid unnecessary recompilation. For the compilation and linking steps, the makefile will employ `libtool`.
5. The `load` method loads the library procedures into the corresponding procedure pointers, using the `dlopen` mechanism via the `dlaccess` subobject.

14.2.3 The module

```

<prclib_interfaces.f90>≡
  <File header>

  module prclib_interfaces

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use io_units
    use system_defs, only: TAB
    use string_utils, only: lower_case
    use diagnostics
    use os_interface

    <Standard module head>

    <Prclib interfaces: public>

    <Prclib interfaces: types>

```

```

    <Prclib interfaces: interfaces>

contains

    <Prclib interfaces: procedures>

end module prclib_interfaces

```

14.2.4 Writers

External matrix element code provides externally visible procedures, which we denote as *features*. The features consist of informational subroutines and functions which are mandatory (universal features) and matrix-element specific subroutines and functions (specific features). The driver interfaces the generic features directly, while it returns the specific features in form of bind(C) procedure pointers to the caller. For instance, function `n_in` is generic, while the matrix matrix-element value itself is specific.

To implement these tasks, the driver needs `use` directives for Fortran module procedures, interface blocks for other external stuff, wrapper code, and Makefile snippets.

Generic writer

In the `prc_writer_t` data type, we collect the procedures which implement the writing tasks. The type is abstract. The concrete implementations are defined by an extension which is specific for the process type.

The MD5 sum stored here should be the MD5 checksum of the current process component, which can be calculated once the process is configured completely. It can be used by implementations which work with external files, such as O'MEGA.

```

    <Prclib interfaces: public>≡
        public :: prc_writer_t

    <Prclib interfaces: types>≡
        type, abstract :: prc_writer_t
            character(32) :: md5sum = ""
        contains
            <Prclib interfaces: prc writer: TBP>
        end type prc_writer_t

```

In any case, it is useful to have a string representation of the writer type. This must be implemented by all extensions.

```

    <Prclib interfaces: prc writer: TBP>≡
        procedure(get_const_string), nopass, deferred :: type_name

    <Prclib interfaces: interfaces>≡
        abstract interface
            function get_const_string () result (string)
                import
                type(string_t) :: string
            end function get_const_string

```

```
end interface
```

Return the name of a procedure that implements a given feature, as it is provided by the external matrix-element code. For a reasonable default, we take the feature name unchanged.

```
<Prclib interfaces: prc writer: TBP>+≡
  procedure, nopass :: get_procname => prc_writer_get_procname

<Prclib interfaces: procedures>≡
  function prc_writer_get_procname (feature) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: feature
    name = feature
  end function prc_writer_get_procname
```

Return the name of a procedure that implements a given feature with the bind(C) property, so it can be accessed via a C procedure pointer and handled by dlopen. We need this for all special features of a matrix element, since the interface has to return a C function pointer for it. For a default implementation, we prefix the external procedure name by the process ID.

```
<Prclib interfaces: prc writer: TBP>+≡
  procedure :: get_c_procname => prc_writer_get_c_procname

<Prclib interfaces: procedures>+≡
  function prc_writer_get_c_procname (writer, id, feature) result (name)
    class(prc_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id, feature
    type(string_t) :: name
    name = id // "_" // feature
  end function prc_writer_get_c_procname
```

Common signature of code-writing procedures. The procedure may use the process ID, and the feature name. (Not necessarily all of them.)

```
<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine write_code_file (writer, id)
      import
      class(prc_writer_t), intent(in) :: writer
      type(string_t), intent(in) :: id
    end subroutine write_code_file
  end interface

  abstract interface
    subroutine write_code (writer, unit, id)
      import
      class(prc_writer_t), intent(in) :: writer
      integer, intent(in) :: unit
      type(string_t), intent(in) :: id
    end subroutine write_code
  end interface

  abstract interface
```



```

subroutine write_code_os &
  (writer, unit, id, os_data, verbose, testflag)
  import
  class(prc_writer_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  type(os_data_t), intent(in) :: os_data
  logical, intent(in) :: verbose
  logical, intent(in), optional :: testflag
end subroutine write_code_os
end interface

abstract interface
  subroutine write_feature_code (writer, unit, id, feature)
    import
    class(prc_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
  end subroutine write_feature_code
end interface

```

There must be a procedure which writes an interface block for a given feature. If the external matrix element is implemented as a Fortran module, this is required only for the specific features which are returned as procedure pointers.

```

<Prclib interfaces: prc writer: TBP>+≡
  procedure(write_feature_code), deferred :: write_interface

```

There must also be a procedure which writes Makefile code which is specific for the current process, but not the feature.

```

<Prclib interfaces: prc writer: TBP>+≡
  procedure(write_code_os), deferred :: write_makefile_code

```

This procedure writes code process-specific source-code file (which need not be Fortran). It is called before `make source` is called. It may be a no-op, if the source code is generated by Make instead.

```

<Prclib interfaces: prc writer: TBP>+≡
  procedure(write_code_file), deferred :: write_source_code

```

This procedure is executed, once for each process, before (after) `make compile` is called, respectively.

```

<Prclib interfaces: prc writer: TBP>+≡
  procedure(write_code_file), deferred :: before_compile
  procedure(write_code_file), deferred :: after_compile

```

Writer for Fortran-module matrix elements

If the matrix element is available as a Fortran module, we have specific requirements: (i) the features are imported via `use` directives, (ii) the specific features require `bind(C)` wrappers.

The type is still abstract, all methods must be implemented explicitly for a specific matrix-element variant.

```

<Prclib interfaces: public>+≡
  public :: prc_writer_f_module_t

```

```

<Prclib interfaces: types>+≡
  type, extends (prc_writer_t), abstract :: prc_writer_f_module_t
  contains
    <Prclib interfaces: prc writer f module: TBP>
  end type prc_writer_f_module_t

```

Return the name of the Fortran module. As a default implementation, we take the process ID unchanged.

```

<Prclib interfaces: prc writer f module: TBP>≡
  procedure, nopass :: get_module_name => prc_writer_get_module_name

<Prclib interfaces: procedures>+≡
  function prc_writer_get_module_name (id) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: id
    name = id
  end function prc_writer_get_module_name

```

Write a use directive that associates the driver reference with the procedure in the matrix element code. By default, we use the C name for this.

```

<Prclib interfaces: prc writer f module: TBP>+≡
  procedure :: write_use_line => prc_writer_write_use_line

<Prclib interfaces: procedures>+≡
  subroutine prc_writer_write_use_line (writer, unit, id, feature)
    class(prc_writer_f_module_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t) :: id, feature
    write (unit, "(2x,9A)") "use ", char (writer%get_module_name (id)), &
      ", only: ", char (writer%get_c_procname (id, feature)), &
      " => ", char (writer%get_procname (feature))
  end subroutine prc_writer_write_use_line

```

Write a wrapper routine for a feature. This also associates a C name the module procedure. The details depend on the writer variant.

```

<Prclib interfaces: prc writer f module: TBP>+≡
  procedure(prc_write_wrapper), deferred :: write_wrapper

<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine prc_write_wrapper (writer, unit, id, feature)
      import
      class(prc_writer_f_module_t), intent(in) :: writer
      integer, intent(in) :: unit
      type(string_t), intent(in) :: id, feature
    end subroutine prc_write_wrapper
  end interface

```

This is used for testing only: initialize the writer with a specific MD5 sum string.

```

<Prclib interfaces: prc writer: TBP>+≡
  procedure :: init_test => prc_writer_init_test

```

```

<Prclib interfaces: procedures>+≡
  subroutine prc_writer_init_test (writer)
    class(prc_writer_t), intent(out) :: writer
    writer%md5sum = "1234567890abcdef1234567890abcdef"
  end subroutine prc_writer_init_test

```

Writer for C-library matrix elements

This applies if the matrix element is available as a C library or a Fortran library with `bind(C)` compatible interface. We can use the basic version.

The type is still abstract, all methods must be implemented explicitly for a specific matrix-element variant.

```

<Prclib interfaces: public>+≡
  public :: prc_writer_c_lib_t

<Prclib interfaces: types>+≡
  type, extends (prc_writer_t), abstract :: prc_writer_c_lib_t
  contains
    <Prclib interfaces: prc writer c lib: TBP>
  end type prc_writer_c_lib_t

```

14.2.5 Process records in the library driver

A process record holds the process (component) ID, the physics `model_name`, and the array of `features` that are implemented by the corresponding matrix element code.

The `writer` component holds procedures. The procedures write source code for the current record, either for the driver or for the Makefile.

```

<Prclib interfaces: types>+≡
  type :: prclib_driver_record_t
    type(string_t) :: id
    type(string_t) :: model_name
    type(string_t), dimension(:), allocatable :: feature
    class(prc_writer_t), pointer :: writer => null ()
  contains
    <Prclib interfaces: prclib driver record: TBP>
  end type prclib_driver_record_t

```

Output routine. We indent the output, so it smoothly integrates into the output routine for the whole driver.

Note: the pointer `writer` is introduced as a workaround for a NAG compiler bug.

```

<Prclib interfaces: prclib driver record: TBP>≡
  procedure :: write => prclib_driver_record_write

<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_record_write (object, unit)
    class(prclib_driver_record_t), intent(in) :: object
    integer, intent(in) :: unit
    integer :: j

```

```

class(prc_writer_t), pointer :: writer
write (unit, "(3x,A,2x,[' ,A,'])") &
    char (object%id), char (object%model_name)
if (allocated (object%feature)) then
    writer => object%writer
    write (unit, "(5x,A,A)", advance="no") &
        char (writer%type_name ()), ":"
    do j = 1, size (object%feature)
        write (unit, "(1x,A)", advance="no") &
            char (object%feature(j))
    end do
    write (unit, *)
end if
end subroutine prclib_driver_record_write

```

Get the C procedure name for a feature.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: get_c_procname => prclib_driver_record_get_c_procname

<Prclib interfaces: procedures>+≡
    function prclib_driver_record_get_c_procname (record, feature) result (name)
        type(string_t) :: name
        class(prclib_driver_record_t), intent(in) :: record
        type(string_t), intent(in) :: feature
        name = record%writer%get_c_procname (record%id, feature)
    end function prclib_driver_record_get_c_procname

```

Write a USE directive for a given feature. Applies only if the record corresponds to a Fortran module.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_use_line => prclib_driver_record_write_use_line

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_record_write_use_line (record, unit, feature)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        type(string_t), intent(in) :: feature
        select type (writer => record%writer)
            class is (prc_writer_f_module_t)
                call writer%write_use_line (unit, record%id, feature)
            end select
    end subroutine prclib_driver_record_write_use_line

```

The alternative: write an interface block for a given feature, unless the record corresponds to a Fortran module.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_interface => prclib_driver_record_write_interface

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_record_write_interface (record, unit, feature)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        type(string_t), intent(in) :: feature
    end subroutine prclib_driver_record_write_interface

```

```

select type (writer => record%writer)
class is (prc_writer_f_module_t)
class default
    call writer%write_interface (unit, record%id, feature)
end select
end subroutine prclib_driver_record_write_interface

```

Write all special feature interfaces for the current record. Do this for all process variants.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_interfaces => prclib_driver_record_write_interfaces

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_record_write_interfaces (record, unit)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        integer :: i
        do i = 1, size (record%feature)
            call record%writer%write_interface (unit, record%id, record%feature(i))
        end do
    end subroutine prclib_driver_record_write_interfaces

```

Write the wrapper routines for this record, if it corresponds to a Fortran module.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_wrappers => prclib_driver_record_write_wrappers

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_record_write_wrappers (record, unit)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        integer :: i
        select type (writer => record%writer)
        class is (prc_writer_f_module_t)
            do i = 1, size (record%feature)
                call writer%write_wrapper (unit, record%id, record%feature(i))
            end do
        end select
    end subroutine prclib_driver_record_write_wrappers

```

Write the Makefile code for this record.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_makefile_code => prclib_driver_record_write_makefile_code

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_record_write_makefile_code &
        (record, unit, os_data, verbose, testflag)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: testflag
        call record%writer%write_makefile_code &
            (unit, record%id, os_data, verbose, testflag)
    end subroutine

```

```
end subroutine prclib_driver_record_write_makefile_code
```

Write source-code files for this record. This can be used as an alternative to handling source code via Makefile. In fact, this procedure is executed before `make source` is called. Usually, does nothing.

```
<Prclib interfaces: prclib driver record: TBP>+≡
  procedure :: write_source_code => prclib_driver_record_write_source_code

<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_record_write_source_code (record)
    class(prclib_driver_record_t), intent(in) :: record
    call record%writer%write_source_code (record%id)
  end subroutine prclib_driver_record_write_source_code
```

Execute commands for this record that depend on the sources, so they cannot be included in the previous procedure. This procedure is executed before (after) `make compile` is called, respectively. Usually, does nothing.

```
<Prclib interfaces: prclib driver record: TBP>+≡
  procedure :: before_compile => prclib_driver_record_before_compile
  procedure :: after_compile => prclib_driver_record_after_compile

<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_record_before_compile (record)
    class(prclib_driver_record_t), intent(in) :: record
    call record%writer%before_compile (record%id)
  end subroutine prclib_driver_record_before_compile

  subroutine prclib_driver_record_after_compile (record)
    class(prclib_driver_record_t), intent(in) :: record
    call record%writer%after_compile (record%id)
  end subroutine prclib_driver_record_after_compile
```

14.2.6 The process library driver object

A `prclib_driver_t` object provides the interface to external matrix element code. The code is provided by an external library which is either statically or dynamically linked.

The dynamic and static versions of the library are two different implementations of the abstract base type.

The `basename` identifies the library, both by file names and by Fortran variable names.

The `loaded` flag becomes true once all procedure pointers to the matrix element have been assigned.

For a dynamical external library, the communication proceeds via a `dlaccess` object.

`n_processes` is the number of external process code components that are referenced by this library. The code is addressed by index (`i.lib` in the process library entry above). This number should be equal to the number returned by `get_n_prc`.

For each external process, there is a separate **record** which holds the data that are needed for the driver parts which are specific for a given process component. The actual pointers for the loaded library will be assigned elsewhere.

The remainder is a collection of procedure pointers, which can be assigned once all external code has been compiled and linked. The procedure pointers all take a process component code index as an argument. Most return information about the process component that should match the process definition. The **get_fptr** procedures return a function pointer, which is the actual means to compute matrix elements or retrieve associated data.

Finally, the **unload_hook** and **reload_hook** pointers allow for the insertion of additional code when a library is loaded.

```

<Prclib interfaces: public>+≡
    public :: prclib_driver_t

<Prclib interfaces: types>+≡
    type, abstract :: prclib_driver_t
        type(string_t) :: basename
        character(32) :: md5sum = ""
        logical :: loaded = .false.
        type(string_t) :: libname
        type(string_t) :: modellibs_ldflags
        integer :: n_processes = 0
        type(prclib_driver_record_t), dimension(:), allocatable :: record
        procedure(prc_get_n_processes), nopass, pointer :: &
            get_n_processes => null ()
        procedure(prc_get_stringptr), nopass, pointer :: &
            get_process_id_ptr => null ()
        procedure(prc_get_stringptr), nopass, pointer :: &
            get_model_name_ptr => null ()
        procedure(prc_get_stringptr), nopass, pointer :: &
            get_md5sum_ptr => null ()
        procedure(prc_get_log), nopass, pointer :: &
            get_omp_status => null ()
        procedure(prc_get_int), nopass, pointer :: get_n_in => null ()
        procedure(prc_get_int), nopass, pointer :: get_n_out => null ()
        procedure(prc_get_int), nopass, pointer :: get_n_flv => null ()
        procedure(prc_get_int), nopass, pointer :: get_n_hel => null ()
        procedure(prc_get_int), nopass, pointer :: get_n_col => null ()
        procedure(prc_get_int), nopass, pointer :: get_n_cin => null ()
        procedure(prc_get_int), nopass, pointer :: get_n_cf => null ()
        procedure(prc_set_int_tab1), nopass, pointer :: &
            set_flv_state_ptr => null ()
        procedure(prc_set_int_tab1), nopass, pointer :: &
            set_hel_state_ptr => null ()
        procedure(prc_set_col_state), nopass, pointer :: &
            set_col_state_ptr => null ()
        procedure(prc_set_color_factors), nopass, pointer :: &
            set_color_factors_ptr => null ()
        procedure(prc_get_fptr), nopass, pointer :: get_fptr => null ()
    contains
    <Prclib interfaces: prclib driver: TBP>
end type prclib_driver_t

```

This is the dynamic version. It contains a `dlaccess` object for communicating with the OS.

```

<Prclib interfaces: public>+≡
    public :: prclib_driver_dynamic_t
<Prclib interfaces: types>+≡
    type, extends (prclib_driver_t) :: prclib_driver_dynamic_t
        type(dlaccess_t) :: dlaccess
    contains
        <Prclib interfaces: prclib driver dynamic: TBP>
    end type prclib_driver_dynamic_t

```

Print just the metadata. Procedure pointers cannot be printed.

```

<Prclib interfaces: prclib driver: TBP>≡
    procedure :: write => prclib_driver_write
<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_write (object, unit, libpath)
        class(prclib_driver_t), intent(in) :: object
        integer, intent(in) :: unit
        logical, intent(in), optional :: libpath
        logical :: write_lib
        integer :: i
        write_lib = .true.
        if (present (libpath)) write_lib = libpath
        write (unit, "(1x,A,A)") &
            "External matrix-element code library: ", char (object%basename)
        select type (object)
        type is (prclib_driver_dynamic_t)
            write (unit, "(3x,A,L1)") "static      = F"
        class default
            write (unit, "(3x,A,L1)") "static      = T"
        end select
        write (unit, "(3x,A,L1)") "loaded       = ", object%loaded
        write (unit, "(3x,A,A,A)") "MD5 sum      = '", object%md5sum, "'"
        if (write_lib) then
            write (unit, "(3x,A,A,A)") "Mdl flags = '", &
                char (object%modellibs_ldflags), "'"
        end if
        select type (object)
        type is (prclib_driver_dynamic_t)
            write (unit, *)
            call object%dlaccess%write (unit)
        end select
        write (unit, *)
        if (allocated (object%record)) then
            write (unit, "(1x,A)") "Matrix-element code entries:"
            do i = 1, object%n_processes
                call object%record(i)%write (unit)
            end do
        else
            write (unit, "(1x,A)") "Matrix-element code entries: [undefined]"
        end if
    end subroutine prclib_driver_write

```


Allocate a library as either static or dynamic. For static libraries, the procedure defers control to an external procedure which knows about the available static libraries. By default, this procedure is empty, but when we build a stand-alone executable, we replace the dummy by an actual dispatcher for the available static libraries. If the static dispatcher was not successful, we allocate a dynamic library.

The default version of `dispatch_prclib_static` resides in the `prebuilt` section of the `WHIZARD` tree, in a separate library. It does nothing, but can be replaced by a different procedure that allocates a static library driver if requested by name.

```

<Prclib interfaces: public>+≡
    public :: dispatch_prclib_driver

<Prclib interfaces: procedures>+≡
    subroutine dispatch_prclib_driver &
        (driver, basename, modellibs_ldflags)
        class(prclib_driver_t), intent(out), allocatable :: driver
        type(string_t), intent(in) :: basename
        type(string_t), intent(in), optional :: modellibs_ldflags
        procedure(dispatch_prclib_driver) :: dispatch_prclib_static
        if (allocated (driver)) deallocate (driver)
        call dispatch_prclib_static (driver, basename)
        if (.not. allocated (driver)) then
            allocate (prclib_driver_dynamic_t :: driver)
        end if
        driver%basename = basename
        driver%modellibs_ldflags = modellibs_ldflags
    end subroutine dispatch_prclib_driver

```

Initialize the ID array and set `n_processes` accordingly.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: init => prclib_driver_init

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_init (driver, n_processes)
        class(prclib_driver_t), intent(inout) :: driver
        integer, intent(in) :: n_processes
        driver%n_processes = n_processes
        allocate (driver%record (n_processes))
    end subroutine prclib_driver_init

```

Set the MD5 sum. This is separate because the MD5 sum may be known only after initialization.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: set_md5sum => prclib_driver_set_md5sum

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_set_md5sum (driver, md5sum)
        class(prclib_driver_t), intent(inout) :: driver
        character(32), intent(in) :: md5sum
        driver%md5sum = md5sum
    end subroutine prclib_driver_set_md5sum

```

Set the process record for a specific library entry. If the index is zero, we do nothing.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: set_record => prclib_driver_set_record
<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_set_record (driver, i, &
    id, model_name, features, writer)
    class(prclib_driver_t), intent(inout) :: driver
    integer, intent(in) :: i
    type(string_t), intent(in) :: id
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: features
    class(prc_writer_t), intent(in), pointer :: writer
    if (i > 0) then
      associate (record => driver%record(i))
        record%id = id
        record%model_name = model_name
        allocate (record%feature (size (features)))
        record%feature = features
        record%writer => writer
      end associate
    end if
  end subroutine prclib_driver_set_record

```

Write all USE directives for a given feature, scanning the array of processes. Only Fortran-module processes count. Then, write interface blocks for the remaining processes.

The implicit none statement must go in-between.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_interfaces => prclib_driver_write_interfaces
<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_write_interfaces (driver, unit, feature)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: feature
    integer :: i
    do i = 1, driver%n_processes
      call driver%record(i)%write_use_line (unit, feature)
    end do
    write (unit, "(2x,9A)") "implicit none"
    do i = 1, driver%n_processes
      call driver%record(i)%write_interface (unit, feature)
    end do
  end subroutine prclib_driver_write_interfaces

```

14.2.7 Write makefile

The makefile contains constant parts, parts that depend on the library name, and parts that depend on the specific processes and their types.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: generate_makefile => prclib_driver_generate_makefile

```

(Prclib interfaces: procedures)+≡

```

subroutine prclib_driver_generate_makefile (driver, unit, os_data, verbose, testflag)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(os_data_t), intent(in) :: os_data
  logical, intent(in) :: verbose
  logical, intent(in), optional :: testflag
  integer :: i
  write (unit, "(A)") "# WHIZARD: Makefile for process library '" &
    // char (driver%basename) // "'"
  write (unit, "(A)") "# Automatically generated file, do not edit"
  write (unit, "(A)") ""
  write (unit, "(A)") "# Integrity check (don't modify the following line!)"
  write (unit, "(A)") "MD5SUM = '" // driver%md5sum // "'"
  write (unit, "(A)") ""
  write (unit, "(A)") "# Library name"
  write (unit, "(A)") "BASE = " // char (driver%basename)
  write (unit, "(A)") ""
  write (unit, "(A)") "# Compiler"
  write (unit, "(A)") "FC = " // char (os_data%fc)
  write (unit, "(A)") "CC = " // char (os_data%cc)
  write (unit, "(A)") ""
  write (unit, "(A)") "# Included libraries"
  write (unit, "(A)") "FCINCL = " // char (os_data%whizard_includes)
  write (unit, "(A)") ""
  write (unit, "(A)") "# Compiler flags"
  write (unit, "(A)") "FCFLAGS = " // char (os_data%fcflags)
  write (unit, "(A)") "FCFLAGS_PIC = " // char (os_data%fcflags_pic)
  write (unit, "(A)") "CFLAGS = " // char (os_data%cflags)
  write (unit, "(A)") "CFLAGS_PIC = " // char (os_data%cflags_pic)
  write (unit, "(A)") "LDFLAGS = " // char (os_data%whizard_ldflags) &
    // " " // char (os_data%ldflags) // " " // &
    char (driver%modellibs_ldflags)
  write (unit, "(A)") ""
  write (unit, "(A)") "# LaTeX setup"
  write (unit, "(A)") "LATEX = " // char (os_data%latex)
  write (unit, "(A)") "MPOST = " // char (os_data%mpost)
  write (unit, "(A)") "DVIPS = " // char (os_data%dvips)
  write (unit, "(A)") "PS2PDF = " // char (os_data%ps2pdf)
  write (unit, "(A)") 'TEX_FLAGS = "$$TEXINPUTS:' // &
    char(os_data%whizard_texpath) // "'"
  write (unit, "(A)") 'MP_FLAGS = "$$MPINPUTS:' // &
    char(os_data%whizard_texpath) // "'"
  write (unit, "(A)") ""
  write (unit, "(A)") "# Libtool"
  write (unit, "(A)") "LIBTOOL = " // char (os_data%whizard_libtool)
  if (verbose) then
    write (unit, "(A)") "FCOMPILE = $(LIBTOOL) --tag=FC --mode=compile"
    write (unit, "(A)") "CCOMPILE = $(LIBTOOL) --tag=CC --mode=compile"
    write (unit, "(A)") "LINK = $(LIBTOOL) --tag=FC --mode=link"
  else
    write (unit, "(A)") "FCOMPILE = @$(LIBTOOL) --silent --tag=FC --mode=compile"
    write (unit, "(A)") "CCOMPILE = @$(LIBTOOL) --silent --tag=CC --mode=compile"
    write (unit, "(A)") "LINK = @$(LIBTOOL) --silent --tag=FC --mode=link"
  end if
end subroutine

```

```

end if
write (unit, "(A)") ""
write (unit, "(A)") "# Compile commands (default)"
write (unit, "(A)") "LTF_COMPILE = $(FC_COMPILE) $(FC) -c &
    &$(FC_INCL) $(FC_FLAGS) $(FC_FLAGS_PIC)"
write (unit, "(A)") "LTCC_COMPILE = $(CC_COMPILE) $(CC) -c &
    &$(C_FLAGS) $(C_FLAGS_PIC)"
write (unit, "(A)") ""
write (unit, "(A)") "# Default target"
write (unit, "(A)") "all: link diags"
write (unit, "(A)") ""
write (unit, "(A)") "# Matrix-element code files"
do i = 1, size (driver%record)
    call driver%record(i)%write_makefile_code (unit, os_data, verbose, testflag)
end do
write (unit, "(A)") ""
write (unit, "(A)") "# Library driver"
write (unit, "(A)") "$(BASE).lo: $(BASE).f90 $(OBJECTS)"
write (unit, "(A)") TAB // "$(LTF_COMPILE) $<"
if (.not. verbose) then
    write (unit, "(A)") TAB // '@echo " FC          " $@"
end if
write (unit, "(A)") ""
write (unit, "(A)") "# Library"
write (unit, "(A)") "$(BASE).la: $(BASE).lo $(OBJECTS)"
if (.not. verbose) then
    write (unit, "(A)") TAB // '@echo " FCLD          " $@"
end if
write (unit, "(A)") TAB // "$(LINK) $(FC) -module -rpath /dev/null &
    &$(FC_FLAGS) $(LD_FLAGS) -o $(BASE).la $"
write (unit, "(A)") ""
write (unit, "(A)") "# Main targets"
write (unit, "(A)") "link: compile $(BASE).la"
write (unit, "(A)") "compile: source $(OBJECTS) $(TEX_OBJECTS) $(BASE).lo"
write (unit, "(A)") "compile_tex: $(TEX_OBJECTS)"
write (unit, "(A)") "source: $(SOURCES) $(BASE).f90 $(TEX_SOURCES)"
write (unit, "(A)") ".PHONY: link diags compile compile_tex source"
write (unit, "(A)") ""
write (unit, "(A)") "# Specific cleanup targets"
do i = 1, size (driver%record)
    write (unit, "(A)") "clean-" // char (driver%record(i)%id) // ":"
    write (unit, "(A)") ".PHONY: clean-" // char (driver%record(i)%id)
end do
write (unit, "(A)") ""
write (unit, "(A)") "# Generic cleanup targets"
write (unit, "(A)") "clean-library:"
if (verbose) then
    write (unit, "(A)") TAB // "rm -f $(BASE).la"
else
    write (unit, "(A)") TAB // '@echo " RM          $(BASE).la"'
    write (unit, "(A)") TAB // "@rm -f $(BASE).la"
end if
write (unit, "(A)") "clean-objects:"
if (verbose) then

```

```

        write (unit, "(A)") TAB // "rm -f $(BASE).lo $(BASE)_driver.mod &
            &$(CLEAN_OBJECTS)"
    else
        write (unit, "(A)") TAB // '@echo " RM          $(BASE).lo &
            &$(BASE)_driver.mod $(CLEAN_OBJECTS)"'
        write (unit, "(A)") TAB // "@rm -f $(BASE).lo $(BASE)_driver.mod &
            &$(CLEAN_OBJECTS)"
    end if
    write (unit, "(A)") "clean-source:"
    if (verbose) then
        write (unit, "(A)") TAB // "rm -f $(CLEAN_SOURCES)"
    else
        write (unit, "(A)") TAB // '@echo " RM          $(CLEAN_SOURCES)"'
        write (unit, "(A)") TAB // "@rm -f $(CLEAN_SOURCES)"
    end if
    write (unit, "(A)") "clean-driver:"
    if (verbose) then
        write (unit, "(A)") TAB // "rm -f $(BASE).f90"
    else
        write (unit, "(A)") TAB // '@echo " RM          $(BASE).f90"'
        write (unit, "(A)") TAB // "@rm -f $(BASE).f90"
    end if
    write (unit, "(A)") "clean-makefile:"
    if (verbose) then
        write (unit, "(A)") TAB // "rm -f $(BASE).makefile"
    else
        write (unit, "(A)") TAB // '@echo " RM          $(BASE).makefile"'
        write (unit, "(A)") TAB // "@rm -f $(BASE).makefile"
    end if
    write (unit, "(A)") ".PHONY: clean-library clean-objects &
        &clean-source clean-driver clean-makefile"
    write (unit, "(A)") ""
    write (unit, "(A)") "clean: clean-library clean-objects clean-source"
    write (unit, "(A)") "distclean: clean clean-driver clean-makefile"
    write (unit, "(A)") ".PHONY: clean distclean"
end subroutine prclib_driver_generate_makefile

```

14.2.8 Write driver file

This procedure writes the process library driver source code to the specified output unit. The individual routines for writing source-code procedures are given below.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: generate_driver_code => prclib_driver_generate_code

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_generate_code (driver, unit)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(string_t) :: prefix
        integer :: i

        prefix = driver%basename // "_"

```

```

write (unit, "(A)")  "! WHIZARD matrix-element code interface"
write (unit, "(A)")  "!"
write (unit, "(A)")  "! Automatically generated file, do not edit"
call driver%write_module (unit, prefix)
call driver%write_lib_md5sum_fun (unit, prefix)
call driver%write_get_n_processes_fun (unit, prefix)
call driver%write_get_process_id_fun (unit, prefix)
call driver%write_get_model_name_fun (unit, prefix)
call driver%write_get_md5sum_fun (unit, prefix)
call driver%write_string_to_array_fun (unit, prefix)
call driver%write_get_openmp_status_fun (unit, prefix)
call driver%write_get_int_fun (unit, prefix, var_str ("n_in"))
call driver%write_get_int_fun (unit, prefix, var_str ("n_out"))
call driver%write_get_int_fun (unit, prefix, var_str ("n_flv"))
call driver%write_get_int_fun (unit, prefix, var_str ("n_hel"))
call driver%write_get_int_fun (unit, prefix, var_str ("n_col"))
call driver%write_get_int_fun (unit, prefix, var_str ("n_cin"))
call driver%write_get_int_fun (unit, prefix, var_str ("n_cf"))
call driver%write_set_int_sub (unit, prefix, var_str ("flv_state"))
call driver%write_set_int_sub (unit, prefix, var_str ("hel_state"))
call driver%write_set_col_state_sub (unit, prefix)
call driver%write_set_color_factors_sub (unit, prefix)
call driver%write_get_fptr_sub (unit, prefix)
do i = 1, driver%n_processes
    call driver%record(i)%write_wrappers (unit)
end do
end subroutine prclib_driver_generate_code

```

The driver module is used and required *only* if we intend to link the library statically. Then, it provides the (static) driver type as a concrete implementation of the abstract library driver. This type contains the internal dispatcher for assigning the library procedures to their appropriate procedure pointers. In the dynamical case, the assignment is done via the base-type dispatcher which invokes the DL mechanism.

However, compiling this together with the rest in any case should not do any harm.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure, nopass :: write_module => prclib_driver_write_module

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_write_module (unit, prefix)
        integer, intent(in) :: unit
        type(string_t), intent(in) :: prefix
        write (unit, "(A)")  ""
        write (unit, "(A)")  "! Module: define library driver as an extension &
            &of the abstract driver type."
        write (unit, "(A)")  "! This is used _only_ by the library dispatcher &
            &of a static executable."
        write (unit, "(A)")  "! For a dynamical library, the stand-alone proce&
            &dures are linked via libdl."
        write (unit, "(A)")  ""
        write (unit, "(A)")  "module " &

```

```

        // char (prefix) // "driver"
write (unit, "(A)") " use iso_c_binding"
write (unit, "(A)") " use iso_varying_string, string_t => varying_string"
write (unit, "(A)") " use diagnostics"
write (unit, "(A)") " use prclib_interfaces"
write (unit, "(A)") ""
write (unit, "(A)") " implicit none"
write (unit, "(A)") ""
write (unit, "(A)") " type, extends (prclib_driver_t) :: " &
        // char (prefix) // "driver_t"
write (unit, "(A)") " contains"
write (unit, "(A)") " procedure :: get_c_funptr => " &
        // char (prefix) // "driver_get_c_funptr"
write (unit, "(A)") " end type " &
        // char (prefix) // "driver_t"
write (unit, "(A)") ""
write (unit, "(A)") "contains"
write (unit, "(A)") ""
write (unit, "(A)") " function " &
        // char (prefix) // "driver_get_c_funptr (driver, feature) result &
        &(c_funptr)"
write (unit, "(A)") " class(" &
        // char (prefix) // "driver_t), intent(inout) :: driver"
write (unit, "(A)") " type(string_t), intent(in) :: feature"
write (unit, "(A)") " type(c_funptr) :: c_funptr"
call write_decl ("get_n_processes", "get_n_processes")
call write_decl ("get_stringptr", "get_process_id_ptr")
call write_decl ("get_stringptr", "get_model_name_ptr")
call write_decl ("get_stringptr", "get_md5sum_ptr")
call write_decl ("get_log", "get_openmp_status")
call write_decl ("get_int", "get_n_in")
call write_decl ("get_int", "get_n_out")
call write_decl ("get_int", "get_n_flv")
call write_decl ("get_int", "get_n_hel")
call write_decl ("get_int", "get_n_col")
call write_decl ("get_int", "get_n_cin")
call write_decl ("get_int", "get_n_cf")
call write_decl ("set_int_tab1", "set_flv_state_ptr")
call write_decl ("set_int_tab1", "set_hel_state_ptr")
call write_decl ("set_col_state", "set_col_state_ptr")
call write_decl ("set_color_factors", "set_color_factors_ptr")
call write_decl ("get_funptr", "get_funptr")
write (unit, "(A)") " select case (char (feature))"
call write_case ("get_n_processes")
call write_case ("get_process_id_ptr")
call write_case ("get_model_name_ptr")
call write_case ("get_md5sum_ptr")
call write_case ("get_openmp_status")
call write_case ("get_n_in")
call write_case ("get_n_out")
call write_case ("get_n_flv")
call write_case ("get_n_hel")
call write_case ("get_n_col")
call write_case ("get_n_cin")

```

```

call write_case ("get_n_cf")
call write_case ("set_flv_state_ptr")
call write_case ("set_hel_state_ptr")
call write_case ("set_col_state_ptr")
call write_case ("set_color_factors_ptr")
call write_case ("get_fp_ptr")
write (unit, "(A)") "      case default"
write (unit, "(A)") "          call msg_bug ('prclib2 driver setup: unknown &
          &function name')"
write (unit, "(A)") "      end select"
write (unit, "(A)") "      end function " &
// char (prefix) // "driver_get_c_fun_ptr"
write (unit, "(A)") ""
write (unit, "(A)") "end module " &
// char (prefix) // "driver"
write (unit, "(A)") ""
write (unit, "(A)") "! Stand-alone external procedures: used for both &
&static and dynamic linkage"
contains
subroutine write_decl (template, feature)
character(*), intent(in) :: template, feature
write (unit, "(A)") "      procedure(prc_" // template // ") &"
write (unit, "(A)") "          :: " &
// char (prefix) // feature
end subroutine write_decl
subroutine write_case (feature)
character(*), intent(in) :: feature
write (unit, "(A)") "      case ('' // feature // '')"
write (unit, "(A)") "          c_fp_ptr = c_funloc (" &
// char (prefix) // feature // ")"
end subroutine write_case
end subroutine prclib_driver_write_module

```

This function provides the overall library MD5sum. The function is for internal use (therefore not bind(C)), the external interface is via the `get_md5sum_ptr` procedure with index 0.

<Prclib interfaces: prclib driver: TBP>+≡

```

procedure :: write_lib_md5sum_fun => prclib_driver_write_lib_md5sum_fun

```

<Prclib interfaces: procedures>+≡

```

subroutine prclib_driver_write_lib_md5sum_fun (driver, unit, prefix)
class(prclib_driver_t), intent(in) :: driver
integer, intent(in) :: unit
type(string_t), intent(in) :: prefix
write (unit, "(A)") ""
write (unit, "(A)") "! The MD5 sum of the library"
write (unit, "(A)") "function " // char (prefix) &
// "md5sum () result (md5sum)"
write (unit, "(A)") "      implicit none"
write (unit, "(A)") "      character(32) :: md5sum"
write (unit, "(A)") "      md5sum = '' // driver%md5sum // ''"
write (unit, "(A)") "end function " // char (prefix) // "md5sum"
end subroutine prclib_driver_write_lib_md5sum_fun

```


14.2.9 Interface bodies for informational functions

These interfaces implement the communication between WHIZARD (the main program) and the process-library driver. The procedures are all BIND(C), so they can safely be exposed by the library and handled by the `dlopen` mechanism, which apparently understands only C calling conventions.

In the sections below, for each procedure, we provide both the interface itself and a procedure that writes the corresponding procedure as source code to the process library driver.

Process count

Return the number of processes contained in the library.

```
<Prclib interfaces: public>+≡
    public :: prc_get_n_processes

<Prclib interfaces: interfaces>+≡
    abstract interface
        function prc_get_n_processes () result (n) bind(C)
            import
                integer(c_int) :: n
            end function prc_get_n_processes
    end interface
```

Here is the code.

```
<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: write_get_n_processes_fun

<Prclib interfaces: procedures>+≡
    subroutine write_get_n_processes_fun (driver, unit, prefix)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(string_t), intent(in) :: prefix
        write (unit, "(A)") ""
        write (unit, "(A)") "! Return the number of processes in this library"
        write (unit, "(A)") "function " // char (prefix) &
            // "get_n_processes () result (n) bind(C)"
        write (unit, "(A)") " use iso_c_binding"
        write (unit, "(A)") " implicit none"
        write (unit, "(A)") " integer(c_int) :: n"
        write (unit, "(A,I0)") " n = ", driver%n_processes
        write (unit, "(A)") "end function " // char (prefix) &
            // "get_n_processes"
    end subroutine write_get_n_processes_fun
```

Informational string functions

These functions return constant information about the matrix-element code.

The following procedures have to return strings. With the BIND(C) constraint, we choose to return the C pointer to a string, and its length, so the procedures implement this interface. They are actually subroutines.

```
<Prclib interfaces: public>+≡
    public :: prc_get_stringptr
```

```

<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine prc_get_stringptr (i, cptr, len) bind(C)
      import
      integer(c_int), intent(in) :: i
      type(c_ptr), intent(out) :: cptr
      integer(c_int), intent(out) :: len
    end subroutine prc_get_stringptr
  end interface

```

To hide this complication, we introduce a subroutine that converts the returned C pointer to a `string_t` object. As a side effect, we deallocate the original after conversion – otherwise, we might have a memory leak.

For the conversion, we first pointer-convert the C pointer to a Fortran character array pointer, length 1 and size `len`. Using argument association and an internal subroutine, we convert this to a character array with length `len` and size 1. Using ordinary assignment, we finally convert this to `string_t`.

The function takes the pointer-returning function as an argument. The index `i` identifies the process in the library.

```

<Prclib interfaces: procedures>+≡
  subroutine get_string_via_cptr (string, i, get_stringptr)
    type(string_t), intent(out) :: string
    integer, intent(in) :: i
    procedure(prc_get_stringptr) :: get_stringptr
    type(c_ptr) :: cptr
    integer(c_int) :: pid, len
    character(kind=c_char), dimension(:), pointer :: c_array
    pid = i
    call get_stringptr (pid, cptr, len)
    if (c_associated (cptr)) then
      call c_f_pointer (cptr, c_array, shape = [len])
      call set_string (c_array)
      call get_stringptr (0_c_int, cptr, len)
    else
      string = ""
    end if
  contains
    subroutine set_string (buffer)
      character(len, kind=c_char), dimension(1), intent(in) :: buffer
      string = buffer(1)
    end subroutine set_string
  end subroutine get_string_via_cptr

```

Since the module procedures return Fortran strings, we have to convert them. This is the necessary auxiliary routine. The routine is not `BIND(C)`, it is not accessed from outside.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure, nopass :: write_string_to_array_fun

<Prclib interfaces: procedures>+≡
  subroutine write_string_to_array_fun (unit, prefix)
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix

```

```

write (unit, "(A)") ""
write (unit, "(A)") "! Auxiliary: convert character string &
&to array pointer"
write (unit, "(A)") "subroutine " // char (prefix) &
// "string_to_array (string, a)"
write (unit, "(A)") " use iso_c_binding"
write (unit, "(A)") " implicit none"
write (unit, "(A)") " character(*), intent(in) :: string"
write (unit, "(A)") " character(kind=c_char), dimension(:), &
&allocatable, intent(out) :: a"
write (unit, "(A)") " integer :: i"
write (unit, "(A)") " allocate (a (len (string)))"
write (unit, "(A)") " do i = 1, size (a)"
write (unit, "(A)") " a(i) = string(i:i)"
write (unit, "(A)") " end do"
write (unit, "(A)") "end subroutine " // char (prefix) &
// "string_to_array"
end subroutine write_string_to_array_fun

```

The above routine is called by other functions. It is not in a module, so they need its interface explicitly.

```

<Prclib interfaces: procedures>+≡
subroutine write_string_to_array_interface (unit, prefix)
integer, intent(in) :: unit
type(string_t), intent(in) :: prefix
write (unit, "(2x,A)") "interface"
write (unit, "(2x,A)") " subroutine " // char (prefix) &
// "string_to_array (string, a)"
write (unit, "(2x,A)") " use iso_c_binding"
write (unit, "(2x,A)") " implicit none"
write (unit, "(2x,A)") " character(*), intent(in) :: string"
write (unit, "(2x,A)") " character(kind=c_char), dimension(:), &
&allocatable, intent(out) :: a"
write (unit, "(2x,A)") " end subroutine " // char (prefix) &
// "string_to_array"
write (unit, "(2x,A)") "end interface"
end subroutine write_string_to_array_interface

```

Here are the info functions which return strings, implementing the interface `prc_get_stringptr`.

Return the process ID for each process.

```

<Prclib interfaces: prclib driver: TBP>+≡
procedure :: write_get_process_id_fun

<Prclib interfaces: procedures>+≡
subroutine write_get_process_id_fun (driver, unit, prefix)
class(prclib_driver_t), intent(in) :: driver
integer, intent(in) :: unit
type(string_t), intent(in) :: prefix
integer :: i
write (unit, "(A)") ""
write (unit, "(A)") "! Return the process ID of process #i &
&(as a C pointer to a character array)"

```

```

write (unit, "(A)") "subroutine " // char (prefix) &
// "get_process_id_ptr (i, cptr, len) bind(C)"
write (unit, "(A)") " use iso_c_binding"
write (unit, "(A)") " implicit none"
write (unit, "(A)") " integer(c_int), intent(in) :: i"
write (unit, "(A)") " type(c_ptr), intent(out) :: cptr"
write (unit, "(A)") " integer(c_int), intent(out) :: len"
write (unit, "(A)") " character(kind=c_char), dimension(:), &
&allocatable, target, save :: a"
call write_string_to_array_interface (unit, prefix)
write (unit, "(A)") " select case (i)"
write (unit, "(A)") " case (0); if (allocated (a)) deallocate (a)"
do i = 1, driver%n_processes
write (unit, "(A,I0,9A)") " case (" , i, ")"; " , &
"call " , char (prefix), "string_to_array ('", &
char (driver%record(i)%id), "'", a)"
end do
write (unit, "(A)") " end select"
write (unit, "(A)") " if (allocated (a)) then"
write (unit, "(A)") " cptr = c_loc (a)"
write (unit, "(A)") " len = size (a)"
write (unit, "(A)") " else"
write (unit, "(A)") " cptr = c_null_ptr"
write (unit, "(A)") " len = 0"
write (unit, "(A)") " end if"
write (unit, "(A)") "end subroutine " // char (prefix) &
// "get_process_id_ptr"
end subroutine write_get_process_id_fun

```

Return the model name, given explicitly.

<Prclib interfaces: prclib driver: TBP>+≡

```
procedure :: write_get_model_name_fun
```

<Prclib interfaces: procedures>+≡

```

subroutine write_get_model_name_fun (driver, unit, prefix)
class(prclib_driver_t), intent(in) :: driver
integer, intent(in) :: unit
type(string_t), intent(in) :: prefix
integer :: i
write (unit, "(A)") ""
write (unit, "(A)") "! Return the model name for process #i &
&(as a C pointer to a character array)"
write (unit, "(A)") "subroutine " // char (prefix) &
// "get_model_name_ptr (i, cptr, len) bind(C)"
write (unit, "(A)") " use iso_c_binding"
write (unit, "(A)") " implicit none"
write (unit, "(A)") " integer(c_int), intent(in) :: i"
write (unit, "(A)") " type(c_ptr), intent(out) :: cptr"
write (unit, "(A)") " integer(c_int), intent(out) :: len"
write (unit, "(A)") " character(kind=c_char), dimension(:), &
&allocatable, target, save :: a"
call write_string_to_array_interface (unit, prefix)
write (unit, "(A)") " select case (i)"
write (unit, "(A)") " case (0); if (allocated (a)) deallocate (a)"

```

```

do i = 1, driver%n_processes
  write (unit, "(A,I0,9A)") " case (" , i, ")"; " , &
    "call ", char (prefix), "string_to_array ('" , &
      char (driver%record(i)%model_name), &
        "'", a)"
end do
write (unit, "(A)") " end select"
write (unit, "(A)") " if (allocated (a)) then"
write (unit, "(A)") "   cptr = c_loc (a)"
write (unit, "(A)") "   len = size (a)"
write (unit, "(A)") " else"
write (unit, "(A)") "   cptr = c_null_ptr"
write (unit, "(A)") "   len = 0"
write (unit, "(A)") " end if"
write (unit, "(A)") "end subroutine " // char (prefix) &
  // "get_model_name_ptr"
end subroutine write_get_model_name_fun

```

Call the MD5 sum function for the process. The function calls the corresponding function of the matrix-element code, and it returns the C address of a character array with length 32.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_get_md5sum_fun

<Prclib interfaces: procedures>+≡
  subroutine write_get_md5sum_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    integer :: i
    write (unit, "(A)") ""
    write (unit, "(A)") "! Return the MD5 sum for the process configuration &
      &(as a C pointer to a character array)"
    write (unit, "(A)") "subroutine " // char (prefix) &
      // "get_md5sum_ptr (i, cptr, len) bind(C)"
    write (unit, "(A)") " use iso_c_binding"
    call driver%write_interfaces (unit, var_str ("md5sum"))
    write (unit, "(A)") " interface"
    write (unit, "(A)") "   function " // char (prefix) &
      // "md5sum () result (md5sum)"
    write (unit, "(A)") "     character(32) :: md5sum"
    write (unit, "(A)") "     end function " // char (prefix) // "md5sum"
    write (unit, "(A)") " end interface"
    write (unit, "(A)") " integer(c_int), intent(in) :: i"
    write (unit, "(A)") " type(c_ptr), intent(out) :: cptr"
    write (unit, "(A)") " integer(c_int), intent(out) :: len"
    write (unit, "(A)") " character(kind=c_char), dimension(32), &
      &target, save :: md5sum"
    write (unit, "(A)") " select case (i)"
    write (unit, "(A)") " case (0)"
    write (unit, "(A)") "   call copy (" // char (prefix) // "md5sum ())"
    write (unit, "(A)") "   cptr = c_loc (md5sum)"
    do i = 1, driver%n_processes
      write (unit, "(A,I0,9A)") " case (" , i, ")"

```

```

        call driver%record(i)%write_md5sum_call (unit)
    end do
    write (unit, "(A)") "   case default"
    write (unit, "(A)") "       cptr = c_null_ptr"
    write (unit, "(A)") "   end select"
    write (unit, "(A)") "   len = 32"
    write (unit, "(A)") "contains"
    write (unit, "(A)") "   subroutine copy (md5sum_tmp)"
    write (unit, "(A)") "       character, dimension(32), intent(in) :: &
        &md5sum_tmp"
    write (unit, "(A)") "       md5sum = md5sum_tmp"
    write (unit, "(A)") "   end subroutine copy"
    write (unit, "(A)") "end subroutine " // char (prefix) &
        // "get_md5sum_ptr"
end subroutine write_get_md5sum_fun

```

The actual call depends on the type of matrix element.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_md5sum_call => prclib_driver_record_write_md5sum_call

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_record_write_md5sum_call (record, unit)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        call record%writer%write_md5sum_call (unit, record%id)
    end subroutine prclib_driver_record_write_md5sum_call

```

The interface goes into the writer base type:

```

<Prclib interfaces: prc writer: TBP>+≡
    procedure(write_code), deferred :: write_md5sum_call

```

In the Fortran module case, we take a detour. The string returned by the Fortran function is copied into a fixed-size array. The copy routine is an internal subroutine of `get_md5sum_ptr`. We return the C address of the target array.

```

<Prclib interfaces: prc writer f module: TBP>+≡
    procedure :: write_md5sum_call => prc_writer_f_module_write_md5sum_call

<Prclib interfaces: procedures>+≡
    subroutine prc_writer_f_module_write_md5sum_call (writer, unit, id)
        class(prc_writer_f_module_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        write (unit, "(5x,9A)") "call copy (", &
            char (writer%get_c_procname (id, var_str ("md5sum"))), " ()"
        write (unit, "(5x,9A)") "cptr = c_loc (md5sum)"
    end subroutine prc_writer_f_module_write_md5sum_call

```

In the C library case, the library function returns a C pointer, which we can just copy.

```

<Prclib interfaces: prc writer c lib: TBP>≡
    procedure :: write_md5sum_call => prc_writer_c_lib_write_md5sum_call

```

```

<Prclib interfaces: procedures>+≡
subroutine prc_writer_c_lib_write_md5sum_call (writer, unit, id)
  class(prc_writer_c_lib_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  write (unit, "(5x,9A)") &
    "cptr = ", &
    char (writer%get_c_procname (id, var_str ("get_md5sum"))), " ()"
end subroutine prc_writer_c_lib_write_md5sum_call

```

Actual references to the info functions

The string-valued info functions return C character arrays. For the API of the library driver, we provide convenience functions which (re)convert those arrays into `string_t` objects.

```

<Prclib interfaces: prclib driver: TBP>+≡
procedure :: get_process_id => prclib_driver_get_process_id
procedure :: get_model_name => prclib_driver_get_model_name
procedure :: get_md5sum => prclib_driver_get_md5sum

<Prclib interfaces: procedures>+≡
function prclib_driver_get_process_id (driver, i) result (string)
  type(string_t) :: string
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: i
  call get_string_via_cptr (string, i, driver%get_process_id_ptr)
end function prclib_driver_get_process_id

function prclib_driver_get_model_name (driver, i) result (string)
  type(string_t) :: string
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: i
  call get_string_via_cptr (string, i, driver%get_model_name_ptr)
end function prclib_driver_get_model_name

function prclib_driver_get_md5sum (driver, i) result (string)
  type(string_t) :: string
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: i
  call get_string_via_cptr (string, i, driver%get_md5sum_ptr)
end function prclib_driver_get_md5sum

```

Informational logical functions

When returning a logical value, we use the C boolean type, which may differ from Fortran.

```

<Prclib interfaces: public>+≡
public :: prc_get_log

```

```

<Prclib interfaces: interfaces>+≡
  abstract interface
    function prc_get_log (pid) result (l) bind(C)
      import
        integer(c_int), intent(in) :: pid
        logical(c_bool) :: l
      end function prc_get_log
  end interface

```

Return a logical flag which tells whether OpenMP is supported for a specific process code.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_get_openmp_status_fun

<Prclib interfaces: procedures>+≡
  subroutine write_get_openmp_status_fun (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    integer :: i
    write (unit, "(A)") ""
    write (unit, "(A)") "! Return the OpenMP support status"
    write (unit, "(A)") "function " // char (prefix) &
      // "get_openmp_status (i) result (openmp_status) bind(C)"
    write (unit, "(A)") " use iso_c_binding"
    call driver%write_interfaces (unit, var_str ("openmp_supported"))
    write (unit, "(A)") " integer(c_int), intent(in) :: i"
    write (unit, "(A)") " logical(c_bool) :: openmp_status"
    write (unit, "(A)") " select case (i)"
    do i = 1, driver%n_processes
      write (unit, "(A,I0,9A)") " case (" , i, "); ", &
        "openmp_status = ", &
        char (driver%record(i)%get_c_procname &
          (var_str ("openmp_supported"))), " ()"
    end do
    write (unit, "(A)") " end select"
    write (unit, "(A)") "end function " // char (prefix) &
      // "get_openmp_status"
  end subroutine write_get_openmp_status_fun

```

Informational integer functions

Various process metadata are integer values. We can use a single interface for all of them.

```

<Prclib interfaces: public>+≡
  public :: prc_get_int

<Prclib interfaces: interfaces>+≡
  abstract interface
    function prc_get_int (pid) result (n) bind(C)
      import
        integer(c_int), intent(in) :: pid
        integer(c_int) :: n
      end function prc_get_int
  end interface

```


end interface

This function returns any data of type integer, for each process.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_get_int_fun
<Prclib interfaces: procedures>+≡
  subroutine write_get_int_fun (driver, unit, prefix, feature)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    type(string_t), intent(in) :: feature
    integer :: i
    write (unit, "(A)") ""
    write (unit, "(9A)") "! Return the value of ", char (feature)
    write (unit, "(9A)") "function ", char (prefix), &
      "get-", char (feature), " (pid)", &
      " result (" , char (feature), ") bind(C)"
    write (unit, "(9A)") " use iso_c_binding"
    call driver%write_interfaces (unit, feature)
    write (unit, "(9A)") " integer(c_int), intent(in) :: pid"
    write (unit, "(9A)") " integer(c_int) :: ", char (feature)
    write (unit, "(9A)") " select case (pid)"
    do i = 1, driver%n_processes
      write (unit, "(2x,A,I0,9A)") "case (" , i, "); ", &
        char (feature), " = ", &
        char (driver%record(i)%get_c_procname (feature)), &
        " ()"
    end do
    write (unit, "(9A)") " end select"
    write (unit, "(9A)") "end function ", char (prefix), &
      "get-", char (feature)
  end subroutine write_get_int_fun

```

Write a `case` line that assigns the value of the external function to the current return value.

```

<Prclib interfaces: procedures>+≡
  subroutine write_case_int_fun (record, unit, i, feature)
    class(prclib_driver_record_t), intent(in) :: record
    integer, intent(in) :: unit
    integer, intent(in) :: i
    type(string_t), intent(in) :: feature
    write (unit, "(5x,A,I0,9A)") "case (" , i, "); ", &
      char (feature), " = ", char (record%get_c_procname (feature))
  end subroutine write_case_int_fun

```

Flavor and helicity tables

Transferring tables is more complicated. First, a two-dimensional array.

```

<Prclib interfaces: public>+≡
  public :: prc_set_int_tab1

```

```

<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine prc_set_int_tab1 (pid, tab, shape) bind(C)
      import
        integer(c_int), intent(in) :: pid
        integer(c_int), dimension(*), intent(out) :: tab
        integer(c_int), dimension(2), intent(in) :: shape
      end subroutine prc_set_int_tab1
  end interface

```

This subroutine returns a table of integers.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_set_int_sub

<Prclib interfaces: procedures>+≡
  subroutine write_set_int_sub (driver, unit, prefix, feature)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    type(string_t), intent(in) :: feature
    integer :: i
    write (unit, "(A)") ""
    write (unit, "(9A)") "! Set table: ", char (feature)
    write (unit, "(9A)") "subroutine ", char (prefix), &
      "set_", char (feature), "_ptr (pid, ", char (feature), &
      ", shape) bind(C)"
    write (unit, "(9A)") " use iso_c_binding"
    call driver%write_interfaces (unit, feature)
    write (unit, "(9A)") " integer(c_int), intent(in) :: pid"
    write (unit, "(9A)") " integer(c_int), dimension(*), intent(out) :: ", &
      char (feature)
    write (unit, "(9A)") " integer(c_int), dimension(2), intent(in) :: shape"
    write (unit, "(9A)") " integer, dimension(:,,:), allocatable :: ", &
      char (feature), "_tmp"
    write (unit, "(9A)") " integer :: i, j"
    write (unit, "(9A)") " select case (pid)"
    do i = 1, driver%n_processes
      write (unit, "(2x,A,IO,A)") "case (", i, ")"
      call driver%record(i)%write_int_sub_call (unit, feature)
    end do
    write (unit, "(9A)") " end select"
    write (unit, "(9A)") "end subroutine ", char (prefix), &
      "set_", char (feature), "_ptr"
  end subroutine write_set_int_sub

```

The actual call depends on the type of matrix element.

```

<Prclib interfaces: prclib driver record: TBP>+≡
  procedure :: write_int_sub_call => prclib_driver_record_write_int_sub_call

<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_record_write_int_sub_call (record, unit, feature)
    class(prclib_driver_record_t), intent(in) :: record
    integer, intent(in) :: unit
    type(string_t), intent(in) :: feature
    call record%writer%write_int_sub_call (unit, record%id, feature)

```

```
end subroutine prclib_driver_record_write_int_sub_call
```

The interface goes into the writer base type:

```
<Prclib interfaces: prc writer: TBP>+≡
```

```
procedure(write_feature_code), deferred :: write_int_sub_call
```

In the Fortran module case, we need an extra copy in the (academical) situation where default integer and `c_int` differ. Otherwise, we just associate a Fortran array with the C pointer and let the matrix-element subroutine fill the array.

```
<Prclib interfaces: prc writer f module: TBP>+≡
```

```
procedure :: write_int_sub_call => prc_writer_f_module_write_int_sub_call
```

```
<Prclib interfaces: procedures>+≡
```

```
subroutine prc_writer_f_module_write_int_sub_call (writer, unit, id, feature)
  class(prc_writer_f_module_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, "(5x,9A)") "allocate (", char (feature), "_tmp ", &
    "(shape(1), shape(2)))"
  write (unit, "(5x,9A)") "call ", &
    char (writer%get_c_procname (id, feature)), &
    " (", char (feature), "_tmp)"
  write (unit, "(5x,9A)") "forall (i=1:shape(1), j=1:shape(2)) "
  write (unit, "(8x,9A)") char (feature), "(i + shape(1)*(j-1)) = ", &
    char (feature), "_tmp", "(i,j)"
  write (unit, "(5x,9A)") "end forall"
end subroutine prc_writer_f_module_write_int_sub_call
```

In the C library case, we just transfer the C pointer to the library function.

```
<Prclib interfaces: prc writer c lib: TBP>+≡
```

```
procedure :: write_int_sub_call => prc_writer_c_lib_write_int_sub_call
```

```
<Prclib interfaces: procedures>+≡
```

```
subroutine prc_writer_c_lib_write_int_sub_call (writer, unit, id, feature)
  class(prc_writer_c_lib_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, "(5x,9A)") "call ", &
    char (writer%get_c_procname (id, feature)), " (", char (feature), ")"
end subroutine prc_writer_c_lib_write_int_sub_call
```

Color state table

The color-state specification needs a table of integers (one array per color flow) and a corresponding array of color-ghost flags.

```
<Prclib interfaces: public>+≡
```

```
public :: prc_set_col_state
```

```
<Prclib interfaces: interfaces>+≡
```

```
abstract interface
```

```
subroutine prc_set_col_state (pid, col_state, ghost_flag, shape) bind(C)
```

```
import
```

```
integer(c_int), intent(in) :: pid
```

```

        integer(c_int), dimension(*), intent(out) :: col_state
        logical(c_bool), dimension(*), intent(out) :: ghost_flag
        integer(c_int), dimension(3), intent(in) :: shape
    end subroutine prc_set_col_state
end interface

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: write_set_col_state_sub

<Prclib interfaces: procedures>+≡
    subroutine write_set_col_state_sub (driver, unit, prefix)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: unit
        type(string_t), intent(in) :: prefix
        integer :: i
        type(string_t) :: feature
        feature = "col_state"
        write (unit, "(A)") ""
        write (unit, "(9A)") "! Set tables: col_state, ghost_flag"
        write (unit, "(9A)") "subroutine ", char (prefix), &
            "set_col_state_ptr (pid, col_state, ghost_flag, shape) bind(C)"
        write (unit, "(9A)") " use iso_c_binding"
        call driver%write_interfaces (unit, feature)
        write (unit, "(9A)") " integer(c_int), intent(in) :: pid"
        write (unit, "(9A)") &
            " integer(c_int), dimension(*), intent(out) :: col_state"
        write (unit, "(9A)") &
            " logical(c_bool), dimension(*), intent(out) :: ghost_flag"
        write (unit, "(9A)") &
            " integer(c_int), dimension(3), intent(in) :: shape"
        write (unit, "(9A)") &
            " integer, dimension(:, :, :), allocatable :: col_state_tmp"
        write (unit, "(9A)") &
            " logical, dimension(:, :, :), allocatable :: ghost_flag_tmp"
        write (unit, "(9A)") " integer :: i, j, k"
        write (unit, "(A)") " select case (pid)"
        do i = 1, driver%n_processes
            write (unit, "(A,I0,A)") " case (" , i, ")"
            call driver%record(i)%write_col_state_call (unit)
        end do
        write (unit, "(A)") " end select"
        write (unit, "(9A)") "end subroutine ", char (prefix), &
            "set_col_state_ptr"
    end subroutine write_set_col_state_sub

```

The actual call depends on the type of matrix element.

```

<Prclib interfaces: prclib driver record: TBP>+≡
    procedure :: write_col_state_call => prclib_driver_record_write_col_state_call

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_record_write_col_state_call (record, unit)
        class(prclib_driver_record_t), intent(in) :: record
        integer, intent(in) :: unit
        call record%writer%write_col_state_call (unit, record%id)
    end subroutine prclib_driver_record_write_col_state_call

```

The interface goes into the writer base type:

```
<Prclib interfaces: prc writer: TBP>+≡
```

```
    procedure(write_code), deferred :: write_col_state_call
```

In the Fortran module case, we need an extra copy in the (academical) situation where default integer and `c_int` differ. Otherwise, we just associate a Fortran array with the C pointer and let the matrix-element subroutine fill the array.

```
<Prclib interfaces: prc writer f module: TBP>+≡
```

```
    procedure :: write_col_state_call => prc_writer_f_module_write_col_state_call
```

```
<Prclib interfaces: procedures>+≡
```

```
    subroutine prc_writer_f_module_write_col_state_call (writer, unit, id)
        class(prc_writer_f_module_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        write (unit, "(9A)") " allocate (col_state_tmp ", &
            "(shape(1), shape(2), shape(3)))"
        write (unit, "(5x,9A)") "allocate (ghost_flag_tmp ", &
            "(shape(2), shape(3)))"
        write (unit, "(5x,9A)") "call ", &
            char (writer%get_c_procname (id, var_str ("col_state"))), &
            " (col_state_tmp, ghost_flag_tmp)"
        write (unit, "(5x,9A)") "forall (i = 1:shape(2), j = 1:shape(3))"
        write (unit, "(8x,9A)") "forall (k = 1:shape(1))"
        write (unit, "(11x,9A)") &
            "col_state(k + shape(1) * (i + shape(2)*(j-1) - 1)) ", &
            "= col_state_tmp(k,i,j)"
        write (unit, "(8x,9A)") "end forall"
        write (unit, "(8x,9A)") &
            "ghost_flag(i + shape(2)*(j-1)) = ghost_flag_tmp(i,j)"
        write (unit, "(5x,9A)") "end forall"
    end subroutine prc_writer_f_module_write_col_state_call
```

In the C library case, we just transfer the C pointer to the library function.

```
<Prclib interfaces: prc writer c lib: TBP>+≡
```

```
    procedure :: write_col_state_call => prc_writer_c_lib_write_col_state_call
```

```
<Prclib interfaces: procedures>+≡
```

```
    subroutine prc_writer_c_lib_write_col_state_call (writer, unit, id)
        class(prc_writer_c_lib_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        write (unit, "(5x,9A)") "call ", &
            char (writer%get_c_procname (id, var_str ("col_state"))), &
            " (col_state, ghost_flag)"
    end subroutine prc_writer_c_lib_write_col_state_call
```

Color factors

For the color-factor information, we return two integer arrays and a complex array.

```
<Prclib interfaces: public>+≡
```

```

public :: prc_set_color_factors
<Prclib interfaces: interfaces>+≡
abstract interface
  subroutine prc_set_color_factors &
    (pid, cf_index1, cf_index2, color_factors, shape) bind(C)
  import
  integer(c_int), intent(in) :: pid
  integer(c_int), dimension(*), intent(out) :: cf_index1, cf_index2
  complex(c_default_complex), dimension(*), intent(out) :: color_factors
  integer(c_int), dimension(1), intent(in) :: shape
  end subroutine prc_set_color_factors
end interface

```

This subroutine returns the color-flavor factor table.

```

<Prclib interfaces: prclib driver: TBP>+≡
procedure :: write_set_color_factors_sub
<Prclib interfaces: procedures>+≡
subroutine write_set_color_factors_sub (driver, unit, prefix)
  class(prclib_driver_t), intent(in) :: driver
  integer, intent(in) :: unit
  type(string_t), intent(in) :: prefix
  integer :: i
  type(string_t) :: feature
  feature = "color_factors"
  write (unit, "(A)") ""
  write (unit, "(A)") "! Set tables: color factors"
  write (unit, "(9A)") "subroutine ", char (prefix), &
    "set_color_factors_ptr (pid, cf_index1, cf_index2, color_factors, ", &
    "shape) bind(C)"
  write (unit, "(A)") " use iso_c_binding"
  write (unit, "(A)") " use kinds"
  write (unit, "(A)") " use omega_color"
  call driver%write_interfaces (unit, feature)
  write (unit, "(A)") " integer(c_int), intent(in) :: pid"
  write (unit, "(A)") " integer(c_int), dimension(1), intent(in) :: shape"
  write (unit, "(A)") " integer(c_int), dimension(*), intent(out) :: &
    &cf_index1, cf_index2"
  write (unit, "(A)") " complex(c_default_complex), dimension(*), &
    &intent(out) :: color_factors"
  write (unit, "(A)") " type(omega_color_factor), dimension(:), &
    &allocatable :: cf"
  write (unit, "(A)") " select case (pid)"
  do i = 1, driver%n_processes
    write (unit, "(2x,A,I0,A)") "case (", i, ")"
    call driver%record(i)%write_color_factors_call (unit)
  end do
  write (unit, "(A)") " end select"
  write (unit, "(A)") "end subroutine " // char (prefix) &
    // "set_color_factors_ptr"
end subroutine write_set_color_factors_sub

```

The actual call depends on the type of matrix element.

```

<Prclib interfaces: prclib driver record: TBP>+≡
  procedure :: write_color_factors_call => prclib_driver_record_write_color_factors_call

<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_record_write_color_factors_call (record, unit)
    class(prclib_driver_record_t), intent(in) :: record
    integer, intent(in) :: unit
    call record%writer%write_color_factors_call (unit, record%id)
  end subroutine prclib_driver_record_write_color_factors_call

```

The interface goes into the writer base type:

```

<Prclib interfaces: prc writer: TBP>+≡
  procedure(write_code), deferred :: write_color_factors_call

```

In the Fortran module case, the matrix-element procedure fills an array of `omega_color_factor` elements. We distribute this array among two integer arrays and one complex-valued array, for which we have the C pointers.

```

<Prclib interfaces: prc writer f module: TBP>+≡
  procedure :: write_color_factors_call => prc_writer_f_module_write_color_factors_call

<Prclib interfaces: procedures>+≡
  subroutine prc_writer_f_module_write_color_factors_call (writer, unit, id)
    class(prc_writer_f_module_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    write (unit, "(5x,A)") "allocate (cf (shape(1)))"
    write (unit, "(5x,9A)") "call ", &
      char (writer%get_c_procname (id, var_str ("color_factors"))), " (cf)"
    write (unit, "(5x,9A)") "cf_index1(1:shape(1)) = cf%i1"
    write (unit, "(5x,9A)") "cf_index2(1:shape(1)) = cf%i2"
    write (unit, "(5x,9A)") "color_factors(1:shape(1)) = cf%factor"
  end subroutine prc_writer_f_module_write_color_factors_call

```

In the C library case, we just transfer the C pointers to the library function. There are three arrays.

```

<Prclib interfaces: prc writer c lib: TBP>+≡
  procedure :: write_color_factors_call => &
    prc_writer_c_lib_write_color_factors_call

<Prclib interfaces: procedures>+≡
  subroutine prc_writer_c_lib_write_color_factors_call (writer, unit, id)
    class(prc_writer_c_lib_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    write (unit, "(5x,9A)") "call ", &
      char (writer%get_c_procname (id, var_str ("color_factors"))), &
      " (cf_index1, cf_index2, color_factors)"
  end subroutine prc_writer_c_lib_write_color_factors_call

```

14.2.10 Interfaces for C-library matrix element

If the matrix element code is not provided as a Fortran module but as a C or bind(C) Fortran library, we need explicit interfaces for the library functions. They are not identical to the Fortran module versions. They transfer pointers directly.

The implementation is part of the `prc_writer_c_lib` type, which serves as base type for all C-library writers. It writes specific interfaces depending on the feature.

We bind this as the method `write_standard_interface` instead of `write_interface`, because we have to override the latter. Otherwise we could not call the method because the writer type is abstract.

```
<Prclib interfaces: prc_writer_c_lib: TBP>+=  
  procedure :: write_standard_interface => prc_writer_c_lib_write_interface  
  
<Prclib interfaces: procedures>+=  
  subroutine prc_writer_c_lib_write_interface (writer, unit, id, feature)  
    class(prc_writer_c_lib_t), intent(in) :: writer  
    integer, intent(in) :: unit  
    type(string_t), intent(in) :: id, feature  
    select case (char (feature))  
    case ("md5sum")  
      write (unit, "(2x,9A)") "interface"  
      write (unit, "(5x,9A)") "function ", &  
        char (writer%get_c_procname (id, var_str ("get_md5sum"))), &  
        " () result (c_ptr) bind(C)"  
      write (unit, "(7x,9A)") "import"  
      write (unit, "(7x,9A)") "implicit none"  
      write (unit, "(7x,9A)") "type(c_ptr) :: c_ptr"  
      write (unit, "(5x,9A)") "end function ", &  
        char (writer%get_c_procname (id, var_str ("get_md5sum")))  
      write (unit, "(2x,9A)") "end interface"  
    case ("openmp_supported")  
      write (unit, "(2x,9A)") "interface"  
      write (unit, "(5x,9A)") "function ", &  
        char (writer%get_c_procname (id, feature)), &  
        " () result (status) bind(C)"  
      write (unit, "(7x,9A)") "import"  
      write (unit, "(7x,9A)") "implicit none"  
      write (unit, "(7x,9A)") "logical(c_bool) :: status"  
      write (unit, "(5x,9A)") "end function ", &  
        char (writer%get_c_procname (id, feature))  
      write (unit, "(2x,9A)") "end interface"  
    case ("n_in", "n_out", "n_flv", "n_hel", "n_col", "n_cin", "n_cf")  
      write (unit, "(2x,9A)") "interface"  
      write (unit, "(5x,9A)") "function ", &  
        char (writer%get_c_procname (id, feature)), &  
        " () result (n) bind(C)"  
      write (unit, "(7x,9A)") "import"  
      write (unit, "(7x,9A)") "implicit none"  
      write (unit, "(7x,9A)") "integer(c_int) :: n"  
      write (unit, "(5x,9A)") "end function ", &  
        char (writer%get_c_procname (id, feature))  
      write (unit, "(2x,9A)") "end interface"
```



```

case ("flv_state", "hel_state")
  write (unit, "(2x,9A)") "interface"
  write (unit, "(5x,9A)") "subroutine ", &
    char (writer%get_c_procname (id, feature)), &
    " (", char (feature), ") bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "implicit none"
  write (unit, "(7x,9A)") "integer(c_int), dimension(*), intent(out) ", &
    ":: ", char (feature)
  write (unit, "(5x,9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
  write (unit, "(2x,9A)") "end interface"
case ("col_state")
  write (unit, "(2x,9A)") "interface"
  write (unit, "(5x,9A)") "subroutine ", &
    char (writer%get_c_procname (id, feature)), &
    " (col_state, ghost_flag) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "implicit none"
  write (unit, "(7x,9A)") "integer(c_int), dimension(*), intent(out) ", &
    ":: col_state"
  write (unit, "(7x,9A)") "logical(c_bool), dimension(*), intent(out) ", &
    ":: ghost_flag"
  write (unit, "(5x,9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
  write (unit, "(2x,9A)") "end interface"
case ("color_factors")
  write (unit, "(2x,9A)") "interface"
  write (unit, "(5x,9A)") "subroutine ", &
    char (writer%get_c_procname (id, feature)), &
    " (cf_index1, cf_index2, color_factors) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "implicit none"
  write (unit, "(7x,9A)") "integer(c_int), dimension(*), &
    &intent(out) :: cf_index1"
  write (unit, "(7x,9A)") "integer(c_int), dimension(*), &
    &intent(out) :: cf_index2"
  write (unit, "(7x,9A)") "complex(c_default_complex), dimension(*), &
    &intent(out) :: color_factors"
  write (unit, "(5x,9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
  write (unit, "(2x,9A)") "end interface"
end select
end subroutine prc_writer_c_lib_write_interface

```

14.2.11 Retrieving the tables

In the previous section we had the writer routines for procedures that return tables, actually C pointers to tables. Here, we write convenience routines that unpack them and move the contents to suitable Fortran arrays.

The flavor and helicity tables are two-dimensional integer arrays. We use intermediate storage for correctly transforming C to Fortran data types.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: set_flv_state => prclib_driver_set_flv_state
  procedure :: set_hel_state => prclib_driver_set_hel_state

<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_set_flv_state (driver, i, flv_state)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    integer, dimension(:,:), allocatable, intent(out) :: flv_state
    integer :: n_tot, n_flv
    integer(c_int) :: pid
    integer(c_int), dimension(:,:), allocatable :: c_flv_state
    pid = i
    n_tot = driver%get_n_in (pid) + driver%get_n_out (pid)
    n_flv = driver%get_n_flv (pid)
    allocate (flv_state (n_tot, n_flv))
    allocate (c_flv_state (n_tot, n_flv))
    call driver%set_flv_state_ptr &
      (pid, c_flv_state, int ([n_tot, n_flv], kind=c_int))
    flv_state = c_flv_state
  end subroutine prclib_driver_set_flv_state

  subroutine prclib_driver_set_hel_state (driver, i, hel_state)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    integer, dimension(:,:), allocatable, intent(out) :: hel_state
    integer :: n_tot, n_hel
    integer(c_int) :: pid
    integer(c_int), dimension(:,:), allocatable, target :: c_hel_state
    pid = i
    n_tot = driver%get_n_in (pid) + driver%get_n_out (pid)
    n_hel = driver%get_n_hel (pid)
    allocate (hel_state (n_tot, n_hel))
    allocate (c_hel_state (n_tot, n_hel))
    call driver%set_hel_state_ptr &
      (pid, c_hel_state, int ([n_tot, n_hel], kind=c_int))
    hel_state = c_hel_state
  end subroutine prclib_driver_set_hel_state

```

The color-flow table is three-dimensional, otherwise similar. We simultaneously set the ghost-flag table, which consists of logical entries.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: set_col_state => prclib_driver_set_col_state

<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_set_col_state (driver, i, col_state, ghost_flag)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    integer, dimension(:,:,:), allocatable, intent(out) :: col_state
    logical, dimension(:,:), allocatable, intent(out) :: ghost_flag
    integer :: n_cin, n_tot, n_col
    integer(c_int) :: pid
    integer(c_int), dimension(:,:,:), allocatable :: c_col_state
    logical(c_bool), dimension(:,:), allocatable :: c_ghost_flag
    pid = i

```

```

n_cin = driver%get_n_cin (pid)
n_tot = driver%get_n_in (pid) + driver%get_n_out (pid)
n_col = driver%get_n_col (pid)
allocate (col_state (n_cin, n_tot, n_col))
allocate (c_col_state (n_cin, n_tot, n_col))
allocate (ghost_flag (n_tot, n_col))
allocate (c_ghost_flag (n_tot, n_col))
call driver%set_col_state_ptr (pid, &
    c_col_state, c_ghost_flag, int ([n_cin, n_tot, n_col], kind=c_int))
col_state = c_col_state
ghost_flag = c_ghost_flag
end subroutine prclib_driver_set_col_state

```

The color-factor table is a sparse matrix: a two-column array of indices and one array which contains the corresponding factors.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: set_color_factors => prclib_driver_set_color_factors

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_set_color_factors (driver, i, color_factors, cf_index)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: i
        complex(default), dimension(:), allocatable, intent(out) :: color_factors
        integer, dimension(:,:), allocatable, intent(out) :: cf_index
        integer :: n_cf
        integer(c_int) :: pid
        complex(c_default_complex), dimension(:), allocatable, target :: c_color_factors
        integer(c_int), dimension(:), allocatable, target :: c_cf_index1
        integer(c_int), dimension(:), allocatable, target :: c_cf_index2
        pid = i
        n_cf = driver%get_n_cf (pid)
        allocate (color_factors (n_cf))
        allocate (c_color_factors (n_cf))
        allocate (c_cf_index1 (n_cf))
        allocate (c_cf_index2 (n_cf))
        call driver%set_color_factors_ptr (pid, &
            c_cf_index1, c_cf_index2, &
            c_color_factors, int ([n_cf], kind=c_int))
        color_factors = c_color_factors
        allocate (cf_index (2, n_cf))
        cf_index(1,:) = c_cf_index1
        cf_index(2,:) = c_cf_index2
    end subroutine prclib_driver_set_color_factors

```

14.2.12 Returning a procedure pointer

The functions that directly access the matrix element, event by event, are assigned to a process-specific driver object as procedure pointers. For the `dlopen` interface, we use C function pointers. This subroutine returns such a pointer:

```

<Prclib interfaces: public>+≡
    public :: prc_get_fptr

```

```

<Prclib interfaces: interfaces>+≡
  abstract interface
    subroutine prc_get_fptr (pid, fid, fptr) bind(C)
      import
        integer(c_int), intent(in) :: pid
        integer(c_int), intent(in) :: fid
        type(c_funptr), intent(out) :: fptr
    end subroutine prc_get_fptr
  end interface

```

This procedure writes the source code for the procedure pointer returning subroutine.

All C functions that are provided by the matrix element code of a specific process are handled here. The selection consists of a double layered **select case** construct.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: write_get_fptr_sub

<Prclib interfaces: procedures>+≡
  subroutine write_get_fptr_sub (driver, unit, prefix)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    integer :: i, j
    write (unit, "(A)") ""
    write (unit, "(A)") "! Return C pointer to a procedure:"
    write (unit, "(A)") "! pid = process index; fid = function index"
    write (unit, "(4A)") "subroutine ", char (prefix), "get_fptr ", &
      "(pid, fid, fptr) bind(C)"
    write (unit, "(A)") " use iso_c_binding"
    write (unit, "(A)") " use kinds"
    write (unit, "(A)") " implicit none"
    write (unit, "(A)") " integer(c_int), intent(in) :: pid"
    write (unit, "(A)") " integer(c_int), intent(in) :: fid"
    write (unit, "(A)") " type(c_funptr), intent(out) :: fptr"
    do i = 1, driver%n_processes
      call driver%record(i)%write_interfaces (unit)
    end do
    write (unit, "(A)") " select case (pid)"
    do i = 1, driver%n_processes
      write (unit, "(2x,A,IO,A)") "case (", i, ")"
      write (unit, "(5x,A)") "select case (fid)"
      associate (record => driver%record(i))
        do j = 1, size (record%feature)
          write (unit, "(5x,A,IO,9A)") "case (", j, "); ", &
            "fptr = c_funloc (", &
            char (record%get_c_procname (record%feature(j))), &
            ")"
        end do
      end associate
      write (unit, "(5x,A)") "end select"
    end do
    write (unit, "(A)") " end select"
    write (unit, "(3A)") "end subroutine ", char (prefix), "get_fptr"
  end subroutine write_get_fptr_sub

```

```
end subroutine write_get_fptr_sub
```

The procedures for which we want to return a pointer (the 'features' of the matrix element code) are actually Fortran module procedures. If we want to have a C signature, we must write wrapper functions for all of them. The procedures, their signatures, and the appropriate writer routines are specific for the process type.

To keep this generic, we do not provide the writer routines here, but just the interface for a writer routine. The actual routines are stored in the process record.

The `prefix` indicates the library, the `id` indicates the process, and `procname` is the bare name of the procedure to be written.

```
<Prclib interfaces: public>+≡
public :: write_driver_code

<Prclib interfaces: interfaces>+≡
abstract interface
  subroutine write_driver_code (unit, prefix, id, procname)
    import
    integer, intent(in) :: unit
    type(string_t), intent(in) :: prefix
    type(string_t), intent(in) :: id
    type(string_t), intent(in) :: procname
  end subroutine write_driver_code
end interface
```

14.2.13 Hooks

Interface for additional library unload / reload hooks (currently unused!)

```
<Prclib interfaces: public>+≡
public :: prclib_unload_hook
public :: prclib_reload_hook

<Prclib interfaces: interfaces>+≡
abstract interface
  subroutine prclib_unload_hook (libname)
    import
    type(string_t), intent(in) :: libname
  end subroutine prclib_unload_hook

  subroutine prclib_reload_hook (libname)
    import
    type(string_t), intent(in) :: libname
  end subroutine prclib_reload_hook
end interface
```

14.2.14 Make source, compile, link

Since we should have written a Makefile, these tasks amount to simple `make` calls. Note that the Makefile targets depend on each other, so calling `link` executes also the `source` and `compile` steps, when necessary.

Optionally, we can use a subdirectory. We construct a prefix for the subdirectory, and generate a shell `cd` call that moves us into the workspace.

The `prefix` version is intended to be prepended to a filename, and can be empty. The `path` version is intended to be prepended with a following slash, so the default is `..`.

```

<Prclib interfaces: public>+≡
  public :: workspace_prefix
  public :: workspace_path
<Prclib interfaces: procedures>+≡
  function workspace_prefix (workspace) result (prefix)
    type(string_t), intent(in), optional :: workspace
    type(string_t) :: prefix
    if (present (workspace)) then
      if (workspace /= "") then
        prefix = workspace // "/"
      else
        prefix = ""
      end if
    else
      prefix = ""
    end if
  end function workspace_prefix

  function workspace_path (workspace) result (path)
    type(string_t), intent(in), optional :: workspace
    type(string_t) :: path
    if (present (workspace)) then
      if (workspace /= "") then
        path = workspace
      else
        path = "."
      end if
    else
      path = "."
    end if
  end function workspace_path

  function workspace_cmd (workspace) result (cmd)
    type(string_t), intent(in), optional :: workspace
    type(string_t) :: cmd
    if (present (workspace)) then
      if (workspace /= "") then
        cmd = "cd " // workspace // " && "
      else
        cmd = ""
      end if
    else
      cmd = ""
    end if
  end function workspace_cmd

```

The first routine writes source-code files for the individual processes. First it calls the writer routines directly for each process, then it calls `make source`.

The make command may either post-process the files, or it may do the complete work, e.g., calling an external program that generates the files.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: make_source => prclib_driver_make_source

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_make_source (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
        integer :: i
        do i = 1, driver%n_processes
            call driver%record(i)%write_source_code ()
        end do
        call os_system_call ( &
            workspace_cmd (workspace) &
            // "make source " // os_data%makeflags &
            // " -f " // driver%basename // ".makefile")
    end subroutine prclib_driver_make_source

```

Compile matrix element source code and the driver source code. As above, we first iterate through all processes and call `before_compile`. This is usually empty, but can execute code that depends on `make_source` already completed. Similarly, `after_compile` scans all processes again.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: make_compile => prclib_driver_make_compile

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_make_compile (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
        integer :: i
        do i = 1, driver%n_processes
            call driver%record(i)%before_compile ()
        end do
        call os_system_call ( &
            workspace_cmd (workspace) &
            // "make compile " // os_data%makeflags &
            // " -f " // driver%basename // ".makefile")
        do i = 1, driver%n_processes
            call driver%record(i)%after_compile ()
        end do
    end subroutine prclib_driver_make_compile

```

Combine all matrix-element code together with the driver in a process library on disk.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: make_link => prclib_driver_make_link

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_make_link (driver, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        type(os_data_t), intent(in) :: os_data

```

```

type(string_t), intent(in), optional :: workspace
integer :: i
call os_system_call ( &
    workspace_cmd (workspace) &
    // "make link " // os_data%makeflags &
    // " -f " // driver%basename // ".makefile")
end subroutine prclib_driver_make_link

```

14.2.15 Clean up generated files

The task of cleaning any generated files should also be deferred to Makefile targets. Apart from removing everything, removing specific files may be useful for partial rebuilds. (Note that removing the makefile itself can only be done once, for obvious reasons.)

If there is no makefile, do nothing.

(Prclib interfaces: prclib_driver: TBP)+≡

```

procedure :: clean_library => prclib_driver_clean_library
procedure :: clean_objects => prclib_driver_clean_objects
procedure :: clean_source => prclib_driver_clean_source
procedure :: clean_driver => prclib_driver_clean_driver
procedure :: clean_makefile => prclib_driver_clean_makefile
procedure :: clean => prclib_driver_clean
procedure :: distclean => prclib_driver_distclean

```

(Prclib interfaces: procedures)+≡

```

subroutine prclib_driver_clean_library (driver, os_data, workspace)
class(prclib_driver_t), intent(in) :: driver
type(os_data_t), intent(in) :: os_data
type(string_t), intent(in), optional :: workspace
if (driver%makefile_exists ()) then
    call os_system_call ( &
        workspace_cmd (workspace) &
        // "make clean-library " // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")
    end if
end subroutine prclib_driver_clean_library

subroutine prclib_driver_clean_objects (driver, os_data, workspace)
class(prclib_driver_t), intent(in) :: driver
type(os_data_t), intent(in) :: os_data
type(string_t), intent(in), optional :: workspace
if (driver%makefile_exists ()) then
    call os_system_call ( &
        workspace_cmd (workspace) &
        // "make clean-objects " // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")
    end if
end subroutine prclib_driver_clean_objects

subroutine prclib_driver_clean_source (driver, os_data, workspace)
class(prclib_driver_t), intent(in) :: driver
type(os_data_t), intent(in) :: os_data

```



```

type(string_t), intent(in), optional :: workspace
if (driver%makefile_exists ()) then
    call os_system_call ( &
        workspace_cmd (workspace) &
        // "make clean-source " // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")
end if
end subroutine prclib_driver_clean_source

subroutine prclib_driver_clean_driver (driver, os_data, workspace)
class(prclib_driver_t), intent(in) :: driver
type(os_data_t), intent(in) :: os_data
type(string_t), intent(in), optional :: workspace
if (driver%makefile_exists ()) then
    call os_system_call ( &
        workspace_cmd (workspace) &
        // "make clean-driver " // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")
end if
end subroutine prclib_driver_clean_driver

subroutine prclib_driver_clean_makefile (driver, os_data, workspace)
class(prclib_driver_t), intent(in) :: driver
type(os_data_t), intent(in) :: os_data
type(string_t), intent(in), optional :: workspace
if (driver%makefile_exists ()) then
    call os_system_call ( &
        workspace_cmd (workspace) &
        // "make clean-makefile " // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")
end if
end subroutine prclib_driver_clean_makefile

subroutine prclib_driver_clean (driver, os_data, workspace)
class(prclib_driver_t), intent(in) :: driver
type(os_data_t), intent(in) :: os_data
type(string_t), intent(in), optional :: workspace
if (driver%makefile_exists ()) then
    call os_system_call ( &
        workspace_cmd (workspace) &
        // "make clean " // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")
end if
end subroutine prclib_driver_clean

subroutine prclib_driver_distclean (driver, os_data, workspace)
class(prclib_driver_t), intent(in) :: driver
type(os_data_t), intent(in) :: os_data
type(string_t), intent(in), optional :: workspace
if (driver%makefile_exists ()) then
    call os_system_call ( &
        workspace_cmd (workspace) &
        // "make distclean " // os_data%makeflags &
        // " -f " // driver%basename // ".makefile")

```

```

        end if
    end subroutine prclib_driver_distclean

```

This Make target should remove all files that apply to a specific process. We execute this when we want to force remaking source code. Note that source targets need not have prerequisites, so just calling `make_source` would not do anything if the files exist.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: clean_proc => prclib_driver_clean_proc

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_clean_proc (driver, i, os_data, workspace)
        class(prclib_driver_t), intent(in) :: driver
        integer, intent(in) :: i
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in), optional :: workspace
        type(string_t) :: id
        if (driver%makefile_exists ()) then
            id = driver%record(i)%id
            call os_system_call ( &
                workspace_cmd (workspace) &
                // "make clean-" // driver%record(i)%id // " " &
                // os_data%makeflags &
                // " -f " // driver%basename // ".makefile")
        end if
    end subroutine prclib_driver_clean_proc

```

14.2.16 Further Tools

Check for the appropriate makefile.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: makefile_exists => prclib_driver_makefile_exists

<Prclib interfaces: procedures>+≡
    function prclib_driver_makefile_exists (driver, workspace) result (flag)
        class(prclib_driver_t), intent(in) :: driver
        type(string_t), intent(in), optional :: workspace
        logical :: flag
        inquire (file = char (workspace_prefix (workspace) &
            & // driver%basename) // ".makefile", &
            exist = flag)
    end function prclib_driver_makefile_exists

```

14.2.17 Load the library

Once the library has been linked, we can dlopen it and assign all procedure pointers to their proper places in the library driver object. The `loaded` flag is set only if all required pointers have become assigned.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure :: load => prclib_driver_load

```

(Prclib interfaces: procedures)+≡

```

subroutine prclib_driver_load (driver, os_data, noerror, workspace)
  class(prclib_driver_t), intent(inout) :: driver
  type(os_data_t), intent(in) :: os_data
  logical, intent(in), optional :: noerror
  type(string_t), intent(in), optional :: workspace
  type(c_funptr) :: c_fptr
  logical :: ignore

  ignore = .false.; if (present (noerror)) ignore = noerror

  driver%libname = os_get_dlname ( &
    workspace_prefix (workspace) // driver%basename, &
    os_data, noerror, noerror)
  if (driver%libname == "") return
  select type (driver)
  type is (prclib_driver_dynamic_t)
    if (.not. dlaccess_is_open (driver%dlaccess)) then
      call dlaccess_init &
        (driver%dlaccess, workspace_path (workspace), &
        driver%libname, os_data)
      if (.not. ignore) call driver%check_dlerror ()
    end if
    driver%loaded = dlaccess_is_open (driver%dlaccess)
  class default
    driver%loaded = .true.
  end select
  if (.not. driver%loaded) return

  c_fptr = driver%get_c_funptr (var_str ("get_n_processes"))
  call c_f_procpointer (c_fptr, driver%get_n_processes)
  driver%loaded = driver%loaded .and. associated (driver%get_n_processes)

  c_fptr = driver%get_c_funptr (var_str ("get_process_id_ptr"))
  call c_f_procpointer (c_fptr, driver%get_process_id_ptr)
  driver%loaded = driver%loaded .and. associated (driver%get_process_id_ptr)

  c_fptr = driver%get_c_funptr (var_str ("get_model_name_ptr"))
  call c_f_procpointer (c_fptr, driver%get_model_name_ptr)
  driver%loaded = driver%loaded .and. associated (driver%get_model_name_ptr)

  c_fptr = driver%get_c_funptr (var_str ("get_md5sum_ptr"))
  call c_f_procpointer (c_fptr, driver%get_md5sum_ptr)
  driver%loaded = driver%loaded .and. associated (driver%get_md5sum_ptr)

  c_fptr = driver%get_c_funptr (var_str ("get_openmp_status"))
  call c_f_procpointer (c_fptr, driver%get_openmp_status)
  driver%loaded = driver%loaded .and. associated (driver%get_openmp_status)

  c_fptr = driver%get_c_funptr (var_str ("get_n_in"))
  call c_f_procpointer (c_fptr, driver%get_n_in)
  driver%loaded = driver%loaded .and. associated (driver%get_n_in)

  c_fptr = driver%get_c_funptr (var_str ("get_n_out"))

```

```

call c_f_procpointer (c_fptr, driver%get_n_out)
driver%loaded = driver%loaded .and. associated (driver%get_n_out)

c_fptr = driver%get_c_funptr (var_str ("get_n_flv"))
call c_f_procpointer (c_fptr, driver%get_n_flv)
driver%loaded = driver%loaded .and. associated (driver%get_n_flv)

c_fptr = driver%get_c_funptr (var_str ("get_n_hel"))
call c_f_procpointer (c_fptr, driver%get_n_hel)
driver%loaded = driver%loaded .and. associated (driver%get_n_hel)

c_fptr = driver%get_c_funptr (var_str ("get_n_col"))
call c_f_procpointer (c_fptr, driver%get_n_col)
driver%loaded = driver%loaded .and. associated (driver%get_n_col)

c_fptr = driver%get_c_funptr (var_str ("get_n_cin"))
call c_f_procpointer (c_fptr, driver%get_n_cin)
driver%loaded = driver%loaded .and. associated (driver%get_n_cin)

c_fptr = driver%get_c_funptr (var_str ("get_n_cf"))
call c_f_procpointer (c_fptr, driver%get_n_cf)
driver%loaded = driver%loaded .and. associated (driver%get_n_cf)

c_fptr = driver%get_c_funptr (var_str ("set_flv_state_ptr"))
call c_f_procpointer (c_fptr, driver%set_flv_state_ptr)
driver%loaded = driver%loaded .and. associated (driver%set_flv_state_ptr)

c_fptr = driver%get_c_funptr (var_str ("set_hel_state_ptr"))
call c_f_procpointer (c_fptr, driver%set_hel_state_ptr)
driver%loaded = driver%loaded .and. associated (driver%set_hel_state_ptr)

c_fptr = driver%get_c_funptr (var_str ("set_col_state_ptr"))
call c_f_procpointer (c_fptr, driver%set_col_state_ptr)
driver%loaded = driver%loaded .and. associated (driver%set_col_state_ptr)

c_fptr = driver%get_c_funptr (var_str ("set_color_factors_ptr"))
call c_f_procpointer (c_fptr, driver%set_color_factors_ptr)
driver%loaded = driver%loaded .and. associated (driver%set_color_factors_ptr)

c_fptr = driver%get_c_funptr (var_str ("get_fptr"))
call c_f_procpointer (c_fptr, driver%get_fptr)
driver%loaded = driver%loaded .and. associated (driver%get_fptr)

end subroutine prclib_driver_load

```

Unload. To be sure, nullify the procedure pointers.

```

<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: unload => prclib_driver_unload

<Prclib interfaces: procedures>+≡
  subroutine prclib_driver_unload (driver)
    class(prclib_driver_t), intent(inout) :: driver
    select type (driver)
      type is (prclib_driver_dynamic_t)

```

```

        if (dlaccess_is_open (driver%dlaccess)) then
            call dlaccess_final (driver%dlaccess)
            call driver%check_dlerror ()
        end if
    end select
    driver%loaded = .false.
    nullify (driver%get_n_processes)
    nullify (driver%get_process_id_ptr)
    nullify (driver%get_model_name_ptr)
    nullify (driver%get_md5sum_ptr)
    nullify (driver%get_openmp_status)
    nullify (driver%get_n_in)
    nullify (driver%get_n_out)
    nullify (driver%get_n_flv)
    nullify (driver%get_n_hel)
    nullify (driver%get_n_col)
    nullify (driver%get_n_cin)
    nullify (driver%get_n_cf)
    nullify (driver%set_flv_state_ptr)
    nullify (driver%set_hel_state_ptr)
    nullify (driver%set_col_state_ptr)
    nullify (driver%set_color_factors_ptr)
    nullify (driver%get_fptr)
end subroutine prclib_driver_unload

```

This subroutine checks the dlerror content and issues a fatal error if it finds an error there.

```

<Prclib interfaces: prclib driver dynamic: TBP>≡
    procedure :: check_dlerror => prclib_driver_check_dlerror

<Prclib interfaces: procedures>+≡
    subroutine prclib_driver_check_dlerror (driver)
        class(prclib_driver_dynamic_t), intent(in) :: driver
        if (dlaccess_has_error (driver%dlaccess)) then
            call msg_fatal (char (dlaccess_get_error (driver%dlaccess)))
        end if
    end subroutine prclib_driver_check_dlerror

```

Get the handle (C function pointer) for a given “feature” of the matrix element code, so it can be assigned to the appropriate procedure pointer slot. In the static case, this is a trivial pointer assignment, hard-coded into the driver type implementation.

```

<Prclib interfaces: prclib driver: TBP>+≡
    procedure (prclib_driver_get_c_funptr), deferred :: get_c_funptr

<Prclib interfaces: interfaces>+≡
    abstract interface
        function prclib_driver_get_c_funptr (driver, feature) result (c_fptr)
            import
            class(prclib_driver_t), intent(inout) :: driver
            type(string_t), intent(in) :: feature
            type(c_funptr) :: c_fptr
        end function prclib_driver_get_c_funptr

```

```
end interface
```

In the dynamic-library case, we call the DL interface to retrieve the C pointer to a named procedure.

```
<Prclib interfaces: prclib driver dynamic: TBP>+≡
  procedure :: get_c_funptr => prclib_driver_dynamic_get_c_funptr

<Prclib interfaces: procedures>+≡
  function prclib_driver_dynamic_get_c_funptr (driver, feature) result (c_fptr)
    class(prclib_driver_dynamic_t), intent(inout) :: driver
    type(string_t), intent(in) :: feature
    type(c_funptr) :: c_fptr
    type(string_t) :: prefix, full_name
    prefix = lower_case (driver%basename) // "_"
    full_name = prefix // feature
    c_fptr = dlaccess_get_c_funptr (driver%dlaccess, full_name)
    call driver%check_dlerror ()
  end function prclib_driver_dynamic_get_c_funptr
```

14.2.18 MD5 sums

Recall the MD5 sum written in the Makefile

```
<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: get_md5sum_makefile => prclib_driver_get_md5sum_makefile

<Prclib interfaces: procedures>+≡
  function prclib_driver_get_md5sum_makefile (driver, workspace) result (md5sum)
    class(prclib_driver_t), intent(in) :: driver
    type(string_t), intent(in), optional :: workspace
    character(32) :: md5sum
    type(string_t) :: filename
    character(80) :: buffer
    logical :: exist
    integer :: u, iostat
    md5sum = ""
    filename = workspace_prefix (workspace) // driver%basename // ".makefile"
    inquire (file = char (filename), exist = exist)
    if (exist) then
      u = free_unit ()
      open (u, file = char (filename), action = "read", status = "old")
      iostat = 0
      do
        read (u, "(A)", iostat = iostat) buffer
        if (iostat /= 0) exit
        buffer = adjustl (buffer)
        select case (buffer(1:9))
          case ("MD5SUM = ")
            read (buffer(11:), "(A32)") md5sum
            exit
        end select
      end do
      close (u)
    end if
  end function
```

```
end function prclib_driver_get_md5sum_makefile
```

Recall the MD5 sum written in the driver source code.

```
<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: get_md5sum_driver => prclib_driver_get_md5sum_driver

<Prclib interfaces: procedures>+≡
  function prclib_driver_get_md5sum_driver (driver, workspace) result (md5sum)
    class(prclib_driver_t), intent(in) :: driver
    type(string_t), intent(in), optional :: workspace
    character(32) :: md5sum
    type(string_t) :: filename
    character(80) :: buffer
    logical :: exist
    integer :: u, iostat
    md5sum = ""
    filename = workspace_prefix (workspace) // driver%basename // ".f90"
    inquire (file = char (filename), exist = exist)
    if (exist) then
      u = free_unit ()
      open (u, file = char (filename), action = "read", status = "old")
      iostat = 0
      do
        read (u, "(A)", iostat = iostat) buffer
        if (iostat /= 0) exit
        buffer = adjustl (buffer)
        select case (buffer(1:9))
          case ("md5sum = ")
            read (buffer(11:), "(A32)") md5sum
            exit
        end select
      end do
      close (u)
    end if
  end function prclib_driver_get_md5sum_driver
```

Recall the MD5 sum written in the matrix element source code.

```
<Prclib interfaces: prclib driver: TBP>+≡
  procedure :: get_md5sum_source => prclib_driver_get_md5sum_source

<Prclib interfaces: procedures>+≡
  function prclib_driver_get_md5sum_source &
    (driver, i, workspace) result (md5sum)
    class(prclib_driver_t), intent(in) :: driver
    integer, intent(in) :: i
    type(string_t), intent(in), optional :: workspace
    character(32) :: md5sum
    type(string_t) :: filename
    character(80) :: buffer
    logical :: exist
    integer :: u, iostat
    md5sum = ""

    filename = workspace_prefix (workspace) // driver%record(i)%id // ".f90"
```

```

inquire (file = char (filename), exist = exist)
if (exist) then
  u = free_unit ()
  open (u, file = char (filename), action = "read", status = "old")
  iostat = 0
  do
    read (u, "(A)", iostat = iostat)  buffer
    if (iostat /= 0)  exit
    buffer = adjustl (buffer)
    select case (buffer(1:9))
    case ("md5sum = ")
      read (buffer(11:), "(A32)")  md5sum
      exit
    end select
  end do
  close (u)
end if
end function prclib_driver_get_md5sum_source

```

14.2.19 Unit Test

Test module, followed by the corresponding implementation module.

`<prclib_interfaces_ut.f90>`≡

<File header>

```

module prclib_interfaces_ut
  use kinds
  use system_dependencies, only: CC_IS_GNU, CC_HAS_QUADMATH
  use unit_tests
  use prclib_interfaces_uti

```

<Standard module head>

<Prclib interfaces: public test>

<Prclib interfaces: public test auxiliary>

contains

<Prclib interfaces: test driver>

```

end module prclib_interfaces_ut

```

`<prclib_interfaces_uti.f90>`≡

<File header>

```

module prclib_interfaces_uti

```

```

  use, intrinsic :: iso_c_binding !NODEP!

```

```

  use kinds

```

```

  use system_dependencies, only: CC_HAS_QUADMATH, DEFAULT_FC_PRECISION

```

<Use strings>


```

    use io_units
    use system_defs, only: TAB
    use os_interface

    use prclib_interfaces

    <Standard module head>

    <Prclib interfaces: public test auxiliary>

    <Prclib interfaces: test declarations>

    <Prclib interfaces: test types>

    contains

    <Prclib interfaces: tests>

    <Prclib interfaces: test auxiliary>

    end module prclib_interfaces_uti
API: driver for the unit tests below.
    <Prclib interfaces: public test>≡
        public :: prclib_interfaces_test
    <Prclib interfaces: test driver>≡
        subroutine prclib_interfaces_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <Prclib interfaces: execute tests>
        end subroutine prclib_interfaces_test

```

Empty process list

Test 1: Create a driver object and display its contents. One of the feature lists references a writer procedure; this is just a dummy that does nothing useful.

```

    <Prclib interfaces: execute tests>≡
        call test (prclib_interfaces_1, "prclib_interfaces_1", &
            "create driver object", &
            u, results)

    <Prclib interfaces: test declarations>≡
        public :: prclib_interfaces_1

    <Prclib interfaces: tests>≡
        subroutine prclib_interfaces_1 (u)
            integer, intent(in) :: u
            class(prclib_driver_t), allocatable :: driver
            character(32), parameter :: md5sum = "prclib_interfaces_1_md5sum"
            class(prc_writer_t), pointer :: test_writer_1

            write (u, "(A)")  "* Test output: prclib_interfaces_1"

```

```

write (u, "(A)")  "* Purpose: display the driver object contents"
write (u, *)
write (u, "(A)")  "* Create a prclib driver object"
write (u, "(A)")

call dispatch_prclib_driver (driver, var_str ("prclib"), var_str (""))
call driver%init (3)
call driver%set_md5sum (md5sum)

allocate (test_writer_1_t :: test_writer_1)

call driver%set_record (1, var_str ("test1"), var_str ("test_model"), &
    [var_str ("init")], test_writer_1)

call driver%set_record (2, var_str ("test2"), var_str ("foo_model"), &
    [var_str ("another_proc")], test_writer_1)

call driver%set_record (3, var_str ("test3"), var_str ("test_model"), &
    [var_str ("init"), var_str ("some_proc")], test_writer_1)

call driver%write (u)

deallocate (test_writer_1)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prclib_interfaces_1"
end subroutine prclib_interfaces_1

```

The writer: the procedures write just comment lines. We can fix an instance of this as a parameter (since it has no mutable content) and just reference the fixed parameter.

NOTE: temporarily made public.

```

<Prclib interfaces: test types>≡
type, extends (prc_writer_t) :: test_writer_1_t
contains
    procedure, nopass :: type_name => test_writer_1_type_name
    procedure :: write_makefile_code => test_writer_1_mk
    procedure :: write_source_code => test_writer_1_src
    procedure :: write_interface => test_writer_1_if
    procedure :: write_md5sum_call => test_writer_1_md5sum
    procedure :: write_int_sub_call => test_writer_1_int_sub
    procedure :: write_col_state_call => test_writer_1_col_state
    procedure :: write_color_factors_call => test_writer_1_col_factors
    procedure :: before_compile => test_writer_1_before_compile
    procedure :: after_compile => test_writer_1_after_compile
end type test_writer_1_t

<Prclib interfaces: test auxiliary>≡
function test_writer_1_type_name () result (string)
    type(string_t) :: string
    string = "test_1"
end function test_writer_1_type_name

```

```

subroutine test_writer_1_mk &
    (writer, unit, id, os_data, verbose, testflag)
    class(test_writer_1_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    write (unit, "(5A)")  "# Makefile code for process ", char (id), &
        " goes here."
end subroutine test_writer_1_mk

subroutine test_writer_1_src (writer, id)
    class(test_writer_1_t), intent(in) :: writer
    type(string_t), intent(in) :: id
end subroutine test_writer_1_src

subroutine test_writer_1_if (writer, unit, id, feature)
    class(test_writer_1_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
    write (unit, "(2x,9A)")  "! Interface code for ", &
        char (id), "_", char (writer%get_procname (feature)), &
        " goes here."
end subroutine test_writer_1_if

subroutine test_writer_1_md5sum (writer, unit, id)
    class(test_writer_1_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    write (unit, "(5x,9A)")  "! MD5sum call for ", char (id), " goes here."
end subroutine test_writer_1_md5sum

subroutine test_writer_1_int_sub (writer, unit, id, feature)
    class(test_writer_1_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
    write (unit, "(5x,9A)")  "! ", char (feature), " call for ", &
        char (id), " goes here."
end subroutine test_writer_1_int_sub

subroutine test_writer_1_col_state (writer, unit, id)
    class(test_writer_1_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    write (unit, "(5x,9A)")  "! col_state call for ", &
        char (id), " goes here."
end subroutine test_writer_1_col_state

subroutine test_writer_1_col_factors (writer, unit, id)
    class(test_writer_1_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    write (unit, "(5x,9A)")  "! color_factors call for ", &

```

```

        char (id), " goes here."
    end subroutine test_writer_1_col_factors

    subroutine test_writer_1_before_compile (writer, id)
        class(test_writer_1_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine test_writer_1_before_compile

    subroutine test_writer_1_after_compile (writer, id)
        class(test_writer_1_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine test_writer_1_after_compile

```

Process library driver file

Test 2: Write the driver file for a test case with two processes. The first process needs no wrapper (C library), the second one needs wrappers (Fortran module library).

```

<Prclib interfaces: execute tests>+≡
    call test (prclib_interfaces_2, "prclib_interfaces_2", &
        "write driver file", &
        u, results)

<Prclib interfaces: test declarations>+≡
    public :: prclib_interfaces_2

<Prclib interfaces: tests>+≡
    subroutine prclib_interfaces_2 (u)
        integer, intent(in) :: u
        class(prclib_driver_t), allocatable :: driver
        character(32), parameter :: md5sum = "prclib_interfaces_2_md5sum"
        class(prc_writer_t), pointer :: test_writer_1, test_writer_2

        write (u, "(A)")  "* Test output: prclib_interfaces_2"
        write (u, "(A)")  "* Purpose: check the generated driver source code"
        write (u, "(A)")
        write (u, "(A)")  "* Create a prclib driver object (2 processes)"
        write (u, "(A)")

        call dispatch_prclib_driver (driver, var_str ("prclib2"), var_str (""))
        call driver%init (2)
        call driver%set_md5sum (md5sum)

        allocate (test_writer_1_t :: test_writer_1)
        allocate (test_writer_2_t :: test_writer_2)

        call driver%set_record (1, var_str ("test1"), var_str ("Test_model"), &
            [var_str ("proc1")], test_writer_1)

        call driver%set_record (2, var_str ("test2"), var_str ("Test_model"), &
            [var_str ("proc1"), var_str ("proc2")], test_writer_2)

        call driver%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Write the driver file"
write (u, "(A)")  "* File contents:"
write (u, "(A)")

call driver%generate_driver_code (u)

deallocate (test_writer_1)
deallocate (test_writer_2)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prclib_interfaces_2"
end subroutine prclib_interfaces_2

```

A writer with wrapper code: the procedures again write just comment lines. Since all procedures are NOPASS, we can reuse two of the TBP.

```

<Prclib interfaces: test types>+≡
type, extends (prc_writer_f_module_t) :: test_writer_2_t
contains
  procedure, nopass :: type_name => test_writer_2_type_name
  procedure :: write_makefile_code => test_writer_2_mk
  procedure :: write_source_code => test_writer_2_src
  procedure :: write_interface => test_writer_2_if
  procedure :: write_wrapper => test_writer_2_wr
  procedure :: before_compile => test_writer_2_before_compile
  procedure :: after_compile => test_writer_2_after_compile
end type test_writer_2_t

<Prclib interfaces: test auxiliary>+≡
function test_writer_2_type_name () result (string)
  type(string_t) :: string
  string = "test_2"
end function test_writer_2_type_name

subroutine test_writer_2_mk &
  (writer, unit, id, os_data, verbose, testflag)
  class(test_writer_2_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id
  type(os_data_t), intent(in) :: os_data
  logical, intent(in) :: verbose
  logical, intent(in), optional :: testflag
  write (unit, "(5A)")  "# Makefile code for process ", char (id), &
    " goes here."
end subroutine test_writer_2_mk

subroutine test_writer_2_src (writer, id)
  class(test_writer_2_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_2_src

subroutine test_writer_2_if (writer, unit, id, feature)
  class(test_writer_2_t), intent(in) :: writer

```

```

integer, intent(in) :: unit
type(string_t), intent(in) :: id, feature
write (unit, "(2x,9A)")  "! Interface code for ", &
    char (writer%get_module_name (id)), "_", &
    char (writer%get_procname (feature)), " goes here."
end subroutine test_writer_2_if

subroutine test_writer_2_wr (writer, unit, id, feature)
    class(test_writer_2_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
    write (unit, *)
    write (unit, "(9A)")  "! Wrapper code for ", &
        char (writer%get_c_procname (id, feature)), " goes here."
end subroutine test_writer_2_wr

subroutine test_writer_2_before_compile (writer, id)
    class(test_writer_2_t), intent(in) :: writer
    type(string_t), intent(in) :: id
end subroutine test_writer_2_before_compile

subroutine test_writer_2_after_compile (writer, id)
    class(test_writer_2_t), intent(in) :: writer
    type(string_t), intent(in) :: id
end subroutine test_writer_2_after_compile

```

Process library makefile

Test 3: Write the makefile for compiling and linking the process library (processes and driver code). There are two processes, one with one method, one with two methods.

To have predictable output, we reset the system-dependent initial components of `os_data` to known values.

```

<Prclib interfaces: execute tests>+≡
    call test (prclib_interfaces_3, "prclib_interfaces_3", &
        "write makefile", &
        u, results)

<Prclib interfaces: test declarations>+≡
    public :: prclib_interfaces_3

<Prclib interfaces: tests>+≡
    subroutine prclib_interfaces_3 (u)
        integer, intent(in) :: u
        class(prclib_driver_t), allocatable :: driver
        type(os_data_t) :: os_data
        character(32), parameter :: md5sum = "prclib_interfaces_3_md5sum"
        class(prc_writer_t), pointer :: test_writer_1, test_writer_2

        call os_data%init ()
        os_data%fc = "fortran-compiler"
        os_data%whizard_includes = "-I module-dir"
        os_data%fcflags = "-C=all"
    end subroutine prclib_interfaces_3

```

```

os_data%fcflags_pic = "-PIC"
os_data%cc = "c-compiler"
os_data%cflags = "-I include-dir"
os_data%cflags_pic = "-PIC"
os_data%whizard_ldflags = ""
os_data%ldflags = ""
os_data%whizard_libtool = "my-libtool"
os_data%latex = "latex -halt-on-error"
os_data%mpost = "mpost --math=scaled -halt-on-error"
os_data%dvips = "dvips"
os_data%ps2pdf = "ps2pdf14"
os_data%whizard_texpath = ""

write (u, "(A)")  "* Test output: prclib_interfaces_3"
write (u, "(A)")  "* Purpose: check the generated Makefile"
write (u, *)
write (u, "(A)")  "* Create a prclib driver object (2 processes)"
write (u, "(A)")

call dispatch_prclib_driver (driver, var_str ("prclib3"), var_str (""))
call driver%init (2)
call driver%set_md5sum (md5sum)

allocate (test_writer_1_t :: test_writer_1)
allocate (test_writer_2_t :: test_writer_2)

call driver%set_record (1, var_str ("test1"), var_str ("Test_model"), &
    [var_str ("proc1")], test_writer_1)

call driver%set_record (2, var_str ("test2"), var_str ("Test_model"), &
    [var_str ("proc1"), var_str ("proc2")], test_writer_2)

call driver%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write Makefile"
write (u, "(A)")  "* File contents:"
write (u, "(A)")

call driver%generate_makefile (u, os_data, verbose = .true.)

deallocate (test_writer_1)
deallocate (test_writer_2)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prclib_interfaces_3"
end subroutine prclib_interfaces_3

```

Compile test with Fortran module

Test 4: Write driver and makefile and try to compile and link the library driver.
 There is a single test process with a single feature. The process code is

provided as a Fortran module, therefore we need a wrapper for the featured procedure.

```

<Prclib interfaces: execute tests>+≡
    call test (prclib_interfaces_4, "prclib_interfaces_4", &
        "compile and link (Fortran module)", &
        u, results)

<Prclib interfaces: test declarations>+≡
    public :: prclib_interfaces_4

<Prclib interfaces: tests>+≡
    subroutine prclib_interfaces_4 (u)
        integer, intent(in) :: u
        class(prclib_driver_t), allocatable :: driver
        class(prc_writer_t), pointer :: test_writer_4
        type(os_data_t) :: os_data
        integer :: u_file

        integer, dimension(:,:), allocatable :: flv_state
        integer, dimension(:,:), allocatable :: hel_state
        integer, dimension(:,:,:), allocatable :: col_state
        logical, dimension(:,:), allocatable :: ghost_flag
        integer, dimension(:,:), allocatable :: cf_index
        complex(default), dimension(:), allocatable :: color_factors
        character(32), parameter :: md5sum = "prclib_interfaces_4_md5sum"
        character(32) :: md5sum_file

        type(c_funptr) :: proc1_ptr
        interface
            subroutine proc1_t (n) bind(C)
                import
                integer(c_int), intent(out) :: n
            end subroutine proc1_t
        end interface
        procedure(proc1_t), pointer :: proc1
        integer(c_int) :: n

        write (u, "(A)")  "*" Test output: prclib_interfaces_4"
        write (u, "(A)")  "*" Purpose: compile, link, and load process library"
        write (u, "(A)")  "*" with (fake) matrix-element code &
            &as a Fortran module"
        write (u, *)
        write (u, "(A)")  "*" Create a prclib driver object (1 process)"
        write (u, "(A)")

        call os_data%init ()

        allocate (test_writer_4_t :: test_writer_4)
        call test_writer_4%init_test ()

        call dispatch_prclib_driver (driver, var_str ("prclib4"), var_str (""))
        call driver%init (1)
        call driver%set_md5sum (md5sum)

        call driver%set_record (1, var_str ("test4"), var_str ("Test_model"), &

```



```

[var_str ("proc1")], test_writer_4)

call driver%write (u)

write (u, *)
write (u, "(A)")  "* Write Makefile"
u_file = free_unit ()
open (u_file, file="prclib4.makefile", status="replace", action="write")
call driver%generate_makefile (u_file, os_data, verbose = .false.)
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Recall MD5 sum from Makefile"
write (u, "(A)")

md5sum_file = driver%get_md5sum_makefile ()
write (u, "(1x,A,A,A)")  "MD5 sum = '", md5sum_file, "'"

write (u, "(A)")
write (u, "(A)")  "* Write driver source code"

u_file = free_unit ()
open (u_file, file="prclib4.f90", status="replace", action="write")
call driver%generate_driver_code (u_file)
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Recall MD5 sum from driver source"
write (u, "(A)")

md5sum_file = driver%get_md5sum_driver ()
write (u, "(1x,A,A,A)")  "MD5 sum = '", md5sum_file, "'"

write (u, "(A)")
write (u, "(A)")  "* Write matrix-element source code"
call driver%make_source (os_data)

write (u, "(A)")
write (u, "(A)")  "* Recall MD5 sum from matrix-element source"
write (u, "(A)")

md5sum_file = driver%get_md5sum_source (1)
write (u, "(1x,A,A,A)")  "MD5 sum = '", md5sum_file, "'"

write (u, "(A)")
write (u, "(A)")  "* Compile source code"
call driver%make_compile (os_data)

write (u, "(A)")  "* Link library"
call driver%make_link (os_data)

write (u, "(A)")  "* Load library"
call driver%load (os_data)

```

```

write (u, *)
call driver%write (u)
write (u, *)

if (driver%loaded) then
  write (u, "(A)")  "* Call library functions:"
  write (u, *)
  write (u, "(1x,A,I0)")  "n_processes   = ", driver%get_n_processes ()
  write (u, "(1x,A,A,A)")  "process_id   = '", &
    char (driver%get_process_id (1)), "'"
  write (u, "(1x,A,A,A)")  "model_name   = '", &
    char (driver%get_model_name (1)), "'"
  write (u, "(1x,A,A,A)")  "md5sum (lib) = '", &
    char (driver%get_md5sum (0)), "'"
  write (u, "(1x,A,A,A)")  "md5sum (proc) = '", &
    char (driver%get_md5sum (1)), "'"
  write (u, "(1x,A,L1)")  "openmp_status = ", driver%get_openmp_status (1)
  write (u, "(1x,A,I0)")  "n_in = ", driver%get_n_in (1)
  write (u, "(1x,A,I0)")  "n_out = ", driver%get_n_out (1)
  write (u, "(1x,A,I0)")  "n_flv = ", driver%get_n_flv (1)
  write (u, "(1x,A,I0)")  "n_hel = ", driver%get_n_hel (1)
  write (u, "(1x,A,I0)")  "n_col = ", driver%get_n_col (1)
  write (u, "(1x,A,I0)")  "n_cin = ", driver%get_n_cin (1)
  write (u, "(1x,A,I0)")  "n_cf = ", driver%get_n_cf (1)

  call driver%set_flv_state (1, flv_state)
  write (u, "(1x,A,10(1x,I0))")  "flv_state =", flv_state

  call driver%set_hel_state (1, hel_state)
  write (u, "(1x,A,10(1x,I0))")  "hel_state =", hel_state

  call driver%set_col_state (1, col_state, ghost_flag)
  write (u, "(1x,A,10(1x,I0))")  "col_state =", col_state
  write (u, "(1x,A,10(1x,L1))")  "ghost_flag =", ghost_flag

  call driver%set_color_factors (1, color_factors, cf_index)
  write (u, "(1x,A,10(1x,F5.3))")  "color_factors =", color_factors
  write (u, "(1x,A,10(1x,I0))")  "cf_index =", cf_index

  call driver%get_fptr (1, 1, proc1_ptr)
  call c_f_procpointer (proc1_ptr, proc1)
  if (associated (proc1)) then
    write (u, *)
    call proc1 (n)
    write (u, "(1x,A,I0)")  "proc1(1) = ", n
  end if

end if

deallocate (test_writer_4)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prclib_interfaces_4"
end subroutine prclib_interfaces_4

```

This version of test-code writer actually writes an interface and wrapper code.
The wrapped function is a no-parameter function with integer result.
The stored MD5 sum may be modified.
We will reuse this later, therefore public.

```

<Prclib interfaces: public test auxiliary>≡
  public :: test_writer_4_t

<Prclib interfaces: test types>+≡
  type, extends (prc_writer_f_module_t) :: test_writer_4_t
  contains
    procedure, nopass :: type_name => test_writer_4_type_name
    procedure, nopass :: get_module_name => &
      test_writer_4_get_module_name
    procedure :: write_makefile_code => test_writer_4_mk
    procedure :: write_source_code => test_writer_4_src
    procedure :: write_interface => test_writer_4_if
    procedure :: write_wrapper => test_writer_4_wr
    procedure :: before_compile => test_writer_4_before_compile
    procedure :: after_compile => test_writer_4_after_compile
  end type test_writer_4_t

<Prclib interfaces: test auxiliary>+≡
  function test_writer_4_type_name () result (string)
    type(string_t) :: string
    string = "test_4"
  end function test_writer_4_type_name

  function test_writer_4_get_module_name (id) result (name)
    type(string_t), intent(in) :: id
    type(string_t) :: name
    name = "tpr_" // id
  end function test_writer_4_get_module_name

  subroutine test_writer_4_mk &
    (writer, unit, id, os_data, verbose, testflag)
    class(test_writer_4_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    write (unit, "(5A)") "SOURCES += ", char (id), ".f90"
    write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
    write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".f90"
    write (unit, "(5A)") "CLEAN_OBJECTS += tpr_", char (id), ".mod"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), ".lo"
    write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
    if (.not. verbose) then
      write (unit, "(5A)") TAB // '@echo " FC "' $@'
    end if
    write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"
  end subroutine test_writer_4_mk

```

```

subroutine test_writer_4_src (writer, id)
  class(test_writer_4_t), intent(in) :: writer
  type(string_t), intent(in) :: id
  call write_test_module_file (id, var_str ("proc1"), writer%md5sum)
end subroutine test_writer_4_src

subroutine test_writer_4_if (writer, unit, id, feature)
  class(test_writer_4_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, "(2x,9A)") "interface"
  write (unit, "(5x,9A)") "subroutine ", &
    char (writer%get_c_procname (id, feature)), &
    " (n) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "implicit none"
  write (unit, "(7x,9A)") "integer(c_int), intent(out) :: n"
  write (unit, "(5x,9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
  write (unit, "(2x,9A)") "end interface"
end subroutine test_writer_4_if

subroutine test_writer_4_wr (writer, unit, id, feature)
  class(test_writer_4_t), intent(in) :: writer
  integer, intent(in) :: unit
  type(string_t), intent(in) :: id, feature
  write (unit, *)
  write (unit, "(9A)") "subroutine ", &
    char (writer%get_c_procname (id, feature)), &
    " (n) bind(C)"
  write (unit, "(2x,9A)") "use iso_c_binding"
  write (unit, "(2x,9A)") "use tpr-", char (id), ", only: ", &
    char (writer%get_procname (feature))
  write (unit, "(2x,9A)") "implicit none"
  write (unit, "(2x,9A)") "integer(c_int), intent(out) :: n"
  write (unit, "(2x,9A)") "call ", char (feature), " (n)"
  write (unit, "(9A)") "end subroutine ", &
    char (writer%get_c_procname (id, feature))
end subroutine test_writer_4_wr

subroutine test_writer_4_before_compile (writer, id)
  class(test_writer_4_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_4_before_compile

subroutine test_writer_4_after_compile (writer, id)
  class(test_writer_4_t), intent(in) :: writer
  type(string_t), intent(in) :: id
end subroutine test_writer_4_after_compile

```

We need a test module file (actually, one for each process in the test above) that allows us to check compilation and linking. The test module implements a colorless $1 \rightarrow 2$ process, and it implements one additional function (feature),

the name given as an argument.

(Prclib interfaces: test auxiliary)+≡

```

subroutine write_test_module_file (basename, feature, md5sum)
  type(string_t), intent(in) :: basename
  type(string_t), intent(in) :: feature
  character(32), intent(in) :: md5sum
  integer :: u
  u = free_unit ()
  open (u, file = char (basename) // ".f90", &
        status = "replace", action = "write")
  write (u, "(A)")  "! (Pseudo) matrix element code file &
    &for WHIZARD self-test"
  write (u, *)
  write (u, "(A)")  "module tpr_" // char (basename)
  write (u, *)
  write (u, "(2x,A)")  "use kinds"
  write (u, "(2x,A)")  "use omega_color, OCF => omega_color_factor"
  write (u, *)
  write (u, "(2x,A)")  "implicit none"
  write (u, "(2x,A)")  "private"
  write (u, *)
  call write_test_me_code_1 (u)
  write (u, *)
  write (u, "(2x,A)")  "public :: " // char (feature)
  write (u, *)
  write (u, "(A)")  "contains"
  write (u, *)
  call write_test_me_code_2 (u, md5sum)
  write (u, *)
  write (u, "(2x,A)")  "subroutine " // char (feature) // " (n)"
  write (u, "(2x,A)")  "  integer, intent(out) :: n"
  write (u, "(2x,A)")  "  n = 42"
  write (u, "(2x,A)")  "end subroutine " // char (feature)
  write (u, *)
  write (u, "(A)")  "end module tpr_" // char (basename)
  close (u)
end subroutine write_test_module_file

```

The following two subroutines provide building blocks for a matrix-element source code file, useful only for testing the workflow. The first routine writes the header part, the other routine the implementation of the procedures listed in the header.

(Prclib interfaces: test auxiliary)+≡

```

subroutine write_test_me_code_1 (u)
  integer, intent(in) :: u
  write (u, "(2x,A)")  "public :: md5sum"
  write (u, "(2x,A)")  "public :: openmp_supported"
  write (u, *)
  write (u, "(2x,A)")  "public :: n_in"
  write (u, "(2x,A)")  "public :: n_out"
  write (u, "(2x,A)")  "public :: n_flv"
  write (u, "(2x,A)")  "public :: n_hel"
  write (u, "(2x,A)")  "public :: n_cin"

```

```

write (u, "(2x,A)") "public :: n_col"
write (u, "(2x,A)") "public :: n_cf"
write (u, *)
write (u, "(2x,A)") "public :: flv_state"
write (u, "(2x,A)") "public :: hel_state"
write (u, "(2x,A)") "public :: col_state"
write (u, "(2x,A)") "public :: color_factors"
end subroutine write_test_me_code_1

subroutine write_test_me_code_2 (u, md5sum)
  integer, intent(in) :: u
  character(32), intent(in) :: md5sum
  write (u, "(2x,A)") "pure function md5sum ()"
  write (u, "(2x,A)") "  character(len=32) :: md5sum"
  write (u, "(2x,A)") "  md5sum = ' " // md5sum // "' "
  write (u, "(2x,A)") "end function md5sum"
  write (u, *)
  write (u, "(2x,A)") "pure function openmp_supported () result (status)"
  write (u, "(2x,A)") "  logical :: status"
  write (u, "(2x,A)") "  status = .false."
  write (u, "(2x,A)") "end function openmp_supported"
  write (u, *)
  write (u, "(2x,A)") "pure function n_in () result (n)"
  write (u, "(2x,A)") "  integer :: n"
  write (u, "(2x,A)") "  n = 1"
  write (u, "(2x,A)") "end function n_in"
  write (u, *)
  write (u, "(2x,A)") "pure function n_out () result (n)"
  write (u, "(2x,A)") "  integer :: n"
  write (u, "(2x,A)") "  n = 2"
  write (u, "(2x,A)") "end function n_out"
  write (u, *)
  write (u, "(2x,A)") "pure function n_flv () result (n)"
  write (u, "(2x,A)") "  integer :: n"
  write (u, "(2x,A)") "  n = 1"
  write (u, "(2x,A)") "end function n_flv"
  write (u, *)
  write (u, "(2x,A)") "pure function n_hel () result (n)"
  write (u, "(2x,A)") "  integer :: n"
  write (u, "(2x,A)") "  n = 1"
  write (u, "(2x,A)") "end function n_hel"
  write (u, *)
  write (u, "(2x,A)") "pure function n_cin () result (n)"
  write (u, "(2x,A)") "  integer :: n"
  write (u, "(2x,A)") "  n = 2"
  write (u, "(2x,A)") "end function n_cin"
  write (u, *)
  write (u, "(2x,A)") "pure function n_col () result (n)"
  write (u, "(2x,A)") "  integer :: n"
  write (u, "(2x,A)") "  n = 1"
  write (u, "(2x,A)") "end function n_col"
  write (u, *)
  write (u, "(2x,A)") "pure function n_cf () result (n)"
  write (u, "(2x,A)") "  integer :: n"

```

```

write (u, "(2x,A)") "  n = 1"
write (u, "(2x,A)") "end function n_cf"
write (u, *)
write (u, "(2x,A)") "pure subroutine flv_state (a)"
write (u, "(2x,A)") "  integer, dimension(:,:), intent(out) :: a"
write (u, "(2x,A)") "  a = reshape ([1,2,3], [3,1])"
write (u, "(2x,A)") "end subroutine flv_state"
write (u, *)
write (u, "(2x,A)") "pure subroutine hel_state (a)"
write (u, "(2x,A)") "  integer, dimension(:,:), intent(out) :: a"
write (u, "(2x,A)") "  a = reshape ([0,0,0], [3,1])"
write (u, "(2x,A)") "end subroutine hel_state"
write (u, *)
write (u, "(2x,A)") "pure subroutine col_state (a, g)"
write (u, "(2x,A)") "  integer, dimension(:,:,:), intent(out) :: a"
write (u, "(2x,A)") "  logical, dimension(:,:), intent(out) :: g"
write (u, "(2x,A)") "  a = reshape ([0,0, 0,0, 0,0], [2,3,1])"
write (u, "(2x,A)") "  g = reshape ([.false., .false., .false.], [3,1])"
write (u, "(2x,A)") "end subroutine col_state"
write (u, *)
write (u, "(2x,A)") "pure subroutine color_factors (cf)"
write (u, "(2x,A)") "  type(OCF), dimension(:), intent(out) :: cf"
write (u, "(2x,A)") "  cf = [ OCF(1,1,+1._default) ]"
write (u, "(2x,A)") "end subroutine color_factors"
end subroutine write_test_me_code_2

```

Compile test with Fortran bind(C) library

Test 5: Write driver and makefile and try to compile and link the library driver.

There is a single test process with a single feature. The process code is provided as a Fortran library of independent procedures. These procedures are bind(C).

```

<Prclib interfaces: execute tests>+≡
  call test (prclib_interfaces_5, "prclib_interfaces_5", &
    "compile and link (Fortran library)", &
    u, results)

<Prclib interfaces: test declarations>+≡
  public :: prclib_interfaces_5

<Prclib interfaces: tests>+≡
  subroutine prclib_interfaces_5 (u)
    integer, intent(in) :: u
    class(prclib_driver_t), allocatable :: driver
    class(prc_writer_t), pointer :: test_writer_5
    type(os_data_t) :: os_data
    integer :: u_file

    integer, dimension(:,:), allocatable :: flv_state
    integer, dimension(:,:), allocatable :: hel_state
    integer, dimension(:,:,:), allocatable :: col_state
    logical, dimension(:,:), allocatable :: ghost_flag
    integer, dimension(:,:), allocatable :: cf_index

```

```

complex(default), dimension(:), allocatable :: color_factors
character(32), parameter :: md5sum = "prclib_interfaces_5_md5sum      "

type(c_funptr) :: proc1_ptr
interface
    subroutine proc1_t (n) bind(C)
        import
        integer(c_int), intent(out) :: n
    end subroutine proc1_t
end interface
procedure(proc1_t), pointer :: proc1
integer(c_int) :: n

write (u, "(A)")  "* Test output: prclib_interfaces_5"
write (u, "(A)")  "*   Purpose: compile, link, and load process library"
write (u, "(A)")  "*               with (fake) matrix-element code &
                &as a Fortran bind(C) library"
write (u, *)
write (u, "(A)")  "* Create a prclib driver object (1 process)"
write (u, "(A)")

call os_data%init ()
allocate (test_writer_5_t :: test_writer_5)

call dispatch_prclib_driver (driver, var_str ("prclib5"), var_str (""))
call driver%init (1)
call driver%set_md5sum (md5sum)

call driver%set_record (1, var_str ("test5"), var_str ("Test_model"), &
    [var_str ("proc1")], test_writer_5)

call driver%write (u)

write (u, *)
write (u, "(A)")  "* Write makefile"
u_file = free_unit ()
open (u_file, file="prclib5.makefile", status="replace", action="write")
call driver%generate_makefile (u_file, os_data, verbose = .false.)
close (u_file)

write (u, "(A)")  "* Write driver source code"
u_file = free_unit ()
open (u_file, file="prclib5.f90", status="replace", action="write")
call driver%generate_driver_code (u_file)
close (u_file)

write (u, "(A)")  "* Write matrix-element source code"
call driver%make_source (os_data)

write (u, "(A)")  "* Compile source code"
call driver%make_compile (os_data)

write (u, "(A)")  "* Link library"
call driver%make_link (os_data)

```



```

write (u, "(A)")  "* Load library"
call driver%load (os_data)

write (u, *)
call driver%write (u)
write (u, *)

if (driver%loaded) then
  write (u, "(A)")  "* Call library functions:"
  write (u, *)
  write (u, "(1x,A,I0)")  "n_processes  = ", driver%get_n_processes ()
  write (u, "(1x,A,A)")  "process_id    = ", &
    char (driver%get_process_id (1))
  write (u, "(1x,A,A)")  "model_name   = ", &
    char (driver%get_model_name (1))
  write (u, "(1x,A,A)")  "md5sum       = ", &
    char (driver%get_md5sum (1))
  write (u, "(1x,A,L1)")  "openmp_status = ", driver%get_openmp_status (1)
  write (u, "(1x,A,I0)")  "n_in      = ", driver%get_n_in (1)
  write (u, "(1x,A,I0)")  "n_out     = ", driver%get_n_out (1)
  write (u, "(1x,A,I0)")  "n_flv     = ", driver%get_n_flv (1)
  write (u, "(1x,A,I0)")  "n_hel     = ", driver%get_n_hel (1)
  write (u, "(1x,A,I0)")  "n_col     = ", driver%get_n_col (1)
  write (u, "(1x,A,I0)")  "n_cin     = ", driver%get_n_cin (1)
  write (u, "(1x,A,I0)")  "n_cf      = ", driver%get_n_cf (1)

  call driver%set_flv_state (1, flv_state)
  write (u, "(1x,A,10(1x,I0))")  "flv_state =", flv_state

  call driver%set_hel_state (1, hel_state)
  write (u, "(1x,A,10(1x,I0))")  "hel_state =", hel_state

  call driver%set_col_state (1, col_state, ghost_flag)
  write (u, "(1x,A,10(1x,I0))")  "col_state =", col_state
  write (u, "(1x,A,10(1x,L1))")  "ghost_flag =", ghost_flag

  call driver%set_color_factors (1, color_factors, cf_index)
  write (u, "(1x,A,10(1x,F5.3))")  "color_factors =", color_factors
  write (u, "(1x,A,10(1x,I0))")  "cf_index =", cf_index

  call driver%get_fptr (1, 1, proc1_ptr)
  call c_f_procpointer (proc1_ptr, proc1)
  if (associated (proc1)) then
    write (u, *)
    call proc1 (n)
    write (u, "(1x,A,I0)")  "proc1(1) = ", n
  end if

end if

deallocate (test_writer_5)

write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: prclib_interfaces_5"
    end subroutine prclib_interfaces_5

```

This version of test-code writer writes interfaces for all standard features plus one specific feature. The interfaces are all bind(C), so no wrapper is needed.

(Prclib interfaces: test types)+≡

```

type, extends (prc_writer_c_lib_t) :: test_writer_5_t
contains
    procedure, nopass :: type_name => test_writer_5_type_name
    procedure :: write_makefile_code => test_writer_5_mk
    procedure :: write_source_code => test_writer_5_src
    procedure :: write_interface => test_writer_5_if
    procedure :: before_compile => test_writer_5_before_compile
    procedure :: after_compile => test_writer_5_after_compile
end type test_writer_5_t

```

The

(Prclib interfaces: test auxiliary)+≡

```

function test_writer_5_type_name () result (string)
    type(string_t) :: string
    string = "test_5"
end function test_writer_5_type_name

subroutine test_writer_5_mk &
    (writer, unit, id, os_data, verbose, testflag)
    class(test_writer_5_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    write (unit, "(5A)")  "SOURCES += ", char (id), ".f90"
    write (unit, "(5A)")  "OBJECTS += ", char (id), ".lo"
    write (unit, "(5A)")  char (id), ".lo: ", char (id), ".f90"
    if (.not. verbose) then
        write (unit, "(5A)")  TAB // '@echo " FC          "$@"
    end if
    write (unit, "(5A)")  TAB, "$(LTF_COMPILE) $<"
end subroutine test_writer_5_mk

subroutine test_writer_5_src (writer, id)
    class(test_writer_5_t), intent(in) :: writer
    type(string_t), intent(in) :: id
    call write_test_f_lib_file (id, var_str ("proc1"))
end subroutine test_writer_5_src

subroutine test_writer_5_if (writer, unit, id, feature)
    class(test_writer_5_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
    select case (char (feature))
    case ("proc1")
        write (unit, "(2x,9A)")  "interface"

```

```

        write (unit, "(5x,9A)") "subroutine ", &
            char (writer%get_c_procname (id, feature)), &
            " (n) bind(C)"
        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "implicit none"
        write (unit, "(7x,9A)") "integer(c_int), intent(out) :: n"
        write (unit, "(5x,9A)") "end subroutine ", &
            char (writer%get_c_procname (id, feature))
        write (unit, "(2x,9A)") "end interface"
    case default
        call writer%write_standard_interface (unit, id, feature)
    end select
end subroutine test_writer_5_if

subroutine test_writer_5_before_compile (writer, id)
    class(test_writer_5_t), intent(in) :: writer
    type(string_t), intent(in) :: id
end subroutine test_writer_5_before_compile

subroutine test_writer_5_after_compile (writer, id)
    class(test_writer_5_t), intent(in) :: writer
    type(string_t), intent(in) :: id
end subroutine test_writer_5_after_compile

```

We need a test module file (actually, one for each process in the test above) that allows us to check compilation and linking. The test module implements a colorless $1 \rightarrow 2$ process, and it implements one additional function (feature), the name given as an argument.

(Prclib interfaces: test auxiliary)+≡

```

subroutine write_test_f_lib_file (basename, feature)
    type(string_t), intent(in) :: basename
    type(string_t), intent(in) :: feature
    integer :: u
    u = free_unit ()
    open (u, file = char (basename) // ".f90", &
        status = "replace", action = "write")
    write (u, "(A)") " ! (Pseudo) matrix element code file &
        &for WHIZARD self-test"
    call write_test_me_code_3 (u, char (basename))
    write (u, *)
    write (u, "(A)") "subroutine " // char (basename) // "_" &
        // char (feature) // " (n) bind(C)"
    write (u, "(A)") " use iso_c_binding"
    write (u, "(A)") " implicit none"
    write (u, "(A)") " integer(c_int), intent(out) :: n"
    write (u, "(A)") " n = 42"
    write (u, "(A)") "end subroutine " // char (basename) // "_" &
        // char (feature)
    close (u)
end subroutine write_test_f_lib_file

```

The following matrix-element source code is identical to the previous one, but modified such as to provide independent procedures without a module envelope.

<Prclib interfaces: test auxiliary>+≡

```

subroutine write_test_me_code_3 (u, id)
  integer, intent(in) :: u
  character(*), intent(in) :: id
  write (u, "(A)") "function " // id // "_get_md5sum () &
    &result (cptr) bind(C)"
  write (u, "(A)") " use iso_c_binding"
  write (u, "(A)") " implicit none"
  write (u, "(A)") " type(c_ptr) :: cptr"
  write (u, "(A)") " character(c_char), dimension(32), &
    &target, save :: md5sum"
  write (u, "(A)") " md5sum = copy (c_char_&
    &'1234567890abcdef1234567890abcdef')"
  write (u, "(A)") " cptr = c_loc (md5sum)"
  write (u, "(A)") "contains"
  write (u, "(A)") " function copy (md5sum)"
  write (u, "(A)") " character(c_char), dimension(32) :: copy"
  write (u, "(A)") " character(c_char), dimension(32), intent(in) :: &
    &md5sum"
  write (u, "(A)") " copy = md5sum"
  write (u, "(A)") " end function copy"
  write (u, "(A)") "end function " // id // "_get_md5sum"
  write (u, *)
  write (u, "(A)") "function " // id // "_openmp_supported () &
    &result (status) bind(C)"
  write (u, "(A)") " use iso_c_binding"
  write (u, "(A)") " implicit none"
  write (u, "(A)") " logical(c_bool) :: status"
  write (u, "(A)") " status = .false."
  write (u, "(A)") "end function " // id // "_openmp_supported"
  write (u, *)
  write (u, "(A)") "function " // id // "_n_in () result (n) bind(C)"
  write (u, "(A)") " use iso_c_binding"
  write (u, "(A)") " implicit none"
  write (u, "(A)") " integer(c_int) :: n"
  write (u, "(A)") " n = 1"
  write (u, "(A)") "end function " // id // "_n_in"
  write (u, *)
  write (u, "(A)") "function " // id // "_n_out () result (n) bind(C)"
  write (u, "(A)") " use iso_c_binding"
  write (u, "(A)") " implicit none"
  write (u, "(A)") " integer(c_int) :: n"
  write (u, "(A)") " n = 2"
  write (u, "(A)") "end function " // id // "_n_out"
  write (u, *)
  write (u, "(A)") "function " // id // "_n_flv () result (n) bind(C)"
  write (u, "(A)") " use iso_c_binding"
  write (u, "(A)") " implicit none"
  write (u, "(A)") " integer(c_int) :: n"
  write (u, "(A)") " n = 1"
  write (u, "(A)") "end function " // id // "_n_flv"
  write (u, *)
  write (u, "(A)") "function " // id // "_n_hel () result (n) bind(C)"
  write (u, "(A)") " use iso_c_binding"

```

```

write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int) :: n"
write (u, "(A)") " n = 1"
write (u, "(A)") "end function " // id // "_n_hel"
write (u, *)
write (u, "(A)") "function " // id // "_n_cin () result (n) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int) :: n"
write (u, "(A)") " n = 2"
write (u, "(A)") "end function " // id // "_n_cin"
write (u, *)
write (u, "(A)") "function " // id // "_n_col () result (n) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int) :: n"
write (u, "(A)") " n = 1"
write (u, "(A)") "end function " // id // "_n_col"
write (u, *)
write (u, "(A)") "function " // id // "_n_cf () result (n) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int) :: n"
write (u, "(A)") " n = 1"
write (u, "(A)") "end function " // id // "_n_cf"
write (u, *)
write (u, "(A)") "subroutine " // id // "_flv_state (flv_state) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) :: flv_state"
write (u, "(A)") " flv_state(1:3) = [1,2,3]"
write (u, "(A)") "end subroutine " // id // "_flv_state"
write (u, *)
write (u, "(A)") "subroutine " // id // "_hel_state (hel_state) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) :: hel_state"
write (u, "(A)") " hel_state(1:3) = [0,0,0]"
write (u, "(A)") "end subroutine " // id // "_hel_state"
write (u, *)
write (u, "(A)") "subroutine " // id // "_col_state &"
write (u, "(A)") " &(col_state, ghost_flag) bind(C)"
write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) &"
write (u, "(A)") " &:: col_state"
write (u, "(A)") " logical(c_bool), dimension(*), intent(out) &"
write (u, "(A)") " &:: ghost_flag"
write (u, "(A)") " col_state(1:6) = [0,0, 0,0, 0,0]"
write (u, "(A)") " ghost_flag(1:3) = [.false., .false., .false.]"
write (u, "(A)") "end subroutine " // id // "_col_state"
write (u, *)
write (u, "(A)") "subroutine " // id // "_color_factors &"
write (u, "(A)") " &(cf_index1, cf_index2, color_factors) bind(C)"

```

```

write (u, "(A)") " use iso_c_binding"
write (u, "(A)") " use kinds"
write (u, "(A)") " implicit none"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) :: cf_index1"
write (u, "(A)") " integer(c_int), dimension(*), intent(out) :: cf_index2"
write (u, "(A)") " complex(c_default_complex), dimension(*), &
    &intent(out) :: color_factors"
write (u, "(A)") " cf_index1(1:1) = [1]"
write (u, "(A)") " cf_index2(1:1) = [1]"
write (u, "(A)") " color_factors(1:1) = [1]"
write (u, "(A)") "end subroutine " // id // "_color_factors"
end subroutine write_test_me_code_3

```

Compile test with genuine C library

Test 6: Write driver and makefile and try to compile and link the library driver.

There is a single test process with a single feature. The process code is provided as a C library of independent procedures. These procedures should match the Fortran bind(C) interface.

```

<Prclib interfaces: execute tests>+≡
  if (default == double .or. (CC_IS_GNU .and. CC_HAS_QUADMATH)) then
    call test (prclib_interfaces_6, "prclib_interfaces_6", &
      "compile and link (C library)", &
      u, results)
  end if

<Prclib interfaces: test declarations>+≡
  public :: prclib_interfaces_6

<Prclib interfaces: tests>+≡
  subroutine prclib_interfaces_6 (u)
    integer, intent(in) :: u
    class(prclib_driver_t), allocatable :: driver
    class(prc_writer_t), pointer :: test_writer_6
    type(os_data_t) :: os_data
    integer :: u_file

    integer, dimension(:,:), allocatable :: flv_state
    integer, dimension(:,:), allocatable :: hel_state
    integer, dimension(:,:,:), allocatable :: col_state
    logical, dimension(:,:), allocatable :: ghost_flag
    integer, dimension(:,:), allocatable :: cf_index
    complex(default), dimension(:), allocatable :: color_factors
    character(32), parameter :: md5sum = "prclib_interfaces_6_md5sum"

    type(c_funptr) :: proc1_ptr
    interface
      subroutine proc1_t (n) bind(C)
        import
        integer(c_int), intent(out) :: n
      end subroutine proc1_t
    end interface
    procedure(proc1_t), pointer :: proc1

```

```

integer(c_int) :: n

write (u, "(A)")  "* Test output: prclib_interfaces_6"
write (u, "(A)")  "* Purpose: compile, link, and load process library"
write (u, "(A)")  "*           with (fake) matrix-element code &
                    &as a C library"
write (u, *)
write (u, "(A)")  "* Create a prclib driver object (1 process)"
write (u, "(A)")

call os_data%init ()
allocate (test_writer_6_t :: test_writer_6)

call dispatch_prclib_driver (driver, var_str ("prclib6"), var_str (""))
call driver%init (1)
call driver%set_md5sum (md5sum)

call driver%set_record (1, var_str ("test6"), var_str ("Test_model"), &
    [var_str ("proc1")], test_writer_6)

call driver%write (u)

write (u, *)
write (u, "(A)")  "* Write makefile"
u_file = free_unit ()
open (u_file, file="prclib6.makefile", status="replace", action="write")
call driver%generate_makefile (u_file, os_data, verbose = .false.)
close (u_file)

write (u, "(A)")  "* Write driver source code"
u_file = free_unit ()
open (u_file, file="prclib6.f90", status="replace", action="write")
call driver%generate_driver_code (u_file)
close (u_file)

write (u, "(A)")  "* Write matrix-element source code"
call driver%make_source (os_data)

write (u, "(A)")  "* Compile source code"
call driver%make_compile (os_data)

write (u, "(A)")  "* Link library"
call driver%make_link (os_data)

write (u, "(A)")  "* Load library"
call driver%load (os_data)

write (u, *)
call driver%write (u)
write (u, *)

if (driver%loaded) then
    write (u, "(A)")  "* Call library functions:"
    write (u, *)

```

```

write (u, "(1x,A,I0)") "n_processes = ", driver%get_n_processes ()
write (u, "(1x,A,A)") "process_id = ", &
    char (driver%get_process_id (1))
write (u, "(1x,A,A)") "model_name = ", &
    char (driver%get_model_name (1))
write (u, "(1x,A,A)") "md5sum = ", &
    char (driver%get_md5sum (1))
write (u, "(1x,A,L1)") "openmp_status = ", driver%get_openmp_status (1)
write (u, "(1x,A,I0)") "n_in = ", driver%get_n_in (1)
write (u, "(1x,A,I0)") "n_out = ", driver%get_n_out (1)
write (u, "(1x,A,I0)") "n_flv = ", driver%get_n_flv (1)
write (u, "(1x,A,I0)") "n_hel = ", driver%get_n_hel (1)
write (u, "(1x,A,I0)") "n_col = ", driver%get_n_col (1)
write (u, "(1x,A,I0)") "n_cin = ", driver%get_n_cin (1)
write (u, "(1x,A,I0)") "n_cf = ", driver%get_n_cf (1)

call driver%set_flv_state (1, flv_state)
write (u, "(1x,A,10(1x,I0))") "flv_state =", flv_state

call driver%set_hel_state (1, hel_state)
write (u, "(1x,A,10(1x,I0))") "hel_state =", hel_state

call driver%set_col_state (1, col_state, ghost_flag)
write (u, "(1x,A,10(1x,I0))") "col_state =", col_state
write (u, "(1x,A,10(1x,L1))") "ghost_flag =", ghost_flag

call driver%set_color_factors (1, color_factors, cf_index)
write (u, "(1x,A,10(1x,F5.3))") "color_factors =", color_factors
write (u, "(1x,A,10(1x,I0))") "cf_index =", cf_index

call driver%get_fptr (1, 1, proc1_ptr)
call c_f_procpointer (proc1_ptr, proc1)
if (associated (proc1)) then
    write (u, *)
    call proc1 (n)
    write (u, "(1x,A,I0)") "proc1(1) = ", n
end if

end if

deallocate (test_writer_6)

write (u, "(A)")
write (u, "(A)") "* Test output end: prclib_interfaces_6"
end subroutine prclib_interfaces_6

```

This version of test-code writer writes interfaces for all standard features plus one specific feature. The interfaces are all `bind(C)`, so no wrapper is needed.

The driver part is identical to the Fortran case, so we simply extend the previous `test_writer_5` type. We only have to override the Makefile writer.

```

(Prclib interfaces: test types)+≡
type, extends (test_writer_5_t) :: test_writer_6_t
contains

```



```

        procedure, nopass :: type_name => test_writer_6_type_name
        procedure :: write_makefile_code => test_writer_6_mk
        procedure :: write_source_code => test_writer_6_src
    end type test_writer_6_t

```

<Prclib interfaces: test auxiliary>+≡

```

function test_writer_6_type_name () result (string)
    type(string_t) :: string
    string = "test_6"
end function test_writer_6_type_name

subroutine test_writer_6_mk &
    (writer, unit, id, os_data, verbose, testflag)
    class(test_writer_6_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(os_data_t), intent(in) :: os_data
    logical, intent(in) :: verbose
    logical, intent(in), optional :: testflag
    write (unit, "(5A)") "SOURCES += ", char (id), ".c"
    write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
    write (unit, "(5A)") char (id), ".lo: ", char (id), ".c"
    if (.not. verbose) then
        write (unit, "(5A)") TAB // '@echo " FC " $@"
    end if
    write (unit, "(5A)") TAB, "$(LTCCOMPILE) $<"
end subroutine test_writer_6_mk

subroutine test_writer_6_src (writer, id)
    class(test_writer_6_t), intent(in) :: writer
    type(string_t), intent(in) :: id
    call write_test_c_lib_file (id, var_str ("proc1"))
end subroutine test_writer_6_src

```

We need a test module file (actually, one for each process in the test above) that allows us to check compilation and linking. The test module implements a colorless $1 \rightarrow 2$ process, and it implements one additional function (feature), the name given as an argument.

<Prclib interfaces: test auxiliary>+≡

```

subroutine write_test_c_lib_file (basename, feature)
    type(string_t), intent(in) :: basename
    type(string_t), intent(in) :: feature
    integer :: u
    u = free_unit ()
    open (u, file = char (basename) // ".c", &
        status = "replace", action = "write")
    write (u, "(A)") "/* (Pseudo) matrix element code file &
        &for WHIZARD self-test */"
    write (u, "(A)") "#include <stdbool.h>"
    if (CC_HAS_QUADMATH) then
        write (u, "(A)") "#include <quadmath.h>"
    end if
    write (u, *)

```

```

call write_test_me_code_4 (u, char (basename))
write (u, *)
write (u, "(A)") "void " // char (basename) // "_" &
// char (feature) // "(int* n) {"
write (u, "(A)") " *n = 42;"
write (u, "(A)") "}"
close (u)
end subroutine write_test_c_lib_file

```

The following matrix-element source code is equivalent to the code in the previous example, but coded in C.

(Prclib interfaces: test auxiliary)+≡

```

subroutine write_test_me_code_4 (u, id)
  integer, intent(in) :: u
  character(*), intent(in) :: id
  write (u, "(A)") "char* " // id // "_get_md5sum() {"
  write (u, "(A)") " return ""1234567890abcdef1234567890abcdef"";"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "bool " // id // "_openmp_supported() {"
  write (u, "(A)") " return false;"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "int " // id // "_n_in() {"
  write (u, "(A)") " return 1;"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "int " // id // "_n_out() {"
  write (u, "(A)") " return 2;"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "int " // id // "_n_flv() {"
  write (u, "(A)") " return 1;"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "int " // id // "_n_hel() {"
  write (u, "(A)") " return 1;"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "int " // id // "_n_cin() {"
  write (u, "(A)") " return 2;"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "int " // id // "_n_col() {"
  write (u, "(A)") " return 1;"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "int " // id // "_n_cf() {"
  write (u, "(A)") " return 1;"
  write (u, "(A)") "}"
  write (u, *)
  write (u, "(A)") "void " // id // "_flv_state( int (*a)[] ) {"
  write (u, "(A)") " static int flv_state[1][3] = { { 1, 2, 3 } };"

```

```

write (u, "(A)") " int j;"
write (u, "(A)") " for (j = 0; j < 3; j++) { (*a)[j] &
&= flv_state[0][j]; }"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "void " // id // "_hel_state( int (*a)[] ) {"
write (u, "(A)") " static int hel_state[1][3] = { { 0, 0, 0 } };"
write (u, "(A)") " int j;"
write (u, "(A)") " for (j = 0; j < 3; j++) { (*a)[j] &
&= hel_state[0][j]; }"
write (u, "(A)") "}"
write (u, *)
write (u, "(A)") "void " // id // "_col_state&
&( int (*a)[], bool (*g)[] ) {"
write (u, "(A)") " static int col_state[1][3][2] = &
&{ { {0, 0}, {0, 0}, {0, 0} } };"
write (u, "(A)") " static bool ghost_flag[1][3] = &
&{ { false, false, false } };"
write (u, "(A)") " int j,k;"
write (u, "(A)") " for (j = 0; j < 3; j++) {"
write (u, "(A)") " for (k = 0; k < 2; k++) {"
write (u, "(A)") " (*a)[j*2+k] = col_state[0][j][k];"
write (u, "(A)") " }"
write (u, "(A)") " (*g)[j] = ghost_flag[0][j];"
write (u, "(A)") " }"
write (u, "(A)") "}"
write (u, *)
select case (DEFAULT_FC_PRECISION)
case ("quadruple")
write (u, "(A)") "void " // id // "_color_factors&
&( int (*cf_index1)[], int (*cf_index2)[], &
&__complex128 (*color_factors)[] ) {"
case ("extended")
write (u, "(A)") "void " // id // "_color_factors&
&( int (*cf_index1)[], int (*cf_index2)[], &
&long double _Complex (*color_factors)[] ) {"
case default
write (u, "(A)") "void " // id // "_color_factors&
&( int (*cf_index1)[], int (*cf_index2)[], &
&double _Complex (*color_factors)[] ) {"
end select
write (u, "(A)") " (*color_factors)[0] = 1;"
write (u, "(A)") " (*cf_index1)[0] = 1;"
write (u, "(A)") " (*cf_index2)[0] = 1;"
write (u, "(A)") "}"
end subroutine write_test_me_code_4

```

Test cleanup targets

Test 7: Repeat test 4 (create, compile, link Fortran module and driver) and properly clean up all generated files.

<Prclib interfaces: execute tests>+≡

```

call test (prclib_interfaces_7, "prclib_interfaces_7", &
          "cleanup", &
          u, results)

<Prclib interfaces: test declarations>+≡
public :: prclib_interfaces_7

<Prclib interfaces: tests>+≡
subroutine prclib_interfaces_7 (u)
  integer, intent(in) :: u
  class(prclib_driver_t), allocatable :: driver
  class(prc_writer_t), pointer :: test_writer_4
  type(os_data_t) :: os_data
  integer :: u_file
  character(32), parameter :: md5sum = "1234567890abcdef1234567890abcdef"

  write (u, "(A)")  "* Test output: prclib_interfaces_7"
  write (u, "(A)")  "* Purpose: compile and link process library"
  write (u, "(A)")  "*           with (fake) matrix-element code &
    &as a Fortran module"
  write (u, "(A)")  "*           then clean up generated files"
  write (u, *)
  write (u, "(A)")  "* Create a prclib driver object (1 process)"

  allocate (test_writer_4_t :: test_writer_4)

  call os_data%init ()
  call dispatch_prclib_driver (driver, var_str ("prclib7"), var_str (""))
  call driver%init (1)
  call driver%set_md5sum (md5sum)
  call driver%set_record (1, var_str ("test7"), var_str ("Test_model"), &
    [var_str ("proc1")], test_writer_4)

  write (u, "(A)")  "* Write makefile"
  u_file = free_unit ()
  open (u_file, file="prclib7.makefile", status="replace", action="write")
  call driver%generate_makefile (u_file, os_data, verbose = .false.)
  close (u_file)

  write (u, "(A)")  "* Write driver source code"
  u_file = free_unit ()
  open (u_file, file="prclib7.f90", status="replace", action="write")
  call driver%generate_driver_code (u_file)
  close (u_file)

  write (u, "(A)")  "* Write matrix-element source code"
  call driver%make_source (os_data)

  write (u, "(A)")  "* Compile source code"
  call driver%make_compile (os_data)

  write (u, "(A)")  "* Link library"
  call driver%make_link (os_data)

```

```

write (u, "(A)")  "* File check"
write (u, *)
call check_file (u, "test7.f90")
call check_file (u, "tpr_test7.mod")
call check_file (u, "test7.lo")
call check_file (u, "prclib7.makefile")
call check_file (u, "prclib7.f90")
call check_file (u, "prclib7.lo")
call check_file (u, "prclib7.la")

write (u, *)
write (u, "(A)")  "* Delete library"
write (u, *)
call driver%clean_library (os_data)
call check_file (u, "prclib7.la")

write (u, *)
write (u, "(A)")  "* Delete object code"
write (u, *)
call driver%clean_objects (os_data)
call check_file (u, "test7.lo")
call check_file (u, "tpr_test7.mod")
call check_file (u, "prclib7.lo")

write (u, *)
write (u, "(A)")  "* Delete source code"
write (u, *)
call driver%clean_source (os_data)
call check_file (u, "test7.f90")

write (u, *)
write (u, "(A)")  "* Delete driver source code"
write (u, *)
call driver%clean_driver (os_data)
call check_file (u, "prclib7.f90")

write (u, *)
write (u, "(A)")  "* Delete makefile"
write (u, *)
call driver%clean_makefile (os_data)
call check_file (u, "prclib7.makefile")

deallocate (test_writer_4)

write (u, *)
write (u, "(A)")  "* Test output end: prclib_interfaces_7"
end subroutine prclib_interfaces_7

```

Auxiliary routine: check and report existence of a file

(Prclib interfaces: test auxiliary)+≡

```

subroutine check_file (u, file)
  integer, intent(in) :: u
  character(*), intent(in) :: file

```

```

    logical :: exist
    inquire (file=file, exist=exist)
    write (u, "(2x,A,A,L1)") file, " = ", exist
end subroutine check_file

```

14.3 Abstract process core configuration

In this module, we define abstract data types that handle the method-specific part of defining a process (including all of its options) and accessing an external matrix element.

There are no unit tests, these are deferred to the `process_libraries` module below.

```

⟨prc_core_def.f90⟩≡
  ⟨File header⟩

  module prc_core_def

    ⟨Use strings⟩
    use io_units
    use diagnostics

    use process_constants
    use prclib_interfaces

    ⟨Standard module head⟩

    ⟨Prc core def: public⟩

    ⟨Prc core def: types⟩

    ⟨Prc core def: interfaces⟩

    contains

    ⟨Prc core def: procedures⟩

  end module prc_core_def

```

14.3.1 Process core definition type

For storing configuration data that depend on the specific process variant, we introduce a polymorphic type. At this point, we just declare an abstract base type. This allows us to defer the implementation to later modules.

There should be no components that need explicit finalization, otherwise we would have to call a finalizer from the `process_component_def_t` wrapper.

Translate a `prc_core_def_t` to above named integers

```

⟨Prc core def: public⟩≡
  public :: prc_core_def_t

```

```

<Prc core def: types>≡
  type, abstract :: prc_core_def_t
    class(prc_writer_t), allocatable :: writer
    contains
      <Prc core def: process core def: TBP>
    end type prc_core_def_t

```

Interfaces for the deferred methods.

This returns a string. No passed argument; the string is constant and depends just on the type.

```

<Prc core def: process core def: TBP>≡
  procedure (prc_core_def_get_string), nopass, deferred :: type_string

<Prc core def: interfaces>≡
  abstract interface
    function prc_core_def_get_string () result (string)
      import
        type(string_t) :: string
    end function prc_core_def_get_string
  end interface

```

The **write** method should display the content completely.

```

<Prc core def: process core def: TBP>+≡
  procedure (prc_core_def_write), deferred :: write

<Prc core def: interfaces>+≡
  abstract interface
    subroutine prc_core_def_write (object, unit)
      import
        class(prc_core_def_t), intent(in) :: object
        integer, intent(in) :: unit
    end subroutine prc_core_def_write
  end interface

```

The **read** method should fill the content completely.

```

<Prc core def: process core def: TBP>+≡
  procedure (prc_core_def_read), deferred :: read

<Prc core def: interfaces>+≡
  abstract interface
    subroutine prc_core_def_read (object, unit)
      import
        class(prc_core_def_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine prc_core_def_read
  end interface

```

This communicates a MD5 checksum to the writer inside the **core_def** object, if there is any. Usually, this checksum is not yet known at the time when the writer is initialized.

```

<Prc core def: process core def: TBP>+≡
  procedure :: set_md5sum => prc_core_def_set_md5sum

```

```

<Prc core def: procedures>≡
  subroutine prc_core_def_set_md5sum (core_def, md5sum)
    class(prc_core_def_t), intent(inout) :: core_def
    character(32) :: md5sum
    if (allocated (core_def%writer)) core_def%writer%md5sum = md5sum
  end subroutine prc_core_def_set_md5sum

```

Allocate an appropriate driver object which corresponds to the chosen process core definition.

For internal matrix element (i.e., those which do not need external code), the driver should have access to all matrix element information from the beginning. In short, it is the matrix-element code.

For external matrix elements, the driver will get access to the external matrix element code.

```

<Prc core def: process core def: TBP>+≡
  procedure(prc_core_def_allocate_driver), deferred :: allocate_driver

<Prc core def: interfaces>+≡
  abstract interface
    subroutine prc_core_def_allocate_driver (object, driver, basename)
      import
      class(prc_core_def_t), intent(in) :: object
      class(prc_core_driver_t), intent(out), allocatable :: driver
      type(string_t), intent(in) :: basename
    end subroutine prc_core_def_allocate_driver
  end interface

```

This flag tells whether the particular variant needs external code. We implement a default function which returns false. The flag depends only on the type, therefore we implement it as **nopass**.

```

<Prc core def: process core def: TBP>+≡
  procedure, nopass :: needs_code => prc_core_def_needs_code

<Prc core def: procedures>+≡
  function prc_core_def_needs_code () result (flag)
    logical :: flag
    flag = .false.
  end function prc_core_def_needs_code

```

This subroutine allocates an array which holds the name of all features that this process core implements. This feature applies to matrix element code that is not coded as a Fortran module but communicates via independent library functions, which follow the C calling conventions. The addresses of those functions are returned as C function pointers, which can be converted into Fortran procedure pointers. The conversion is done in code specific for the process variant; here we just retrieve the C function pointer.

The array returned here serves the purpose of writing specific driver code. The driver interfaces only those C functions which are supported for the given process core.

If the process core does not require external code, this array is meaningless.

```

<Prc core def: process core def: TBP>+≡

```



```

        procedure(prc_core_def_get_features), nopass, deferred &
            :: get_features
    <Prc core def: interfaces>+≡
    abstract interface
        subroutine prc_core_def_get_features (features)
            import
            type(string_t), dimension(:), allocatable, intent(out) :: features
        end subroutine prc_core_def_get_features
    end interface

```

Assign pointers to the process-specific procedures to the driver, if the process is external.

```

    <Prc core def: process core def: TBP>+≡
        procedure(prc_core_def_connect), deferred :: connect
    <Prc core def: interfaces>+≡
    abstract interface
        subroutine prc_core_def_connect (def, lib_driver, i, proc_driver)
            import
            class(prc_core_def_t), intent(in) :: def
            class(prclib_driver_t), intent(in) :: lib_driver
            integer, intent(in) :: i
            class(prc_core_driver_t), intent(inout) :: proc_driver
        end subroutine prc_core_def_connect
    end interface

```

14.3.2 Process core template

We must be able to automatically allocate a process core definition object with the appropriate type, given only the type name.

To this end, we introduce a `prc_template_t` type which is simply a wrapper for an empty `prc_core_def_t` object. Choosing one of the templates from an array, we can allocate the target object.

```

    <Prc core def: public>+≡
        public :: prc_template_t
    <Prc core def: types>+≡
        type :: prc_template_t
            class(prc_core_def_t), allocatable :: core_def
        end type prc_template_t

```

The allocation routine. We use the `source` option of the `allocate` statement. The `mold` option would probably more appropriate, but is a F2008 feature.

```

    <Prc core def: public>+≡
        public :: allocate_core_def
    <Prc core def: procedures>+≡
        subroutine allocate_core_def (template, name, core_def)
            type(prc_template_t), dimension(:), intent(in) :: template
            type(string_t), intent(in) :: name
            class(prc_core_def_t), allocatable :: core_def

```

```

integer :: i
do i = 1, size (template)
  if (template(i)%core_def%type_string () == name) then
    allocate (core_def, source = template(i)%core_def)
    return
  end if
end do
end subroutine allocate_core_def

```

14.3.3 Process driver

For each process component, we implement a driver object which holds the calls to the matrix element and various auxiliary routines as procedure pointers. Any actual calculation will use this object to communicate with the process.

Depending on the type of process (as described by a corresponding `prc_core_def` object), the procedure pointers may refer to external or internal code, and there may be additional procedures for certain types. The base type defined here is abstract.

```

<Prc core def: public>+≡
  public :: prc_core_driver_t
<Prc core def: types>+≡
  type, abstract :: prc_core_driver_t
  contains
  <Prc core def: process driver: TBP>
end type prc_core_driver_t

```

This returns the process type. No reference to contents.

```

<Prc core def: process driver: TBP>≡
  procedure(prc_core_driver_type_name), nopass, deferred :: type_name
<Prc core def: interfaces>+≡
  abstract interface
    function prc_core_driver_type_name () result (type)
      import
      type(string_t) :: type
    end function prc_core_driver_type_name
  end interface

```

14.3.4 Process driver for intrinsic process

This is an abstract extension for the driver type. It has one additional method, namely a subroutine that fills the record of constant process data. For an external process, this task is performed by the external library driver instead.

```

<Prc core def: public>+≡
  public :: process_driver_internal_t

```

```

<Prc core def: types>+≡
  type, extends (prc_core_driver_t), abstract :: process_driver_internal_t
  contains
    <Prc core def: process driver internal: TBP>
  end type process_driver_internal_t

<Prc core def: process driver internal: TBP>≡
  procedure(process_driver_fill_constants), deferred :: fill_constants

<Prc core def: interfaces>+≡
  abstract interface
    subroutine process_driver_fill_constants (driver, data)
      import
        class(process_driver_internal_t), intent(in) :: driver
        type(process_constants_t), intent(out) :: data
    end subroutine process_driver_fill_constants
  end interface

```

14.4 Process library access

Processes (the code and data that are necessary for evaluating matrix elements of a particular process or process component) are organized in process libraries. In full form, process libraries contain generated and dynamically compiled and linked code, so they are actual libraries on the OS level. Alternatively, there may be simple processes that can be generated without referring to external libraries, and external libraries that are just linked in.

This module interfaces the OS to create, build, and use process libraries.

We work with two related data structures. There is the list of process configurations that stores the user input and data derived from it. A given process configuration list is scanned for creating a process library, which consists of both data and code. The creation step involves calling external programs and incorporating external code.

For the subsequent integration and event generation steps, we read the process library. We also support partial (re)creation of the process library. To this end, we should be able to reconstruct the configuration data records from the process library.

```

<process_libraries.f90>≡
  <File header>

  module process_libraries

    use, intrinsic :: iso_c_binding !NODEP!

    <Use strings>
    use io_units
    use diagnostics
    use md5
    use physics_defs
    use os_interface
    use model_data

```

```

    use particle_specifiers
    use process_constants
    use prclib_interfaces
    use prc_core_def

    <Standard module head>

    <Process libraries: public>

    <Process libraries: parameters>

    <Process libraries: types>

    contains

    <Process libraries: procedures>

end module process_libraries

```

14.4.1 Auxiliary stuff

Here is a small subroutine that strips the left-hand side and the equals sign off an equation.

```

    <Process libraries: public>≡
        public :: strip_equation_lhs

    <Process libraries: procedures>≡
        subroutine strip_equation_lhs (buffer)
            character(*), intent(inout) :: buffer
            type(string_t) :: string, prefix
            string = buffer
            call split (string, prefix, "=")
            buffer = string
        end subroutine strip_equation_lhs

```

14.4.2 Process definition objects

We collect process configuration data in a derived type, `process_def_t`. A process can be a collection of several components which are treated as a single entity for the purpose of observables and event generation. Multiple process components may initially be defined by the user. The system may add additional components, e.g., subtraction terms. The common data type is `process_component_def_t`. Within each component, there are several universal data items, and a part which depend on the particular process variant. The latter is covered by an abstract type `prc_core_def_t` and its extensions.

Wrapper for components

We define a wrapper type for the configuration of individual components.

The string `basename` is used for building file, module, and function names for the current process component. Initially, it will be built from the corresponding process basename by appending an alphanumeric suffix.

The logical `initial` tells whether this is a user-defined (true) or system-generated (false) configuration.

The numbers `n_in`, `n_out`, and `n_tot` denote the incoming, outgoing and total number of particles (partons) participating in the process component, respectively. These are the nominal particles, as input by the user (recombination may change the particle content, for the output events).

The string arrays `prt_in` and `prt_out` hold the particle specifications as provided by the user. For a system-generated process component, they remain deallocated.

The `method` string is used to determine the type of process matrix element and how it is obtained.

The `description` string collects the information about particle content and method in a single human-readable string.

The pointer object `core_def` is allocated according to the actual process variant, which depends on the method. The subobject holds any additional configuration data that is relevant for the process component.

We assume that no finalizer is needed.

```

(Process libraries: public)+≡
    public :: process_component_def_t

(Process libraries: types)≡
    type :: process_component_def_t
        private
        type(string_t) :: basename
        logical :: initial = .false.
        integer :: n_in = 0
        integer :: n_out = 0
        integer :: n_tot = 0
        type(prt_spec_t), dimension(:), allocatable :: prt_in
        type(prt_spec_t), dimension(:), allocatable :: prt_out
        type(string_t) :: method
        type(string_t) :: description
        class(prc_core_def_t), allocatable :: core_def
        character(32) :: md5sum = ""
        integer :: nlo_type = BORN
        integer, dimension(N_ASSOCIATED_COMPONENTS) :: associated_components = 0
        logical :: active
        integer :: fixed_emitter = -1
        integer :: alpha_power = 0
        integer :: alphas_power = 0
    contains
        (Process libraries: process component def: TBP)
    end type process_component_def_t

```

Display the complete content.

```

(Process libraries: process component def: TBP)≡
    procedure :: write => process_component_def_write

(Process libraries: procedures)+≡
    subroutine process_component_def_write (object, unit)
        class(process_component_def_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
    end subroutine

```

```

u = given_output_unit (unit)
write (u, "(3x,A,A)") "Component ID          = ", char (object%basename)
write (u, "(3x,A,L1)") "Initial component    = ", object%initial
write (u, "(3x,A,I0,1x,I0,1x,I0)") "N (in, out, tot)    = ", &
    object%n_in, object%n_out, object%n_tot
write (u, "(3x,A)", advance="no") "Particle content    = "
if (allocated (object%prt_in)) then
    call prt_spec_write (object%prt_in, u, advance="no")
else
    write (u, "(A)", advance="no") "[undefined]"
end if
write (u, "(A)", advance="no") " => "
if (allocated (object%prt_out)) then
    call prt_spec_write (object%prt_out, u, advance="no")
else
    write (u, "(A)", advance="no") "[undefined]"
end if
write (u, "(A)")
if (object%method /= "") then
    write (u, "(3x,A,A)") "Method              = ", &
        char (object%method)
else
    write (u, "(3x,A)") "Method              = [undefined]"
end if
if (allocated (object%core_def)) then
    write (u, "(3x,A,A)") "Process variant      = ", &
        char (object%core_def%type_string ())
    call object%core_def%write (u)
else
    write (u, "(3x,A)") "Process variant      = [undefined]"
end if
write (u, "(3x,A,A,A)") "MD5 sum (def)        = '", object%md5sum, "'"
end subroutine process_component_def_write

```

Read the process component definition. Allocate the process variant definition with appropriate type, matching the type name on file with the provided templates.

(Process libraries: process component def: TBP)+≡

```
procedure :: read => process_component_def_read
```

(Process libraries: procedures)+≡

```

subroutine process_component_def_read (component, unit, core_def_templates)
class(process_component_def_t), intent(out) :: component
integer, intent(in) :: unit
type(prc_template_t), dimension(:), intent(in) :: core_def_templates
character(80) :: buffer
type(string_t) :: var_buffer, prefix, in_state, out_state
type(string_t) :: variant_type

read (unit, "(A)") buffer
call strip_equation_lhs (buffer)
component%basename = trim (adjustl (buffer))

read (unit, "(A)") buffer

```

```

call strip_equation_lhs (buffer)
read (buffer, *) component%initial

read (unit, "(A)") buffer
call strip_equation_lhs (buffer)
read (buffer, *) component%n_in, component%n_out, component%n_tot

call get (unit, var_buffer)
call split (var_buffer, prefix, "=") ! keeps 'in => out'
call split (var_buffer, prefix, "=") ! actually: separator is '=>'

in_state = prefix
if (component%n_in > 0) then
  call prt_spec_read (component%prt_in, in_state)
end if

out_state = extract (var_buffer, 2)
if (component%n_out > 0) then
  call prt_spec_read (component%prt_out, out_state)
end if

read (unit, "(A)") buffer
call strip_equation_lhs (buffer)
component%method = trim (adjustl (buffer))
if (component%method == "[undefined]") &
  component%method = ""

read (unit, "(A)") buffer
call strip_equation_lhs (buffer)
variant_type = trim (adjustl (buffer))
call allocate_core_def &
  (core_def_templates, variant_type, component%core_def)
if (allocated (component%core_def)) then
  call component%core_def%read (unit)
end if

read (unit, "(A)") buffer
call strip_equation_lhs (buffer)
read (buffer(3:34), "(A32)") component%md5sum

end subroutine process_component_def_read

```

Short account.

```

<Process libraries: process component def: TBP>+≡
  procedure :: show => process_component_def_show

<Process libraries: procedures>+≡
  subroutine process_component_def_show (object, unit)
    class(process_component_def_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(6x,A)", advance="no") char (object%basename)
    if (.not. object%initial) &

```

```

        write (u, "('*')", advance="no")
write (u, "(:',1x)", advance="no")
if (allocated (object%prt_in)) then
    call prt_spec_write (object%prt_in, u, advance="no")
else
    write (u, "(A)", advance="no") "[undefined]"
end if
write (u, "(A)", advance="no") " => "
if (allocated (object%prt_out)) then
    call prt_spec_write (object%prt_out, u, advance="no")
else
    write (u, "(A)", advance="no") "[undefined]"
end if
if (object%method /= "") then
    write (u, "(2x,['A,'])" char (object%method)
else
    write (u, *)
end if
end subroutine process_component_def_show

```

Compute the MD5 sum of a process component. We reset the stored MD5 sum to the empty string (so a previous value is not included in the calculation), then write a temporary file and calculate the MD5 sum of that file.

This implies that all data that are displayed by the `write` method become part of the MD5 sum calculation.

The `model` is not part of the object, but must be included in the MD5 sum. Otherwise, modifying the model and nothing else would not trigger remaking the process-component source. Note that the model parameters may change later and therefore are not incorporated.

After the MD5 sum of the component has been computed, we communicate it to the `writer` subobject of the specific `core_def` component. Although these types are abstract, the MD5-related features are valid for the abstract types.

(Process libraries: process component def: TBP)+≡

```

procedure :: compute_md5sum => process_component_def_compute_md5sum

```

(Process libraries: procedures)+≡

```

subroutine process_component_def_compute_md5sum (component, model)
class(process_component_def_t), intent(inout) :: component
class(model_data_t), intent(in), optional, target :: model
integer :: u
component%md5sum = ""
u = free_unit ()
open (u, status = "scratch", action = "readwrite")
if (present (model)) write (u, "(A32)") model%get_md5sum ()
call component%write (u)
rewind (u)
component%md5sum = md5sum (u)
close (u)
if (allocated (component%core_def)) then
    call component%core_def%set_md5sum (component%md5sum)
end if
end subroutine process_component_def_compute_md5sum

```



```

<Process libraries: process component def: TBP>+≡
    procedure :: get_def_type_string => process_component_def_get_def_type_string

<Process libraries: procedures>+≡
    function process_component_def_get_def_type_string (component) result (type_string)
        type(string_t) :: type_string
        class(process_component_def_t), intent(in) :: component
        type_string = component%core_def%type_string ()
    end function process_component_def_get_def_type_string

```

Allocate the process driver (with a suitable type) for a process component. For internal processes, we may set all data already at this stage.

```

<Process libraries: process component def: TBP>+≡
    procedure :: allocate_driver => process_component_def_allocate_driver

<Process libraries: procedures>+≡
    subroutine process_component_def_allocate_driver (component, driver)
        class(process_component_def_t), intent(in) :: component
        class(prc_core_driver_t), intent(out), allocatable :: driver
        if (allocated (component%core_def)) then
            call component%core_def%allocate_driver (driver, component%basename)
        end if
    end subroutine process_component_def_allocate_driver

```

Tell whether the process core needs external code.

```

<Process libraries: process component def: TBP>+≡
    procedure :: needs_code => process_component_def_needs_code

<Process libraries: procedures>+≡
    function process_component_def_needs_code (component) result (flag)
        class(process_component_def_t), intent(in) :: component
        logical :: flag
        flag = component%core_def%needs_code ()
    end function process_component_def_needs_code

```

If there is external code, the `core_def` subobject should provide a writer object. This method returns a pointer to the writer.

```

<Process libraries: process component def: TBP>+≡
    procedure :: get_writer_ptr => process_component_def_get_writer_ptr

<Process libraries: procedures>+≡
    function process_component_def_get_writer_ptr (component) result (writer)
        class(process_component_def_t), intent(in), target :: component
        class(prc_writer_t), pointer :: writer
        writer => component%core_def%writer
    end function process_component_def_get_writer_ptr

```

Return an array which holds the names of all C functions that this process component implements.

```

<Process libraries: process component def: TBP>+≡
    procedure :: get_features => process_component_def_get_features

```

```

(Process libraries: procedures)+≡
function process_component_def_get_features (component) result (features)
  class(process_component_def_t), intent(in) :: component
  type(string_t), dimension(:), allocatable :: features
  call component%core_def%get_features (features)
end function process_component_def_get_features

```

Assign procedure pointers in the driver component (external processes). For internal processes, this is meaningless.

```

(Process libraries: process component def: TBP)+≡
procedure :: connect => process_component_def_connect

(Process libraries: procedures)+≡
subroutine process_component_def_connect &
  (component, lib_driver, i, proc_driver)
  class(process_component_def_t), intent(in) :: component
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
  select type (proc_driver)
  class is (process_driver_internal_t)
    !!! Nothing to do
  class default
    call component%core_def%connect (lib_driver, i, proc_driver)
  end select
end subroutine process_component_def_connect

```

Return a pointer to the process core definition, which is of abstract type.

```

(Process libraries: process component def: TBP)+≡
procedure :: get_core_def_ptr => process_component_get_core_def_ptr

(Process libraries: procedures)+≡
function process_component_get_core_def_ptr (component) result (ptr)
  class(process_component_def_t), intent(in), target :: component
  class(prc_core_def_t), pointer :: ptr
  ptr => component%core_def
end function process_component_get_core_def_ptr

```

Return nominal particle counts, as input by the user.

```

(Process libraries: process component def: TBP)+≡
procedure :: get_n_in => process_component_def_get_n_in
procedure :: get_n_out => process_component_def_get_n_out
procedure :: get_n_tot => process_component_def_get_n_tot

(Process libraries: procedures)+≡
function process_component_def_get_n_in (component) result (n_in)
  class(process_component_def_t), intent(in) :: component
  integer :: n_in
  n_in = component%n_in
end function process_component_def_get_n_in

function process_component_def_get_n_out (component) result (n_out)
  class(process_component_def_t), intent(in) :: component

```

```

integer :: n_out
n_out = component%n_out
end function process_component_def_get_n_out

function process_component_def_get_n_tot (component) result (n_tot)
class(process_component_def_t), intent(in) :: component
integer :: n_tot
n_tot = component%n_tot
end function process_component_def_get_n_tot

```

Allocate and return string arrays for the incoming and outgoing particles.

```

(Process libraries: process component def: TBP)+≡
procedure :: get_prt_in => process_component_def_get_prt_in
procedure :: get_prt_out => process_component_def_get_prt_out

(Process libraries: procedures)+≡
subroutine process_component_def_get_prt_in (component, prt)
class(process_component_def_t), intent(in) :: component
type(string_t), dimension(:), intent(out), allocatable :: prt
integer :: i
allocate (prt (component%n_in))
do i = 1, component%n_in
prt(i) = component%prt_in(i)%to_string ()
end do
end subroutine process_component_def_get_prt_in

subroutine process_component_def_get_prt_out (component, prt)
class(process_component_def_t), intent(in) :: component
type(string_t), dimension(:), intent(out), allocatable :: prt
integer :: i
allocate (prt (component%n_out))
do i = 1, component%n_out
prt(i) = component%prt_out(i)%to_string ()
end do
end subroutine process_component_def_get_prt_out

```

Return the incoming and outgoing particle specifiers as-is.

```

(Process libraries: process component def: TBP)+≡
procedure :: get_prt_spec_in => process_component_def_get_prt_spec_in
procedure :: get_prt_spec_out => process_component_def_get_prt_spec_out

(Process libraries: procedures)+≡
function process_component_def_get_prt_spec_in (component) result (prt)
class(process_component_def_t), intent(in) :: component
type(prt_spec_t), dimension(:), allocatable :: prt
allocate (prt (component%n_in))
prt(:) = component%prt_in(:)
end function process_component_def_get_prt_spec_in

function process_component_def_get_prt_spec_out (component) result (prt)
class(process_component_def_t), intent(in) :: component
type(prt_spec_t), dimension(:), allocatable :: prt
allocate (prt (component%n_out))
prt(:) = component%prt_out(:)
end function process_component_def_get_prt_spec_out

```

```
end function process_component_def_get_prt_spec_out
```

Return the combination of incoming particles as a PDG code

```
(Process libraries: process component def: TBP)+≡
  procedure :: get_pdg_in => process_component_def_get_pdg_in

(Process libraries: procedures)+≡
  subroutine process_component_def_get_pdg_in (component, model, pdg)
    class(process_component_def_t), intent(in) :: component
    class(model_data_t), intent(in), target :: model
    integer, intent(out), dimension(:) :: pdg
    integer :: i
    do i = 1, size (pdg)
      pdg(i) = model%get_pdg (component%prt_in(i)%to_string ())
    end do
  end subroutine process_component_def_get_pdg_in
```

Return the MD5 sum.

```
(Process libraries: process component def: TBP)+≡
  procedure :: get_md5sum => process_component_def_get_md5sum

(Process libraries: procedures)+≡
  pure function process_component_def_get_md5sum (component) result (md5sum)
    class(process_component_def_t), intent(in) :: component
    character(32) :: md5sum
    md5sum = component%md5sum
  end function process_component_def_get_md5sum
```

Get NLO data

```
(Process libraries: process component def: TBP)+≡
  procedure :: get_nlo_type => process_component_def_get_nlo_type
  procedure :: get_associated_born &
    => process_component_def_get_associated_born
  procedure :: get_associated_real_fin &
    => process_component_def_get_associated_real_fin
  procedure :: get_associated_real_sing &
    => process_component_def_get_associated_real_sing
  procedure :: get_associated_subtraction &
    => process_component_def_get_associated_subtraction
  procedure :: get_association_list &
    => process_component_def_get_association_list
  procedure :: can_be_integrated &
    => process_component_def_can_be_integrated
  procedure :: get_associated_real => process_component_def_get_associated_real

(Process libraries: procedures)+≡
  elemental function process_component_def_get_nlo_type (component) result (nlo_type)
    integer :: nlo_type
    class(process_component_def_t), intent(in) :: component
    nlo_type = component%nlo_type
  end function process_component_def_get_nlo_type

  elemental function process_component_def_get_associated_born (component) result (i_born)
    integer :: i_born
```

```

        class(process_component_def_t), intent(in) :: component
        i_born = component%associated_components(ASSOCIATED_BORN)
    end function process_component_def_get_associated_born

    elemental function process_component_def_get_associated_real_fin (component) result (i_rfin)
        integer :: i_rfin
        class(process_component_def_t), intent(in) :: component
        i_rfin = component%associated_components(ASSOCIATED_REAL_FIN)
    end function process_component_def_get_associated_real_fin

    elemental function process_component_def_get_associated_real_sing (component) result (i_rsing)
        integer :: i_rsing
        class(process_component_def_t), intent(in) :: component
        i_rsing = component%associated_components(ASSOCIATED_REAL_SING)
    end function process_component_def_get_associated_real_sing

    elemental function process_component_def_get_associated_subtraction (component) result (i_sub)
        integer :: i_sub
        class(process_component_def_t), intent(in) :: component
        i_sub = component%associated_components(ASSOCIATED_SUB)
    end function process_component_def_get_associated_subtraction

    elemental function process_component_def_can_be_integrated (component) result (active)
        logical :: active
        class(process_component_def_t), intent(in) :: component
        active = component%active
    end function process_component_def_can_be_integrated

    function process_component_def_get_association_list (component, i_skip_in) result (list)
        integer, dimension(:), allocatable :: list
        class(process_component_def_t), intent(in) :: component
        integer, intent(in), optional :: i_skip_in
        integer :: i, j, n, i_skip
        logical :: valid
        i_skip = 0; if (present (i_skip_in)) i_skip = i_skip_in
        n = count (component%associated_components /= 0) - 1
        if (i_skip > 0) then
            if (component%associated_components(i_skip) > 0) n = n - 1
        end if
        allocate (list (n))
        j = 1
        do i = 1, size(component%associated_components)
            valid = component%associated_components(i) /= 0 &
                .and. i /= ASSOCIATED_SUB .and. i /= i_skip
            if (valid) then
                list(j) = component%associated_components(i)
                j = j + 1
            end if
        end do
    end function process_component_def_get_association_list

    function process_component_def_get_associated_real (component) result (i_real)
        integer :: i_real
        class(process_component_def_t), intent(in) :: component

```

```

        i_real = component%associated_components(ASSOCIATED_REAL)
    end function process_component_def_get_associated_real

<Process libraries: process component def: TBP>+≡
    procedure :: get_me_method => process_component_def_get_me_method

<Process libraries: procedures>+≡
    elemental function process_component_def_get_me_method (component) result (method)
        type(string_t) :: method
        class(process_component_def_t), intent(in) :: component
        method = component%method
    end function process_component_def_get_me_method

<Process libraries: process component def: TBP>+≡
    procedure :: get_fixed_emitter => process_component_def_get_fixed_emitter

<Process libraries: procedures>+≡
    function process_component_def_get_fixed_emitter (component) result (emitter)
        integer :: emitter
        class(process_component_def_t), intent(in) :: component
        emitter = component%fixed_emitter
    end function process_component_def_get_fixed_emitter

<Process libraries: process component def: TBP>+≡
    procedure :: get_coupling_powers => process_component_def_get_coupling_powers

<Process libraries: procedures>+≡
    pure subroutine process_component_def_get_coupling_powers (component, alpha_power, alphas_power)
        class(process_component_def_t), intent(in) :: component
        integer, intent(out) :: alpha_power, alphas_power
        alpha_power = component%alpha_power
        alphas_power = component%alphas_power
    end subroutine process_component_def_get_coupling_powers

```

Process definition

The process component definitions are collected in a common process definition object.

The `id` is the ID string that the user has provided for identifying this process. It must be a string that is allowed as part of a Fortran variable name, since it may be used for generating code.

The number `n_in` is 1 or 2 for a decay or scattering process, respectively. This must be identical to `n_in` for all components.

The initial and extra component definitions (see above) are allocated as the `initial` and `extra` arrays, respectively. The latter are determined from the former.

The `md5sum` is used to verify the integrity of the configuration.

```

<Process libraries: public>+≡
    public :: process_def_t

```

```

<Process libraries: types>+≡
  type :: process_def_t
    private
      type(string_t) :: id
      integer :: num_id = 0
      class(model_data_t), pointer :: model => null ()
      type(string_t) :: model_name
      integer :: n_in = 0
      integer :: n_initial = 0
      integer :: n_extra = 0
      type(process_component_def_t), dimension(:), allocatable :: initial
      type(process_component_def_t), dimension(:), allocatable :: extra
      character(32) :: md5sum = ""
      logical :: nlo_process = .false.
      logical :: negative_sf = .false.
      logical :: requires_resonances = .false.
    contains
      <Process libraries: process def: TBP>
    end type process_def_t

```

Write the process definition including components:

```

<Process libraries: process def: TBP>≡
  procedure :: write => process_def_write

<Process libraries: procedures>+≡
  subroutine process_def_write (object, unit)
    class(process_def_t), intent(in) :: object
    integer, intent(in) :: unit
    integer :: i
    write (unit, "(1x,A,A,A)") "ID = '", char (object%id), "'"
    if (object%num_id /= 0) &
      write (unit, "(1x,A,IO)") "ID(num) = ", object%num_id
    select case (object%n_in)
    case (1); write (unit, "(1x,A)") "Decay"
    case (2); write (unit, "(1x,A)") "Scattering"
    case default
      write (unit, "(1x,A)") "[Undefined process]"
      return
    end select
    if (object%model_name /= "") then
      write (unit, "(1x,A,A)") "Model = ", char (object%model_name)
    else
      write (unit, "(1x,A)") "Model = [undefined]"
    end if
    write (unit, "(1x,A,IO)") "Initially defined component(s) = ", &
      object%n_initial
    write (unit, "(1x,A,IO)") "Extra generated component(s) = ", &
      object%n_extra
    if (object%requires_resonances) then
      ! This line has to matched with the reader below!
      write (unit, "(1x,A,IO)") "Resonant subprocesses required"
    end if
    write (unit, "(1x,A,A,A)") "MD5 sum = '", object%md5sum, "'"
    if (allocated (object%initial)) then

```

```

        do i = 1, size (object%initial)
            write (unit, "(1x,A,I0)") "Component #", i
            call object%initial(i)%write (unit)
        end do
    end if
    if (allocated (object%extra)) then
        do i = 1, size (object%extra)
            write (unit, "(1x,A,I0)") "Component #", object%n_initial + i
            call object%extra(i)%write (unit)
        end do
    end if
end subroutine process_def_write

```

Read the process definition including components.

(Process libraries: process def: TBP)+≡

```

procedure :: read => process_def_read

```

(Process libraries: procedures)+≡

```

subroutine process_def_read (object, unit, core_def_templates)
    class(process_def_t), intent(out) :: object
    integer, intent(in) :: unit
    type(prc_template_t), dimension(:), intent(in) :: core_def_templates
    integer :: i, i1, i2
    character(80) :: buffer, ref
    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    i1 = scan (buffer, "'")
    i2 = scan (buffer, "\"", back=.true.)
    if (i2 > i1) then
        object%id = buffer(i1+1:i2-1)
    else
        object%id = ""
    end if

    read (unit, "(A)") buffer
    select case (buffer(2:11))
    case ("Decay      "); object%n_in = 1
    case ("Scattering"); object%n_in = 2
    case default
        return
    end select

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    object%model_name = trim (adjustl (buffer))
    if (object%model_name == "[undefined]") object%model_name = ""

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer, *) object%n_initial

    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer, *) object%n_extra

```



```

read (unit, "(A)")  buffer
if (buffer(1:9) == " Resonant") then
    object%requires_resonances = .true.
    read (unit, "(A)")  buffer
else
    object%requires_resonances = .false.
end if

call strip_equation_lhs (buffer)
read (buffer(3:34), "(A32)")  object%md5sum

if (object%n_initial > 0) then
    allocate (object%initial (object%n_initial))
    do i = 1, object%n_initial
        read (unit, "(A)")  buffer
        write (ref, "(1x,A,I0)")  "Component #", i
        if (buffer /= ref) return ! Wrong component header
        call object%initial(i)%read (unit, core_def_templates)
    end do
end if

end subroutine process_def_read

```

Short account.

```

<Process libraries: process def: TBP>+≡
    procedure :: show => process_def_show

<Process libraries: procedures>+≡
    subroutine process_def_show (object, unit)
        class(process_def_t), intent(in) :: object
        integer, intent(in) :: unit
        integer :: i
        write (unit, "(4x,A)", advance="no") char (object%id)
        if (object%num_id /= 0) &
            write (unit, "(1x,'(,I0,')')", advance="no")  object%num_id
        if (object%model_name /= "") &
            write (unit, "(1x,['A,']')", advance="no")  char (object%model_name)
        if (object%requires_resonances) then
            write (unit, "(1x,A)", advance="no")  "[+ resonant subprocesses]"
        end if
        write (unit, *)
        if (allocated (object%initial)) then
            do i = 1, size (object%initial)
                call object%initial(i)%show (unit)
            end do
        end if
        if (allocated (object%extra)) then
            do i = 1, size (object%extra)
                call object%extra(i)%show (unit)
            end do
        end if
    end subroutine process_def_show

```

Initialize an entry (initialize the process definition inside). We allocate the 'initial' set of components. Extra components remain unallocated.

The model should be present as a pointer. This allows us to retrieve the model's MD5 sum. However, for various tests it is sufficient to have the name.

We create the basenames for the process components by appending a suffix which we increment for each component.

```

(Process libraries: process def: TBP)+≡
  procedure :: init => process_def_init

(Process libraries: procedures)+≡
  subroutine process_def_init (def, id, &
    model, model_name, n_in, n_components, num_id, &
    nlo_process, negative_sf, requires_resonances)
    class(process_def_t), intent(out) :: def
    type(string_t), intent(in), optional :: id
    class(model_data_t), intent(in), optional, target :: model
    type(string_t), intent(in), optional :: model_name
    integer, intent(in), optional :: n_in
    integer, intent(in), optional :: n_components
    integer, intent(in), optional :: num_id
    logical, intent(in), optional :: nlo_process
    logical, intent(in), optional :: negative_sf
    logical, intent(in), optional :: requires_resonances
    character(16) :: suffix
    integer :: i
    if (present (id)) then
      def%id = id
    else
      def%id = ""
    end if
    if (present (num_id)) then
      def%num_id = num_id
    end if
    if (present (model)) then
      def%model => model
      def%model_name = model%get_name ()
    else
      def%model => null ()
      if (present (model_name)) then
        def%model_name = model_name
      else
        def%model_name = ""
      end if
    end if
    if (present (n_in)) def%n_in = n_in
    if (present (n_components)) then
      def%n_initial = n_components
      allocate (def%initial (n_components))
    end if
    if (present (nlo_process)) then
      def%nlo_process = nlo_process
    end if
    if (present (negative_sf)) then
      def%negative_sf = negative_sf

```

```

end if
if (present (requires_resonances)) then
  def%requires_resonances = requires_resonances
end if
def%initial%initial = .true.
def%initial%method   = ""
do i = 1, def%n_initial
  write (suffix, "(A,I0)")  "_i", i
  def%initial(i)%basename = def%id // trim (suffix)
end do
def%initial%description = ""
end subroutine process_def_init

```

Explicitly set the model name (for unit test).

```

<Process libraries: process def: TBP>+≡
  procedure :: set_model_name => process_def_set_model_name

<Process libraries: procedures>+≡
  subroutine process_def_set_model_name (def, model_name)
    class(process_def_t), intent(inout) :: def
    type(string_t), intent(in) :: model_name
    def%model_name = model_name
  end subroutine process_def_set_model_name

```

Initialize an initial component. The particle content must be specified. The process core block is not (yet) allocated.

We assume that the particle arrays match the `n_in` and `n_out` values in size. The model is referred to by name; it is identified as an existing model later. The index `i` must refer to an existing element of the component array.

Data specific for the process core of a component are imported as the `core_def` argument. We should allocate an object of class `prc_core_def_t` with the appropriate specific type, fill it, and transfer it to the process component definition here. The allocation is moved, so the original allocated object is returned empty.

```

<Process libraries: process def: TBP>+≡
  procedure :: import_component => process_def_import_component

<Process libraries: procedures>+≡
  subroutine process_def_import_component (def, &
    i, n_out, prt_in, prt_out, method, variant, &
    nlo_type, can_be_integrated)
    class(process_def_t), intent(inout) :: def
    integer, intent(in) :: i
    integer, intent(in), optional :: n_out
    type(prt_spec_t), dimension(:), intent(in), optional :: prt_in
    type(prt_spec_t), dimension(:), intent(in), optional :: prt_out
    type(string_t), intent(in), optional :: method
    integer, intent(in), optional :: nlo_type
    logical, intent(in), optional :: can_be_integrated
    type(string_t) :: nlo_type_string
    class(prc_core_def_t), &
      intent(inout), allocatable, optional :: variant
    integer :: p

```

```

associate (comp => def%initial(i))
  if (present (n_out)) then
    comp%n_in = def%n_in
    comp%n_out = n_out
    comp%n_tot = def%n_in + n_out
  end if
  if (present (prt_in)) then
    allocate (comp%prt_in (size (prt_in)))
    comp%prt_in = prt_in
  end if
  if (present (prt_out)) then
    allocate (comp%prt_out (size (prt_out)))
    comp%prt_out = prt_out
  end if
  if (present (method)) comp%method = method
  if (present (variant)) then
    call move_alloc (variant, comp%core_def)
  end if
  if (present (nlo_type)) then
    comp%nlo_type = nlo_type
  end if
  if (present (can_be_integrated)) then
    comp%active = can_be_integrated
  else
    comp%active = .true.
  end if
  if (allocated (comp%prt_in) .and. allocated (comp%prt_out)) then
    associate (d => comp%description)
      d = ""
      do p = 1, size (prt_in)
        if (p > 1) d = d // ", "
        d = d // comp%prt_in(p)%to_string ()
      end do
      d = d // " => "
      do p = 1, size (prt_out)
        if (p > 1) d = d // ", "
        d = d // comp%prt_out(p)%to_string ()
      end do
      if (comp%method /= "") then
        if ((def%nlo_process .and. .not. comp%active) .or. &
            comp%nlo_type == NLO_SUBTRACTION) then
          d = d // " [inactive]"
        else
          d = d // " [" // comp%method // "]"
        end if
      end if
      nlo_type_string = component_status (comp%nlo_type)
      if (nlo_type_string /= "born") then
        d = d // ", [" // nlo_type_string // "]"
      end if
    end associate
  end if
end associate
end subroutine process_def_import_component

```

```

<Process libraries: process def: TBP>+≡
    procedure :: get_n_components => process_def_get_n_components

<Process libraries: procedures>+≡
    function process_def_get_n_components (def) result (n)
        class(process_def_t), intent(in) :: def
        integer :: n
        n = size (def%initial)
    end function process_def_get_n_components

<Process libraries: process def: TBP>+≡
    procedure :: set_fixed_emitter => process_def_set_fixed_emitter

<Process libraries: procedures>+≡
    subroutine process_def_set_fixed_emitter (def, i, emitter)
        class(process_def_t), intent(inout) :: def
        integer, intent(in) :: i, emitter
        def%initial(i)%fixed_emitter = emitter
    end subroutine process_def_set_fixed_emitter

<Process libraries: process def: TBP>+≡
    procedure :: set_coupling_powers => process_def_set_coupling_powers

<Process libraries: procedures>+≡
    subroutine process_def_set_coupling_powers (def, alpha_power, alphas_power)
        class(process_def_t), intent(inout) :: def
        integer, intent(in) :: alpha_power, alphas_power
        def%initial(1)%alpha_power = alpha_power
        def%initial(1)%alphas_power = alphas_power
    end subroutine process_def_set_coupling_powers

<Process libraries: process def: TBP>+≡
    procedure :: set_associated_components => &
        process_def_set_associated_components

<Process libraries: procedures>+≡
    subroutine process_def_set_associated_components (def, i, &
        i_list, remnant, real_finite, mismatch)
        class(process_def_t), intent(inout) :: def
        logical, intent(in) :: remnant, real_finite, mismatch
        integer, intent(in) :: i
        integer, dimension(:), intent(in) :: i_list
        integer :: add_index
        add_index = 0
        associate (comp => def%initial(i)%associated_components)
            comp(ASSOCIATED_BORN) = i_list(1)
            comp(ASSOCIATED_REAL) = i_list(2)
            comp(ASSOCIATED_VIRT) = i_list(3)
            comp(ASSOCIATED_SUB) = i_list(4)
            if (remnant) then
                comp(ASSOCIATED_PDF) = i_list(5)
                add_index = add_index + 1
            end if
        end associate
    end subroutine

```

```

        if (real_finite) then
            comp(ASSOCIATED_REAL_FIN) = i_list(5+add_index)
            add_index = add_index + 1
        end if
        if (mismatch) then
            !!! incomplete
        end if
    end associate
end subroutine process_def_set_associated_components

```

Compute the MD5 sum for this process definition. We compute the MD5 sums for all components individually, then concatenate a string of those and compute the MD5 sum of this string. We also include the model name. All other data part of the component definitions.

```

<Process libraries: process def: TBP>+≡
    procedure :: compute_md5sum => process_def_compute_md5sum

<Process libraries: procedures>+≡
    subroutine process_def_compute_md5sum (def, model)
        class(process_def_t), intent(inout) :: def
        class(model_data_t), intent(in), optional, target :: model
        integer :: i
        type(string_t) :: buffer
        buffer = def%model_name
        do i = 1, def%n_initial
            call def%initial(i)%compute_md5sum (model)
            buffer = buffer // def%initial(i)%md5sum
        end do
        do i = 1, def%n_extra
            call def%extra(i)%compute_md5sum (model)
            buffer = buffer // def%initial(i)%md5sum
        end do
        def%md5sum = md5sum (char (buffer))
    end subroutine process_def_compute_md5sum

```

Return the MD5 sum of the process or of a process component.

```

<Process libraries: process def: TBP>+≡
    procedure :: get_md5sum => process_def_get_md5sum

<Process libraries: procedures>+≡
    function process_def_get_md5sum (def, i_component) result (md5sum)
        class(process_def_t), intent(in) :: def
        integer, intent(in), optional :: i_component
        character(32) :: md5sum
        if (present (i_component)) then
            md5sum = def%initial(i_component)%md5sum
        else
            md5sum = def%md5sum
        end if
    end function process_def_get_md5sum

```

Return a pointer to the definition of a particular component (for test purposes).

```

<Process libraries: process def: TBP>+≡
    procedure :: get_core_def_ptr => process_def_get_core_def_ptr

```

```

<Process libraries: procedures>+≡
function process_def_get_core_def_ptr (def, i_component) result (ptr)
  class(process_def_t), intent(in), target :: def
  integer, intent(in) :: i_component
  class(prc_core_def_t), pointer :: ptr
  ptr => def%initial(i_component)%get_core_def_ptr ()
end function process_def_get_core_def_ptr

```

This query tells whether a specific process component relies on external code. This includes all traditional WHIZARD matrix elements which rely on O'MEGA for code generation. Other process components (trivial decays, subtraction terms) do not require external code.

NOTE: Implemented only for initial component.

The query is passed to the process component.

```

<Process libraries: process def: TBP>+≡
procedure :: needs_code => process_def_needs_code

<Process libraries: procedures>+≡
function process_def_needs_code (def, i_component) result (flag)
  class(process_def_t), intent(in) :: def
  integer, intent(in) :: i_component
  logical :: flag
  flag = def%initial(i_component)%needs_code ()
end function process_def_needs_code

```

Return the first entry for the incoming particle(s), PDG code, of this process.

```

<Process libraries: process def: TBP>+≡
procedure :: get_pdg_in_1 => process_def_get_pdg_in_1

<Process libraries: procedures>+≡
subroutine process_def_get_pdg_in_1 (def, pdg)
  class(process_def_t), intent(in), target :: def
  integer, dimension(:), intent(out) :: pdg
  call def%initial(1)%get_pdg_in (def%model, pdg)
end subroutine process_def_get_pdg_in_1

```

```

<Process libraries: process def: TBP>+≡
procedure :: is_nlo => process_def_is_nlo

<Process libraries: procedures>+≡
elemental function process_def_is_nlo (def) result (flag)
  logical :: flag
  class(process_def_t), intent(in) :: def
  flag = def%nlo_process
end function process_def_is_nlo

```

```

<Process libraries: process def: TBP>+≡
procedure :: get_nlo_type => process_def_get_nlo_type

<Process libraries: procedures>+≡
elemental function process_def_get_nlo_type (def, i_component) result (nlo_type)
  integer :: nlo_type
  class(process_def_t), intent(in) :: def

```

```

integer, intent(in) :: i_component
nlo_type = def%initial(i_component)%nlo_type
end function process_def_get_nlo_type

```

```

<Process libraries: process def: TBP>+≡
  procedure :: get_negative_sf => process_def_get_negative_sf

<Process libraries: procedures>+≡
  elemental function process_def_get_negative_sf (def) result (neg_sf)
    logical :: neg_sf
    class(process_def_t), intent(in) :: def
    neg_sf = def%negative_sf
  end function process_def_get_negative_sf

```

Number of incoming particles, common to all components.

```

<Process libraries: process def: TBP>+≡
  procedure :: get_n_in => process_def_get_n_in

<Process libraries: procedures>+≡
  function process_def_get_n_in (def) result (n_in)
    class(process_def_t), intent(in) :: def
    integer :: n_in
    n_in = def%n_in
  end function process_def_get_n_in

```

Pointer to a particular component definition record.

```

<Process libraries: process def: TBP>+≡
  procedure :: get_component_def_ptr => process_def_get_component_def_ptr

<Process libraries: procedures>+≡
  function process_def_get_component_def_ptr (def, i) result (component)
    type(process_component_def_t), pointer :: component
    class(process_def_t), intent(in), target :: def
    integer, intent(in) :: i
    if (i <= def%n_initial) then
      component => def%initial(i)
    else
      component => null ()
    end if
  end function process_def_get_component_def_ptr

```

Process definition list

A list of process definitions is the starting point for creating a process library. The list is built when reading the user input. When reading an existing process library, the list is used for cross-checking and updating the configuration.

We need a type for the list entry. The simplest way is to extend the process definition type, so all methods apply to the process definition directly.

```

<Process libraries: public>+≡
  public :: process_def_entry_t

```



```

<Process libraries: types>+≡
  type, extends (process_def_t) :: process_def_entry_t
  private
    type(process_def_entry_t), pointer :: next => null ()
  end type process_def_entry_t

```

This is the type for the list itself.

```

<Process libraries: public>+≡
  public :: process_def_list_t

<Process libraries: types>+≡
  type :: process_def_list_t
  private
    type(process_def_entry_t), pointer :: first => null ()
    type(process_def_entry_t), pointer :: last => null ()
  contains
    <Process libraries: process def list: TBP>
  end type process_def_list_t

```

The deallocates the list iteratively. We assume that the list entries do not need finalization themselves.

```

<Process libraries: process def list: TBP>≡
  procedure :: final => process_def_list_final

<Process libraries: procedures>+≡
  subroutine process_def_list_final (list)
    class(process_def_list_t), intent(inout) :: list
    type(process_def_entry_t), pointer :: current
    nullify (list%last)
    do while (associated (list%first))
      current => list%first
      list%first => current%next
      deallocate (current)
    end do
  end subroutine process_def_list_final

```

Write the complete list.

```

<Process libraries: process def list: TBP>+≡
  procedure :: write => process_def_list_write

<Process libraries: procedures>+≡
  subroutine process_def_list_write (object, unit, libpath)
    class(process_def_list_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: libpath
    type(process_def_entry_t), pointer :: entry
    integer :: i, u
    u = given_output_unit (unit)
    if (associated (object%first)) then
      i = 1
      entry => object%first
      do while (associated (entry))
        write (u, "(1x,A,I0,A)" "Process #", i, ":")

```

```

        call entry%write (u)
        i = i + 1
        entry => entry%next
        if (associated (entry)) write (u, *)
    end do
else
    write (u, "(1x,A)") "Process definition list: [empty]"
end if
end subroutine process_def_list_write

```

Short account.

```

<Process libraries: process def list: TBP>+=
    procedure :: show => process_def_list_show

<Process libraries: procedures>+=
    subroutine process_def_list_show (object, unit)
        class(process_def_list_t), intent(in) :: object
        integer, intent(in), optional :: unit
        type(process_def_entry_t), pointer :: entry
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%first)) then
            write (u, "(2x,A)") "Processes:"
            entry => object%first
            do while (associated (entry))
                call entry%show (u)
                entry => entry%next
            end do
        else
            write (u, "(2x,A)") "Processes: [empty]"
        end if
    end subroutine process_def_list_show

```

Read the complete list. We need an array of templates for the component sub-objects of abstract `prc_core_t` type, to allocate them with the correct specific type.

NOTE: Error handling is missing. Reading will just be aborted on error, or an I/O error occurs.

```

<Process libraries: process def list: TBP>+=
    procedure :: read => process_def_list_read

<Process libraries: procedures>+=
    subroutine process_def_list_read (object, unit, core_def_templates)
        class(process_def_list_t), intent(out) :: object
        integer, intent(in) :: unit
        type(prc_template_t), dimension(:), intent(in) :: core_def_templates
        type(process_def_entry_t), pointer :: entry
        character(80) :: buffer, ref
        integer :: i
        read (unit, "(A)") buffer
        write (ref, "(1x,A)") "Process definition list: [empty]"
        if (buffer == ref) return ! OK: empty library
        backspace (unit)
    end subroutine process_def_list_read

```

```

READ_ENTRIES: do i = 1, huge (0)
  if (i > 1) read (unit, *, end=1)
  read (unit, "(A)") buffer

  write (ref, "(1x,A,I0,A)") "Process #", i, ":"
  if (buffer /= ref) return      ! Wrong process header: done.
  allocate (entry)
  call entry%read (unit, core_def_templates)
  call object%append (entry)
end do READ_ENTRIES
1  continue                      ! EOF: done
end subroutine process_def_list_read

```

Append an entry to the list. The entry should be allocated as a pointer, and the pointer allocation is transferred. The original pointer is returned null.

```

<Process libraries: process def list: TBP>+=
  procedure :: append => process_def_list_append

<Process libraries: procedures>+=
  subroutine process_def_list_append (list, entry)
    class(process_def_list_t), intent(inout) :: list
    type(process_def_entry_t), intent(inout), pointer :: entry
    if (list%contains (entry%id)) then
      call msg_fatal ("Recording process: '" // char (entry%id) &
        // "' has already been defined")
    end if
    if (associated (list%first)) then
      list%last%next => entry
    else
      list%first => entry
    end if
    list%last => entry
    entry => null ()
  end subroutine process_def_list_append

```

Probe the process definition list

Return the number of processes supported by the library.

```

<Process libraries: process def list: TBP>+=
  procedure :: get_n_processes => process_def_list_get_n_processes

<Process libraries: procedures>+=
  function process_def_list_get_n_processes (list) result (n)
    integer :: n
    class(process_def_list_t), intent(in) :: list
    type(process_def_entry_t), pointer :: current
    n = 0
    current => list%first
    do while (associated (current))
      n = n + 1
      current => current%next
    end do
  end function process_def_list_get_n_processes

```

Allocate an array with the process IDs supported by the library.

```

(Process libraries: process def list: TBP)+≡
  procedure :: get_process_id_list => process_def_list_get_process_id_list

(Process libraries: procedures)+≡
  subroutine process_def_list_get_process_id_list (list, id)
    class(process_def_list_t), intent(in) :: list
    type(string_t), dimension(:), allocatable, intent(out) :: id
    type(process_def_entry_t), pointer :: current
    integer :: i
    allocate (id (list%get_n_processes ()))
    i = 0
    current => list%first
    do while (associated (current))
      i = i + 1
      id(i) = current%id
      current => current%next
    end do
  end subroutine process_def_list_get_process_id_list

```

Return just the processes which require resonant subprocesses.

```

(Process libraries: process def list: TBP)+≡
  procedure :: get_process_id_req_resonant => &
    process_def_list_get_process_id_req_resonant

(Process libraries: procedures)+≡
  subroutine process_def_list_get_process_id_req_resonant (list, id)
    class(process_def_list_t), intent(in) :: list
    type(string_t), dimension(:), allocatable, intent(out) :: id
    type(process_def_entry_t), pointer :: current
    integer :: i
    allocate (id (list%get_n_processes ()))
    i = 0
    current => list%first
    do while (associated (current))
      if (current%requires_resonances) then
        i = i + 1
        id(i) = current%id
      end if
      current => current%next
    end do
    id = id(1:i)
  end subroutine process_def_list_get_process_id_req_resonant

```

Return a pointer to a particular process entry.

```

(Process libraries: process def list: TBP)+≡
  procedure :: get_process_def_ptr => process_def_list_get_process_def_ptr

(Process libraries: procedures)+≡
  function process_def_list_get_process_def_ptr (list, id) result (entry)
    type(process_def_entry_t), pointer :: entry
    class(process_def_list_t), intent(in) :: list
    type(string_t), intent(in) :: id

```

```

    type(process_def_entry_t), pointer :: current
    current => list%first
    do while (associated (current))
        if (id == current%id) exit
        current => current%next
    end do
    entry => current
end function process_def_list_get_process_def_ptr

```

Return true if a given process is in the library.

```

⟨Process libraries: process def list: TBP⟩+≡
    procedure :: contains => process_def_list_contains

⟨Process libraries: procedures⟩+≡
    function process_def_list_contains (list, id) result (flag)
        logical :: flag
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(process_def_entry_t), pointer :: current
        current => list%get_process_def_ptr (id)
        flag = associated (current)
    end function process_def_list_contains

```

Return the index of the entry that corresponds to a given process.

```

⟨Process libraries: process def list: TBP⟩+≡
    procedure :: get_entry_index => process_def_list_get_entry_index

⟨Process libraries: procedures⟩+≡
    function process_def_list_get_entry_index (list, id) result (n)
        integer :: n
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(process_def_entry_t), pointer :: current
        n = 0
        current => list%first
        do while (associated (current))
            n = n + 1
            if (id == current%id) then
                return
            end if
            current => current%next
        end do
        n = 0
    end function process_def_list_get_entry_index

```

Return the numerical ID for a process.

```

⟨Process libraries: process def list: TBP⟩+≡
    procedure :: get_num_id => process_def_list_get_num_id

⟨Process libraries: procedures⟩+≡
    function process_def_list_get_num_id (list, id) result (num_id)
        integer :: num_id
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id

```

```

type(process_def_entry_t), pointer :: current
current => list%get_process_def_ptr (id)
if (associated (current)) then
    num_id = current%num_id
else
    num_id = 0
end if
end function process_def_list_get_num_id

```

Return the model name for a given process in the library.

```

(Process libraries: process def list: TBP)+≡
    procedure :: get_model_name => process_def_list_get_model_name

(Process libraries: procedures)+≡
    function process_def_list_get_model_name (list, id) result (model_name)
        type(string_t) :: model_name
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(process_def_entry_t), pointer :: current
        current => list%get_process_def_ptr (id)
        if (associated (current)) then
            model_name = current%model_name
        else
            model_name = ""
        end if
    end function process_def_list_get_model_name

```

Return the number of incoming particles of a given process in the library. This tells us whether the process is a decay or a scattering.

```

(Process libraries: process def list: TBP)+≡
    procedure :: get_n_in => process_def_list_get_n_in

(Process libraries: procedures)+≡
    function process_def_list_get_n_in (list, id) result (n)
        integer :: n
        class(process_def_list_t), intent(in) :: list
        type(string_t), intent(in) :: id
        type(process_def_entry_t), pointer :: current
        current => list%get_process_def_ptr (id)
        if (associated (current)) then
            n = current%n_in
        else
            n = 0
        end if
    end function process_def_list_get_n_in

```

Return the incoming particle pdg codesnumber of incoming particles of a given process in the library. If there is a PDG array, return only the first code for each beam. This serves as a quick way for (re)constructing beam properties.

```

(Process libraries: process def list: TBP)+≡
    procedure :: get_pdg_in_1 => process_def_list_get_pdg_in_1

```

```

(Process libraries: procedures)+≡
subroutine process_def_list_get_pdg_in_1 (list, id, pdg)
  class(process_def_list_t), intent(in) :: list
  type(string_t), intent(in) :: id
  integer, dimension(:), intent(out) :: pdg
  type(process_def_entry_t), pointer :: current
  current => list%get_process_def_ptr (id)
  if (associated (current)) then
    call current%get_pdg_in_1 (pdg)
  else
    pdg = 0
  end if
end subroutine process_def_list_get_pdg_in_1

```

Return the list of component IDs of a given process in the library.

```

(Process libraries: process def list: TBP)+≡
procedure :: get_component_list => process_def_list_get_component_list

(Process libraries: procedures)+≡
subroutine process_def_list_get_component_list (list, id, cid)
  class(process_def_list_t), intent(in) :: list
  type(string_t), intent(in) :: id
  type(string_t), dimension(:), allocatable, intent(out) :: cid
  type(process_def_entry_t), pointer :: current
  integer :: i, n
  current => list%get_process_def_ptr (id)
  if (associated (current)) then
    allocate (cid (current%n_initial + current%n_extra))
    do i = 1, current%n_initial
      cid(i) = current%initial(i)%basename
    end do
    n = current%n_initial
    do i = 1, current%n_extra
      cid(n + i) = current%extra(i)%basename
    end do
  end if
end subroutine process_def_list_get_component_list

```

Return the list of component description strings for a given process in the library.

```

(Process libraries: process def list: TBP)+≡
procedure :: get_component_description_list => &
  process_def_list_get_component_description_list

(Process libraries: procedures)+≡
subroutine process_def_list_get_component_description_list &
  (list, id, description)
  class(process_def_list_t), intent(in) :: list
  type(string_t), intent(in) :: id
  type(string_t), dimension(:), allocatable, intent(out) :: description
  type(process_def_entry_t), pointer :: current
  integer :: i, n
  current => list%get_process_def_ptr (id)
  if (associated (current)) then
    allocate (description (current%n_initial + current%n_extra))

```

```

do i = 1, current%n_initial
  description(i) = current%initial(i)%description
end do
n = current%n_initial
do i = 1, current%n_extra
  description(n + i) = current%extra(i)%description
end do
end if
end subroutine process_def_list_get_component_description_list

```

Return whether the entry requires construction of a resonant subprocess set.

(Process libraries: process def list: TBP)+≡

```

procedure :: req_resonant => process_def_list_req_resonant

```

(Process libraries: procedures)+≡

```

function process_def_list_req_resonant (list, id) result (flag)
  class(process_def_list_t), intent(in) :: list
  type(string_t), intent(in) :: id
  logical :: flag
  type(process_def_entry_t), pointer :: current
  current => list%get_process_def_ptr (id)
  if (associated (current)) then
    flag = current%requires_resonances
  else
    flag = .false.
  end if
end function process_def_list_req_resonant

```

14.4.3 Process library

The process library object is the interface between the process definition data, as provided by the user, generated or linked process code on file, and the process run data that reference the process code.

Process library entry

For each process component that is part of the library, there is a separate library entry (`process_library_entry_t`). The library entry connects a process definition with the specific code (if any) in the compiled driver library.

The **status** indicates how far the process has been processed by the system (definition, code generation, compilation, linking). A process with status `STAT_LOADED` is accessible for computing matrix elements.

The **def** pointer identifies the corresponding process definition. The process component within that definition is identified by the **i_component** index.

The **i_external** index refers to the compiled library driver. If it is zero, there is no associated matrix-element code.

The **driver** component holds the pointers to the matrix-element specific functions, in particular the matrix element function itself.

(Process libraries: types)+≡

```

type :: process_library_entry_t
  private

```



```

integer :: status = STAT_UNKNOWN
type(process_def_t), pointer :: def => null ()
integer :: i_component = 0
integer :: i_external = 0
class(prc_core_driver_t), allocatable :: driver
contains
  <Process libraries: process library entry: TBP>
end type process_library_entry_t

```

Here are the available status codes. An entry starts with UNKNOWN status. Once the association with a valid process definition is established, the status becomes CONFIGURED. If matrix element source code is to be generated by the system or provided from elsewhere, CODE.GENERATED indicates that this is done. The COMPILED status is next, it also applies to processes which are accessed as pre-compiled binaries. Finally, the library is linked and process pointers are set; this is marked as LOADED.

For a process library, the initial status is OPEN, since process definitions may be added. After configuration, the process content is fixed and the status becomes CONFIGURED. The further states are as above, always referring to the lowest status among the process entries.

```

<Process libraries: parameters>≡
integer, parameter, public :: STAT_UNKNOWN = 0
integer, parameter, public :: STAT_OPEN = 1
integer, parameter, public :: STAT_CONFIGURED = 2
integer, parameter, public :: STAT_SOURCE = 3
integer, parameter, public :: STAT_COMPILED = 4
integer, parameter, public :: STAT_LINKED = 5
integer, parameter, public :: STAT_ACTIVE = 6

integer, parameter, public :: ASSOCIATED_BORN = 1
integer, parameter, public :: ASSOCIATED_REAL = 2
integer, parameter, public :: ASSOCIATED_VIRT = 3
integer, parameter, public :: ASSOCIATED_SUB = 4
integer, parameter, public :: ASSOCIATED_PDF = 5
integer, parameter, public :: ASSOCIATED_REAL_SING = 6
integer, parameter, public :: ASSOCIATED_REAL_FIN = 7
integer, parameter, public :: N_ASSOCIATED_COMPONENTS = 7

```

These are the associated code letters, for output:

```

<Process libraries: parameters>+≡
character, dimension(0:6), parameter :: STATUS_LETTER = &
  ["?", "o", "f", "s", "c", "l", "a"]

```

This produces a condensed account of the library entry. The status is indicated by a letter in brackets, then the ID and component index of the associated process definition, finally the library index, if available.

```

<Process libraries: process library entry: TBP>≡
procedure :: to_string => process_library_entry_to_string

<Process libraries: procedures>+≡
function process_library_entry_to_string (object) result (string)
  type(string_t) :: string

```

```

class(process_library_entry_t), intent(in) :: object
character(32) :: buffer
string = "[" // STATUS_LETTER(object%status) // "]"
select case (object%status)
case (STAT_UNKNOWN)
case default
    if (associated (object%def)) then
        write (buffer, "(IO)") object%i_component
        string = string // " " // object%def%id // "." // trim (buffer)
    end if
    if (object%i_external /= 0) then
        write (buffer, "(IO)") object%i_external
        string = string // " = ext:" // trim (buffer)
    else
        string = string // " = int"
    end if
    if (allocated (object%driver)) then
        string = string // " (" // object%driver%type_name () // ")"
    end if
end select
end function process_library_entry_to_string

```

Initialize with data. Used for the unit tests.

```

<Process libraries: process library entry: TBP>+≡
    procedure :: init => process_library_entry_init

<Process libraries: procedures>+≡
    subroutine process_library_entry_init (object, &
        status, def, i_component, i_external, driver_template)
        class(process_library_entry_t), intent(out) :: object
        integer, intent(in) :: status
        type(process_def_t), target, intent(in) :: def
        integer, intent(in) :: i_component
        integer, intent(in) :: i_external
        class(prc_core_driver_t), intent(inout), allocatable, optional &
            :: driver_template
        object%status = status
        object%def => def
        object%i_component = i_component
        object%i_external = i_external
        if (present (driver_template)) then
            call move_alloc (driver_template, object%driver)
        end if
    end subroutine process_library_entry_init

```

Assign pointers for all process-specific features. We have to combine the method from the `core_def` specification, the assigned pointers within the library driver, the index within that driver, and the process driver which should receive the links.

```

<Process libraries: process library entry: TBP>+≡
    procedure :: connect => process_library_entry_connect

<Process libraries: procedures>+≡
    subroutine process_library_entry_connect (entry, lib_driver, i)

```

```

class(process_library_entry_t), intent(inout) :: entry
class(prclib_driver_t), intent(in) :: lib_driver
integer, intent(in) :: i
call entry%def%initial(entry%i_component)%connect &
    (lib_driver, i, entry%driver)
end subroutine process_library_entry_connect

```

The process library object

The `process_library_t` type is an extension of the `process_def_list_t` type. Thus, it automatically contains the process definition list.

The `basename` identifies the library generically.

The `external` flag is true if any process within the library needs external code, so the library must correspond to an actual code library (statically or dynamically linked).

The `entry` array contains all process components that can be handled by this library. Each entry refers to the process (component) definition and to the associated external matrix element code, if there is any.

The `driver` object is needed only if `external` is true. This object handles all interactions with external matrix-element code.

The `md5sum` summarizes the complete `process_def_list_t` base object. It can be used to check if the library configuration has changed.

```

(Process libraries: public)+≡
    public :: process_library_t

(Process libraries: types)+≡
    type, extends (process_def_list_t) :: process_library_t
    private
    type(string_t) :: basename
    integer :: n_entries = 0
    logical :: external = .false.
    integer :: status = STAT_UNKNOWN
    logical :: static = .false.
    logical :: driver_exists = .false.
    logical :: makefile_exists = .false.
    integer :: update_counter = 0
    type(process_library_entry_t), dimension(:), allocatable :: entry
    class(prclib_driver_t), allocatable :: driver
    character(32) :: md5sum = ""
    contains
    (Process libraries: process library: TBP)
end type process_library_t

```

For the output, we write first the metadata and the DL access record, then the library entries in short form, and finally the process definition list which is the base object.

Don't write the MD5 sum since this is used to generate it.

```

(Process libraries: process library: TBP)≡
    procedure :: write => process_library_write

```

<Process libraries: procedures>+≡

```

subroutine process_library_write (object, unit, libpath)
  class(process_library_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: libpath
  integer :: i, u
  u = given_output_unit (unit)
  write (u, "(1x,A,A)") "Process library: ", char (object%basename)
  write (u, "(3x,A,L1)") "external      = ", object%external
  write (u, "(3x,A,L1)") "makefile exists = ", object%makefile_exists
  write (u, "(3x,A,L1)") "driver exists  = ", object%driver_exists
  write (u, "(3x,A,A1)") "code status   = ", &
    STATUS_LETTER (object%status)
  write (u, *)
  if (allocated (object%entry)) then
    write (u, "(1x,A)", advance="no") "Process library entries:"
    write (u, "(1x,I0)") object%n_entries
    do i = 1, size (object%entry)
      write (u, "(1x,A,I0,A,A)") "Entry #", i, ": ", &
        char (object%entry(i)%to_string ())
    end do
    write (u, *)
  end if
  if (object%external) then
    call object%driver%write (u, libpath)
    write (u, *)
  end if
  call object%process_def_list_t%write (u)
end subroutine process_library_write

```

Condensed version for screen output.

<Process libraries: process library: TBP>+≡

procedure :: show => process_library_show

<Process libraries: procedures>+≡

```

subroutine process_library_show (object, unit)
  class(process_library_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(A,A)") "Process library: ", char (object%basename)
  write (u, "(2x,A,L1)") "external      = ", object%external
  if (object%static) then
    write (u, "(2x,A,L1)") "static          = ", .true.
  else
    write (u, "(2x,A,L1)") "makefile exists = ", object%makefile_exists
    write (u, "(2x,A,L1)") "driver exists  = ", object%driver_exists
  end if
  write (u, "(2x,A,A1)", advance="no") "code status   = "
  select case (object%status)
  case (STAT_UNKNOWN);   write (u, "(A)") "[unknown]"
  case (STAT_OPEN);      write (u, "(A)") "open"
  case (STAT_CONFIGURED); write (u, "(A)") "configured"
  case (STAT_SOURCE);    write (u, "(A)") "source code exists"

```

```

        case (STAT_COMPILED);   write (u, "(A)") "compiled"
        case (STAT_LINKED);    write (u, "(A)") "linked"
        case (STAT_ACTIVE);    write (u, "(A)") "active"
    end select
    call object%process_def_list_t%show (u)
end subroutine process_library_show

```

The initializer defines just the basename. We may now add process definitions to the library.

```

<Process libraries: process library: TBP>+=
    procedure :: init => process_library_init

<Process libraries: procedures>+=
    subroutine process_library_init (lib, basename)
        class(process_library_t), intent(out) :: lib
        type(string_t), intent(in) :: basename
        lib%basename = basename
        lib%status = STAT_OPEN
        call msg_message ("Process library '" // char (basename) &
            // "': initialized")
    end subroutine process_library_init

```

This alternative initializer declares the library as static. We should now add process definitions to the library, but all external process code exists already. We need the driver object, and we should check the defined processes against the stored ones.

```

<Process libraries: process library: TBP>+=
    procedure :: init_static => process_library_init_static

<Process libraries: procedures>+=
    subroutine process_library_init_static (lib, basename)
        class(process_library_t), intent(out) :: lib
        type(string_t), intent(in) :: basename
        lib%basename = basename
        lib%status = STAT_OPEN
        lib%static = .true.
        call msg_message ("Static process library '" // char (basename) &
            // "': initialized")
    end subroutine process_library_init_static

```

The `configure` procedure scans the allocated entries in the process definition list. The configuration proceeds in three passes.

In the first pass, we scan the process definition list and count the number of process components and the number of components which need external code. This is used to allocate the `entry` array.

In the second pass, we initialize the `entry` elements which connect process definitions, process driver objects, and external code.

In the third pass, we initialize the library driver object, allocating an entry for each external matrix element.

NOTE: Currently we handle only `initial` process components; `extra` components are ignored.

```

<Process libraries: process library: TBP>+=
    procedure :: configure => process_library_configure

```

```

(Process libraries: procedures)+≡
subroutine process_library_configure (lib, os_data)
  class(process_library_t), intent(inout) :: lib
  type(os_data_t), intent(in) :: os_data
  type(process_def_entry_t), pointer :: def_entry
  integer :: n_entries, n_external, i_entry, i_external
  type(string_t) :: model_name
  integer :: i_component

  n_entries = 0
  n_external = 0
  if (allocated (lib%entry)) deallocate (lib%entry)

  def_entry => lib%first
  do while (associated (def_entry))
    do i_component = 1, def_entry%n_initial
      n_entries = n_entries + 1
      if (def_entry%initial(i_component)%needs_code ()) then
        n_external = n_external + 1
        lib%external = .true.
      end if
    end do
    def_entry => def_entry%next
  end do

  call lib%allocate_entries (n_entries)

  i_entry = 0
  i_external = 0
  def_entry => lib%first
  do while (associated (def_entry))
    do i_component = 1, def_entry%n_initial
      i_entry = i_entry + 1
      associate (lib_entry => lib%entry(i_entry))
        lib_entry%status = STAT_CONFIGURED
        lib_entry%def => def_entry%process_def_t
        lib_entry%i_component = i_component
        if (def_entry%initial(i_component)%needs_code ()) then
          i_external = i_external + 1
          lib_entry%i_external = i_external
        end if
        call def_entry%initial(i_component)%allocate_driver &
          (lib_entry%driver)
      end associate
    end do
    def_entry => def_entry%next
  end do

  call dispatch_prclib_driver (lib%driver, &
    lib%basename, lib%get_modellibs_ldflags (os_data))
  call lib%driver%init (n_external)
  do i_entry = 1, n_entries
    associate (lib_entry => lib%entry(i_entry))
      i_component = lib_entry%i_component
    end associate
  end do

```

```

        model_name = lib_entry%def%model_name
        associate (def => lib_entry%def%initial(i_component))
            if (def%needs_code ()) then
                call lib%driver%set_record (lib_entry%i_external, &
                    def%basename, &
                    model_name, &
                    def%get_features (), def%get_writer_ptr ())
            end if
        end associate
    end associate
end do

if (lib%static) then
    if (lib%n_entries /= 0) lib_entry%status = STAT_LINKED
    lib%status = STAT_LINKED
else if (lib%external) then
    where (lib_entry%i_external == 0) lib_entry%status = STAT_LINKED
    lib%status = STAT_CONFIGURED
    lib%makefile_exists = .false.
    lib%driver_exists = .false.
else
    if (lib%n_entries /= 0) lib_entry%status = STAT_LINKED
    lib%status = STAT_LINKED
end if
end subroutine process_library_configure

```

Basic setup: allocate the entry array.

```

<Process libraries: process library: TBP>+≡
    procedure :: allocate_entries => process_library_allocate_entries

<Process libraries: procedures>+≡
    subroutine process_library_allocate_entries (lib, n_entries)
        class(process_library_t), intent(inout) :: lib
        integer, intent(in) :: n_entries
        lib%n_entries = n_entries
        allocate (lib%entry (n_entries))
    end subroutine process_library_allocate_entries

```

Initialize an entry with data (used by unit tests).

```

<Process libraries: process library: TBP>+≡
    procedure :: init_entry => process_library_init_entry

<Process libraries: procedures>+≡
    subroutine process_library_init_entry (lib, i, &
        status, def, i_component, i_external, driver_template)
        class(process_library_t), intent(inout) :: lib
        integer, intent(in) :: i
        integer, intent(in) :: status
        type(process_def_t), target, intent(in) :: def
        integer, intent(in) :: i_component
        integer, intent(in) :: i_external
        class(prc_core_driver_t), intent(inout), allocatable, optional &
            :: driver_template
        call lib%entry(i)%init (status, def, i_component, i_external, &

```

```

        driver_template)
    end subroutine process_library_init_entry

```

Compute the MD5 sum. We concatenate the individual MD5 sums of all processes (which, in turn, are derived from the MD5 sums of their components) and compute the MD5 sum of that.

This should be executed *after* configuration, where the driver was initialized, since otherwise the MD5 sum stored in the driver would be overwritten.

```

(Process libraries: process library: TBP)+≡
    procedure :: compute_md5sum => process_library_compute_md5sum

(Process libraries: procedures)+≡
    subroutine process_library_compute_md5sum (lib, model)
        class(process_library_t), intent(inout) :: lib
        class(model_data_t), intent(in), optional, target :: model
        type(process_def_entry_t), pointer :: def_entry
        type(string_t) :: buffer
        buffer = lib%basename
        def_entry => lib%first
        do while (associated (def_entry))
            call def_entry%compute_md5sum (model)
            buffer = buffer // def_entry%md5sum
            def_entry => def_entry%next
        end do
        lib%md5sum = md5sum (char (buffer))
        call lib%driver%set_md5sum (lib%md5sum)
    end subroutine process_library_compute_md5sum

```

Write an appropriate makefile, if there are external processes. Unless **force** is in effect, first check if there is already a makefile with the correct MD5 sum. If yes, do nothing.

The **workspace** optional argument puts any library code in a subdirectory.

```

(Process libraries: process library: TBP)+≡
    procedure :: write_makefile => process_library_write_makefile

(Process libraries: procedures)+≡
    subroutine process_library_write_makefile &
        (lib, os_data, force, verbose, testflag, workspace)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: force, verbose
        logical, intent(in), optional :: testflag
        type(string_t), intent(in), optional :: workspace
        character(32) :: md5sum_file
        logical :: generate
        integer :: unit
        if (lib%external .and. .not. lib%static) then
            generate = .true.
            if (.not. force) then
                md5sum_file = lib%driver%get_md5sum_makefile (workspace)
                if (lib%md5sum == md5sum_file) then
                    call msg_message ("Process library '" // char (lib%basename) &
                        // "' : keeping makefile")

```



```

        generate = .false.
    end if
end if
if (generate) then
    call msg_message ("Process library '" // char (lib%basename) &
        // "': writing makefile")
    unit = free_unit ()
    open (unit, &
        file = char (workspace_prefix (workspace) &
            & // lib%driver%basename // ".makefile"), &
        status="replace", action="write")
    call lib%driver%generate_makefile (unit, os_data, verbose, testflag)
    close (unit)
end if
lib%makefile_exists = .true.
end if
end subroutine process_library_write_makefile

```

Write the driver source code for the library to file, if there are external processes.

```

<Process libraries: process library: TBP>+≡
    procedure :: write_driver => process_library_write_driver

<Process libraries: procedures>+≡
    subroutine process_library_write_driver (lib, force, workspace)
        class(process_library_t), intent(inout) :: lib
        logical, intent(in) :: force
        type(string_t), intent(in), optional :: workspace
        character(32) :: md5sum_file
        logical :: generate
        integer :: unit
        if (lib%external .and. .not. lib%static) then
            generate = .true.
            if (.not. force) then
                md5sum_file = lib%driver%get_md5sum_driver (workspace)
                if (lib%md5sum == md5sum_file) then
                    call msg_message ("Process library '" // char (lib%basename) &
                        // "': keeping driver")
                    generate = .false.
                end if
            end if
            if (generate) then
                call msg_message ("Process library '" // char (lib%basename) &
                    // "': writing driver")
                unit = free_unit ()
                open (unit, &
                    file = char (workspace_prefix (workspace) &
                        & // lib%driver%basename // ".f90"), &
                    status="replace", action="write")
                call lib%driver%generate_driver_code (unit)
                close (unit)
            end if
            lib%driver_exists = .true.
        end if
    end subroutine process_library_write_driver

```

Update the compilation status of an external library.

Strictly speaking, this is not necessary for a one-time run, since the individual library methods will update the status themselves. However, it allows us to identify compilation steps that we can skip because the file exists or is already loaded, for the whole library or for particular entries.

Independently, the building process is controlled by a makefile. Thus, previous files are reused if they are not modified by the current compilation.

1. If it is not already loaded, attempt to load the library. If successful, check the overall MD5 sum. If it matches, just keep it loaded and mark as ACTIVE. If not, check the MD5 sum for all linked process components. Where it matches, mark the entry as COMPILED. Then, unload the library and mark as CONFIGURED.

Thus, we can identify compiled files for all matrix elements which are accessible via the previous compiled library, even if it is no longer up to date.

2. If the library is now in CONFIGURED state, look for valid source files. Each entry that is just in CONFIGURED state will advance to SOURCE if the MD5 sum matches. Finally, advance the whole library to SOURCE if all entries are at least in this condition.

(Process libraries: process library: TBP)+≡

```
procedure :: update_status => process_library_update_status
```

(Process libraries: procedures)+≡

```
subroutine process_library_update_status (lib, os_data, workspace)
  class(process_library_t), intent(inout) :: lib
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(in), optional :: workspace
  character(32) :: md5sum_file
  integer :: i, i_external, i_component
  if (lib%external) then
    select case (lib%status)
    case (STAT_CONFIGURED:STAT_LINKED)
      call lib%driver%load (os_data, noerror=.true., workspace=workspace)
    end select
  if (lib%driver%loaded) then
    md5sum_file = lib%driver%get_md5sum (0)
    if (lib%md5sum == md5sum_file) then
      call lib%load_entries ()
      lib%entry%status = STAT_ACTIVE
      lib%status = STAT_ACTIVE
      call msg_message ("Process library '" // char (lib%basename) &
        // "': active")
    else
      do i = 1, lib%n_entries
        associate (entry => lib%entry(i))
          i_external = entry%i_external
          i_component = entry%i_component
          if (i_external /= 0) then
            md5sum_file = lib%driver%get_md5sum (i_external)
```

```

        if (entry%def%get_md5sum (i_component) == md5sum_file) then
            entry%status = STAT_COMPILED
        else
            entry%status = STAT_CONFIGURED
        end if
    end if
end associate
end do
call lib%driver%unload ()
lib%status = STAT_CONFIGURED
end if
end if
select case (lib%status)
case (STAT_CONFIGURED)
    do i = 1, lib%n_entries
        associate (entry => lib%entry(i))
            i_external = entry%i_external
            i_component = entry%i_component
            if (i_external /= 0) then
                select case (entry%status)
                case (STAT_CONFIGURED)
                    md5sum_file = lib%driver%get_md5sum_source &
                        (i_external, workspace)
                    if (entry%def%get_md5sum (i_component) == md5sum_file) then
                        entry%status = STAT_SOURCE
                    end if
                end select
            end if
        end associate
    end do
    if (all (lib%entry%status >= STAT_SOURCE)) then
        md5sum_file = lib%driver%get_md5sum_driver (workspace)
        if (lib%md5sum == md5sum_file) then
            lib%status = STAT_SOURCE
        end if
    end if
end select
end if
end subroutine process_library_update_status

```

This procedure triggers code generation for all processes where this is possible.

We generate code only for external processes of status `STAT_CONFIGURED`, which then advance to `STAT_SOURCE`. If, for a particular process, the status is already advanced, we do not remove previous files, so `make` will consider them as up to date if they exist. Otherwise, we remove those files to force a fresh `make`.

Finally, if any source code has been generated, we need a driver file.

```

<Process libraries: process library: TBP>+≡
    procedure :: make_source => process_library_make_source

<Process libraries: procedures>+≡
    subroutine process_library_make_source &
        (lib, os_data, keep_old_source, workspace)

```

```

class(process_library_t), intent(inout) :: lib
type(os_data_t), intent(in) :: os_data
logical, intent(in), optional :: keep_old_source
type(string_t), intent(in), optional :: workspace
logical :: keep_old
integer :: i, i_external
keep_old = .false.
if (present (keep_old_source)) keep_old = keep_old_source
if (lib%external .and. .not. lib%static) then
  select case (lib%status)
  case (STAT_CONFIGURED)
    if (keep_old) then
      call msg_message ("Process library '" // char (lib%basename) &
        // "': keeping source code")
    else
      call msg_message ("Process library '" // char (lib%basename) &
        // "': creating source code")
      do i = 1, size (lib%entry)
        associate (entry => lib%entry(i))
          i_external = entry%i_external
          if (i_external /= 0 &
            .and. lib%entry(i)%status == STAT_CONFIGURED) then
            call lib%driver%clean_proc &
              (i_external, os_data, workspace)
          end if
        end associate
      end do
      call lib%driver%make_source (os_data, workspace)
    end if
    lib%status = STAT_SOURCE
    where (lib%entry%i_external /= 0 &
      .and. lib%entry%status == STAT_CONFIGURED)
      lib%entry%status = STAT_SOURCE
    end where
    lib%status = STAT_SOURCE
  end select
end if
end subroutine process_library_make_source

```

Compile the generated code and update the status codes. Try to make the sources first, just in case. This includes compiling possible L^AT_EX Feynman diagram files.

```

⟨Process libraries: process library: TBP⟩+≡
  procedure :: make_compile => process_library_make_compile

⟨Process libraries: procedures⟩+≡
  subroutine process_library_make_compile &
    (lib, os_data, keep_old_source, workspace)
    class(process_library_t), intent(inout) :: lib
    type(os_data_t), intent(in) :: os_data
    logical, intent(in), optional :: keep_old_source
    type(string_t), intent(in), optional :: workspace
    if (lib%external .and. .not. lib%static) then

```

```

select case (lib%status)
case (STAT_CONFIGURED)
    call lib%make_source (os_data, keep_old_source, workspace)
end select
if (signal_is_pending ()) return
select case (lib%status)
case (STAT_SOURCE)
    call msg_message ("Process library '" // char (lib%basename) &
        // "': compiling sources")
    call lib%driver%make_compile (os_data, workspace)
    where (lib%entry%i_external /= 0 &
        .and. lib%entry%status == STAT_SOURCE)
        lib%entry%status = STAT_COMPILED
    end where
    lib%status = STAT_COMPILED
end select
end if
end subroutine process_library_make_compile

```

Link the process library. Try to compile first, just in case.

```

<Process libraries: process library: TBP>+≡
    procedure :: make_link => process_library_make_link

<Process libraries: procedures>+≡
    subroutine process_library_make_link &
        (lib, os_data, keep_old_source, workspace)
    class(process_library_t), intent(inout) :: lib
    type(os_data_t), intent(in) :: os_data
    logical, intent(in), optional :: keep_old_source
    type(string_t), intent(in), optional :: workspace
    if (lib%external .and. .not. lib%static) then
        select case (lib%status)
        case (STAT_CONFIGURED:STAT_SOURCE)
            call lib%make_compile (os_data, keep_old_source, workspace)
        end select
        if (signal_is_pending ()) return
        select case (lib%status)
        case (STAT_COMPILED)
            call msg_message ("Process library '" // char (lib%basename) &
                // "': linking")
            call lib%driver%make_link (os_data, workspace)
            lib%entry%status = STAT_LINKED
            lib%status = STAT_LINKED
        end select
    end if
end subroutine process_library_make_link

```

Load the process library, i.e., assign pointers to the library functions.

```

<Process libraries: process library: TBP>+≡
    procedure :: load => process_library_load

<Process libraries: procedures>+≡
    subroutine process_library_load (lib, os_data, keep_old_source, workspace)
    class(process_library_t), intent(inout) :: lib

```

```

type(os_data_t), intent(in) :: os_data
logical, intent(in), optional :: keep_old_source
type(string_t), intent(in), optional :: workspace
select case (lib%status)
case (STAT_CONFIGURED:STAT_COMPILED)
    call lib%make_link (os_data, keep_old_source, workspace)
end select
if (signal_is_pending ()) return
select case (lib%status)
case (STAT_LINKED)
    if (lib%external) then
        call msg_message ("Process library '" // char (lib%basename) &
            // "': loading")
        call lib%driver%load (os_data, workspace=workspace)
        call lib%load_entries ()
    end if
    lib%entry%status = STAT_ACTIVE
    lib%status = STAT_ACTIVE
end select
end subroutine process_library_load

```

This is the actual loading part for the process methods.

```

<Process libraries: process library: TBP>+≡
    procedure :: load_entries => process_library_load_entries

<Process libraries: procedures>+≡
    subroutine process_library_load_entries (lib)
        class(process_library_t), intent(inout) :: lib
        integer :: i
        do i = 1, size (lib%entry)
            associate (entry => lib%entry(i))
                if (entry%i_external /= 0) then
                    call entry%connect (lib%driver, entry%i_external)
                end if
            end associate
        end do
    end subroutine process_library_load_entries

```

Unload the library, if possible. This reverts the status to “linked”.

```

<Process libraries: process library: TBP>+≡
    procedure :: unload => process_library_unload

<Process libraries: procedures>+≡
    subroutine process_library_unload (lib)
        class(process_library_t), intent(inout) :: lib
        select case (lib%status)
        case (STAT_ACTIVE)
            if (lib%external) then
                call msg_message ("Process library '" // char (lib%basename) &
                    // "': unloading")
                call lib%driver%unload ()
            end if
            lib%entry%status = STAT_LINKED
            lib%status = STAT_LINKED

```

```

        end select
    end subroutine process_library_unload

```

Unload, clean all generated files and revert the library status. If `distclean` is set, also remove the makefile and the driver source.

```

<Process libraries: process library: TBP>+≡
    procedure :: clean => process_library_clean

<Process libraries: procedures>+≡
    subroutine process_library_clean (lib, os_data, distclean, workspace)
        class(process_library_t), intent(inout) :: lib
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: distclean
        type(string_t), intent(in), optional :: workspace
        call lib%unload ()
        if (lib%external .and. .not. lib%static) then
            call msg_message ("Process library '" // char (lib%basename) &
                // "' : removing old files")
            if (distclean) then
                call lib%driver%distclean (os_data, workspace)
            else
                call lib%driver%clean (os_data, workspace)
            end if
        end if
        where (lib%entry%i_external /= 0)
            lib%entry%status = STAT_CONFIGURED
        elsewhere
            lib%entry%status = STAT_LINKED
        end where
        if (lib%external) then
            lib%status = STAT_CONFIGURED
        else
            lib%status = STAT_LINKED
        end if
    end subroutine process_library_clean

```

Unload and revert the library status to INITIAL. This allows for appending new processes. No files are deleted.

```

<Process libraries: process library: TBP>+≡
    procedure :: open => process_library_open

<Process libraries: procedures>+≡
    subroutine process_library_open (lib)
        class(process_library_t), intent(inout) :: lib
        select case (lib%status)
        case (STAT_OPEN)
        case default
            call lib%unload ()
            if (.not. lib%static) then
                lib%entry%status = STAT_OPEN
                lib%status = STAT_OPEN
                if (lib%external) lib%update_counter = lib%update_counter + 1
                call msg_message ("Process library '" // char (lib%basename) &
                    // "' : open")
            end if
        end select
    end subroutine process_library_open

```

```

        else
            call msg_error ("Static process library '" // char (lib%basename) &
                // "': processes can't be appended")
        end if
    end select
end subroutine process_library_open

```

14.4.4 Use the library

Return the base name of the library

```

<Process libraries: process library: TBP>+≡
    procedure :: get_name => process_library_get_name

<Process libraries: procedures>+≡
    function process_library_get_name (lib) result (name)
        class(process_library_t), intent(in) :: lib
        type(string_t) :: name
        name = lib%basename
    end function process_library_get_name

```

Once activated, we view the process library object as an interface for accessing the matrix elements.

```

<Process libraries: process library: TBP>+≡
    procedure :: is_active => process_library_is_active

<Process libraries: procedures>+≡
    function process_library_is_active (lib) result (flag)
        logical :: flag
        class(process_library_t), intent(in) :: lib
        flag = lib%status == STAT_ACTIVE
    end function process_library_is_active

```

Return the current status code of the library. If an index is provided, return the status of that entry.

```

<Process libraries: process library: TBP>+≡
    procedure :: get_status => process_library_get_status

<Process libraries: procedures>+≡
    function process_library_get_status (lib, i) result (status)
        class(process_library_t), intent(in) :: lib
        integer, intent(in), optional :: i
        integer :: status
        if (present (i)) then
            status = lib%entry(i)%status
        else
            status = lib%status
        end if
    end function process_library_get_status

```


Return the update counter. Since this is incremented each time the library is re-opened, we can use this to check if existing pointers to matrix element code are still valid.

```

(Process libraries: process library: TBP)+≡
  procedure :: get_update_counter => process_library_get_update_counter

(Process libraries: procedures)+≡
  function process_library_get_update_counter (lib) result (counter)
    class(process_library_t), intent(in) :: lib
    integer :: counter
    counter = lib%update_counter
  end function process_library_get_update_counter

```

Manually set the current status code of the library. If the optional flag is set, set also the entry status codes. This is used for unit tests.

```

(Process libraries: process library: TBP)+≡
  procedure :: set_status => process_library_set_status

(Process libraries: procedures)+≡
  subroutine process_library_set_status (lib, status, entries)
    class(process_library_t), intent(inout) :: lib
    integer, intent(in) :: status
    logical, intent(in), optional :: entries
    lib%status = status
    if (present (entries)) then
      if (entries) lib%entry%status = status
    end if
  end subroutine process_library_set_status

```

Return the load status of the associated driver.

```

(Process libraries: process library: TBP)+≡
  procedure :: is_loaded => process_library_is_loaded

(Process libraries: procedures)+≡
  function process_library_is_loaded (lib) result (flag)
    class(process_library_t), intent(in) :: lib
    logical :: flag
    flag = lib%driver%loaded
  end function process_library_is_loaded

```

Retrieve constants using the process library driver. We assume that the process code has been loaded, if external.

```

(Process libraries: process library entry: TBP)+≡
  procedure :: fill_constants => process_library_entry_fill_constants

(Process libraries: procedures)+≡
  subroutine process_library_entry_fill_constants (entry, driver, data)
    class(process_library_entry_t), intent(in) :: entry
    class(prclib_driver_t), intent(in) :: driver
    type(process_constants_t), intent(out) :: data
    integer :: i
    if (entry%i_external /= 0) then
      i = entry%i_external
    end if
  end subroutine process_library_entry_fill_constants

```

```

        data%id          = driver%get_process_id (i)
        data%model_name = driver%get_model_name (i)
        data%md5sum      = driver%get_md5sum (i)
        data%openmp_supported = driver%get_openmp_status (i)
        data%n_in  = driver%get_n_in  (i)
        data%n_out = driver%get_n_out (i)
        data%n_flv = driver%get_n_flv (i)
        data%n_hel = driver%get_n_hel (i)
        data%n_col = driver%get_n_col (i)
        data%n_cin = driver%get_n_cin (i)
        data%n_cf  = driver%get_n_cf  (i)
        call driver%set_flv_state (i, data%flv_state)
        call driver%set_hel_state (i, data%hel_state)
        call driver%set_col_state (i, data%col_state, data%ghost_flag)
        call driver%set_color_factors (i, data%color_factors, data%cf_index)
    else
        select type (proc_driver => entry%driver)
        class is (process_driver_internal_t)
            call proc_driver%fill_constants (data)
        end select
    end if
end subroutine process_library_entry_fill_constants

```

Retrieve the constants for a process

```

<Process libraries: process library: TBP>+≡
    procedure :: fill_constants => process_library_fill_constants

<Process libraries: procedures>+≡
    subroutine process_library_fill_constants (lib, id, i_component, data)
        class(process_library_t), intent(in) :: lib
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        type(process_constants_t), intent(out) :: data
        integer :: i
        do i = 1, size (lib%entry)
            associate (entry => lib%entry(i))
                if (entry%def%id == id .and. entry%i_component == i_component) then
                    call entry%fill_constants (lib%driver, data)
                    return
                end if
            end associate
        end do
    end subroutine process_library_fill_constants

```

Retrieve the constants and a connected driver for a process, identified by a process ID and a subprocess index. We scan the process entries until we have found a match.

```

<Process libraries: process library: TBP>+≡
    procedure :: connect_process => process_library_connect_process

<Process libraries: procedures>+≡
    subroutine process_library_connect_process &
        (lib, id, i_component, data, proc_driver)
        class(process_library_t), intent(in) :: lib

```

```

type(string_t), intent(in) :: id
integer, intent(in) :: i_component
type(process_constants_t), intent(out) :: data
class(prc_core_driver_t), allocatable, intent(out) :: proc_driver
integer :: i
do i = 1, size (lib%entry)
    associate (entry => lib%entry(i))
        if (entry%def%id == id .and. entry%i_component == i_component) then
            call entry%fill_constants (lib%driver, data)
            allocate (proc_driver, source = entry%driver)
            return
        end if
    end associate
end do
call msg_fatal ("Process library '" // char (lib%basename) &
               // "': process '" // char (id) // "' not found")
end subroutine process_library_connect_process

```

Shortcut for use in unit tests: fetch the MD5sum from a specific library entry and inject it into the writer of a specific record.

```

<Process libraries: process library: TBP>+≡
    procedure :: test_transfer_md5sum => process_library_test_transfer_md5sum

```

```

<Process libraries: procedures>+≡
    subroutine process_library_test_transfer_md5sum (lib, r, e, c)
        class(process_library_t), intent(inout) :: lib
        integer, intent(in) :: r, e, c
        associate (writer => lib%driver%record(r)%writer)
            writer%md5sum = lib%entry(e)%def%get_md5sum (c)
        end associate
    end subroutine process_library_test_transfer_md5sum

```

```

<Process libraries: process library: TBP>+≡
    procedure :: get_nlo_type => process_library_get_nlo_type

```

```

<Process libraries: procedures>+≡
    function process_library_get_nlo_type (lib, id, i_component) result (nlo_type)
        integer :: nlo_type
        class(process_library_t), intent(in) :: lib
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        integer :: i
        do i = 1, size (lib%entry)
            if (lib%entry(i)%def%id == id .and. lib%entry(i)%i_component == i_component) then
                nlo_type = lib%entry(i)%def%get_nlo_type (i_component)
                exit
            end if
        end do
    end function process_library_get_nlo_type

```

14.4.5 Collect model-specific libraries

This returns appropriate linker flags for the model parameter libraries that are used by the generated matrix element. At the end, the main libwhizard is appended (again), because functions from that may be required.

Extra models in the local user space need to be treated individually.

```

(Process libraries: process library: TBP)+≡
  procedure :: get_modellibs_ldflags => process_library_get_modellibs_ldflags
(Process libraries: procedures)+≡
  function process_library_get_modellibs_ldflags (prc_lib, os_data) result (flags)
    class(process_library_t), intent(in) :: prc_lib
    type(os_data_t), intent(in) :: os_data
    type(string_t) :: flags
    type(string_t), dimension(:), allocatable :: models
    type(string_t) :: modelname, modellib, modellib_full
    logical :: exist
    integer :: i, j, mi
    flags = " -lomega"
    if ((.not. os_data%use_testfiles) .and. &
        os_dir_exist (os_data%whizard_models_libpath_local)) &
        flags = flags // " -L" // os_data%whizard_models_libpath_local
    flags = flags // " -L" // os_data%whizard_models_libpath
    allocate (models(prc_lib%n_entries + 1))
    models = ""
    mi = 1
    if (allocated (prc_lib%entry)) then
      SCAN: do i = 1, prc_lib%n_entries
        if (associated (prc_lib%entry(i)%def)) then
          if (prc_lib%entry(i)%def%model_name /= "") then
            modelname = prc_lib%entry(i)%def%model_name
          else
            cycle SCAN
          end if
        else
          cycle SCAN
        end if
      end do
      models(mi) = modelname
      mi = mi + 1
      if (os_data%use_libtool) then
        modellib = "libparameters_" // modelname // ".la"
      else
        modellib = "libparameters_" // modelname // ".a"
      end if
      exist = .false.
      if (.not. os_data%use_testfiles) then
        modellib_full = os_data%whizard_models_libpath_local &
          // "/" // modellib
        inquire (file=char (modellib_full), exist=exist)
      end if
      if (.not. exist) then
        modellib_full = os_data%whizard_models_libpath &

```

```

        // "/" // modellib
        inquire (file=char (modellib_full), exist=exist)
    end if
    if (exist) flags = flags // " -lparameters_" // modelname
end do SCAN
end if
deallocate (models)
flags = flags // " -lwhizard"
end function process_library_get_modellibs_ldflags

```

(Process libraries: process library: TBP)+≡

```

procedure :: get_static_modelname => process_library_get_static_modelname

```

(Process libraries: procedures)+≡

```

function process_library_get_static_modelname (prc_lib, os_data) result (name)
    class(process_library_t), intent(in) :: prc_lib
    type(os_data_t), intent(in) :: os_data
    type(string_t) :: name
    type(string_t), dimension(:), allocatable :: models
    type(string_t) :: modelname, modellib, modellib_full
    logical :: exist
    integer :: i, j, mi
    name = ""
    allocate (models(prc_lib%n_entries + 1))
    models = ""
    mi = 1
    if (allocated (prc_lib%entry)) then
        SCAN: do i = 1, prc_lib%n_entries
            if (associated (prc_lib%entry(i)%def)) then
                if (prc_lib%entry(i)%def%model_name /= "") then
                    modelname = prc_lib%entry(i)%def%model_name
                else
                    cycle SCAN
                end if
            else
                cycle SCAN
            end if
        end do
        models(mi) = modelname
        mi = mi + 1
        modellib = "libparameters_" // modelname // ".a"
        exist = .false.
        if (.not. os_data%use_testfiles) then
            modellib_full = os_data%whizard_models_libpath_local &
                // "/" // modellib
            inquire (file=char (modellib_full), exist=exist)
        end if
        if (.not. exist) then
            modellib_full = os_data%whizard_models_libpath &
                // "/" // modellib
            inquire (file=char (modellib_full), exist=exist)
        end if
    end if
end function

```

```

        if (exist) name = name // " " // modellib_full
    end do SCAN
end if
deallocate (models)
end function process_library_get_static_modelname

```

14.4.6 Unit Test

Test module, followed by the corresponding implementation module.

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

```

module process_libraries_ut
    use unit_tests
    use process_libraries_uti

```

<Standard module head>

<Process libraries: public test>

contains

<Process libraries: test driver>

```

end module process_libraries_ut

```

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

```

module process_libraries_uti

    use, intrinsic :: iso_c_binding !NODEP!

<Use strings>
    use io_units
    use os_interface
    use particle_specifiers, only: new_prt_spec
    use process_constants
    use prclib_interfaces
    use prc_core_def

```

```

    use process_libraries

```

```

    use prclib_interfaces_ut, only: test_writer_4_t

```

<Standard module head>

<Process libraries: test declarations>

<Process libraries: test types>

contains

⟨Process libraries: tests⟩

⟨Process libraries: test auxiliary⟩

```
end module process_libraries_util
```

API: driver for the unit tests below.

⟨Process libraries: public test⟩≡

```
public :: process_libraries_test
```

⟨Process libraries: test driver⟩≡

```
subroutine process_libraries_test (u, results)
```

```
integer, intent(in) :: u
```

```
type(test_results_t), intent(inout) :: results
```

⟨Process libraries: execute tests⟩

```
end subroutine process_libraries_test
```

Empty process list

Test 1: Write an empty process list.

⟨Process libraries: execute tests⟩≡

```
call test (process_libraries_1, "process_libraries_1", &  
  "empty process list", &  
  u, results)
```

⟨Process libraries: test declarations⟩≡

```
public :: process_libraries_1
```

⟨Process libraries: tests⟩≡

```
subroutine process_libraries_1 (u)
```

```
integer, intent(in) :: u
```

```
type(process_def_list_t) :: process_def_list
```

```
write (u, "(A)")  "* Test output: process_libraries_1"
```

```
write (u, "(A)")  "* Purpose: Display an empty process definition list"
```

```
write (u, "(A)")
```

```
call process_def_list%write (u)
```

```
write (u, "(A)")
```

```
write (u, "(A)")  "* Test output end: process_libraries_1"
```

```
end subroutine process_libraries_1
```

Process definition list

Test 2: Process definition list with processes and components. Construct the list, write to file, read it in again, and display. Finalize and delete the list after use.

We define a trivial 'test' type for the process variant. The test type contains just one (meaningless) data item, which is an integer.

⟨Process libraries: test types⟩≡

```
type, extends (prc_core_def_t) :: prcdef_2_t
```

```

        integer :: data = 0
        logical :: file = .false.
contains
  <Process libraries: prcdef 2: TBP>
end type prcdef_2_t

```

The process variant is named 'test'.

```

<Process libraries: prcdef 2: TBP>≡
  procedure, nopass :: type_string => prcdef_2_type_string
<Process libraries: test auxiliary>≡
  function prcdef_2_type_string () result (string)
    type(string_t) :: string
    string = "test"
  end function prcdef_2_type_string

```

Write the contents (the integer value).

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: write => prcdef_2_write
<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_write (object, unit)
    class(prcdef_2_t), intent(in) :: object
    integer, intent(in) :: unit
    write (unit, "(3x,A,I0)") "Test data          = ", object%data
  end subroutine prcdef_2_write

```

Recover the integer value.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: read => prcdef_2_read
<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_read (object, unit)
    class(prcdef_2_t), intent(out) :: object
    integer, intent(in) :: unit
    character(80) :: buffer
    read (unit, "(A)") buffer
    call strip_equation_lhs (buffer)
    read (buffer, *) object%data
  end subroutine prcdef_2_read

```

No external procedures.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure, nopass :: get_features => prcdef_2_get_features
<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (0))
  end subroutine prcdef_2_get_features

```

No code generated.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: generate_code => prcdef_2_generate_code

```



```

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_generate_code (object, &
    basename, model_name, prt_in, prt_out)
    class(prcdef_2_t), intent(in) :: object
    type(string_t), intent(in) :: basename
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
  end subroutine prcdef_2_generate_code

```

Allocate the driver with the appropriate type.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: allocate_driver => prcdef_2_allocate_driver

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_allocate_driver (object, driver, basename)
    class(prcdef_2_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    allocate (prctest_2_t :: driver)
  end subroutine prcdef_2_allocate_driver

```

Nothing to connect.

```

<Process libraries: prcdef 2: TBP>+≡
  procedure :: connect => prcdef_2_connect

<Process libraries: test auxiliary>+≡
  subroutine prcdef_2_connect (def, lib_driver, i, proc_driver)
    class(prcdef_2_t), intent(in) :: def
    class(prclib_driver_t), intent(in) :: lib_driver
    integer, intent(in) :: i
    class(prc_core_driver_t), intent(inout) :: proc_driver
  end subroutine prcdef_2_connect

```

The associated driver type.

```

<Process libraries: test types>+≡
  type, extends (process_driver_internal_t) :: prctest_2_t
  contains
    <Process libraries: prctest 2: TBP>
  end type prctest_2_t

```

Return the type name.

```

<Process libraries: prctest 2: TBP>≡
  procedure, nopass :: type_name => prctest_2_type_name

<Process libraries: test auxiliary>+≡
  function prctest_2_type_name () result (type)
    type(string_t) :: type
    type = "test"
  end function prctest_2_type_name

```

This should fill constant process data. We do not check those here, however, therefore nothing done.

```

(Process libraries: prctest 2: TBP)+≡
  procedure :: fill_constants => prctest_2_fill_constants

(Process libraries: test auxiliary)+≡
  subroutine prctest_2_fill_constants (driver, data)
    class(prctest_2_t), intent(in) :: driver
    type(process_constants_t), intent(out) :: data
  end subroutine prctest_2_fill_constants

```

Here is the actual test.

For reading, we need a list of templates, i.e., an array containing allocated objects for all available process variants. This is the purpose of `process_core_templates`. Here, we have only a single template for the 'test' variant.

```

(Process libraries: execute tests)+≡
  call test (process_libraries_2, "process_libraries_2", &
    "process definition list", &
    u, results)

(Process libraries: test declarations)+≡
  public :: process_libraries_2

(Process libraries: tests)+≡
  subroutine process_libraries_2 (u)
    integer, intent(in) :: u
    type(prc_template_t), dimension(:), allocatable :: process_core_templates
    type(process_def_list_t) :: process_def_list
    type(process_def_entry_t), pointer :: entry => null ()
    class(prc_core_def_t), allocatable :: test_def
    integer :: scratch_unit

    write (u, "(A)")  "*" Test output: process_libraries_2"
    write (u, "(A)")  "*" Purpose: Construct a process definition list,"
    write (u, "(A)")  "*"           write it to file and reread it"
    write (u, "(A)")  ""
    write (u, "(A)")  "*" Construct a process definition list"
    write (u, "(A)")  "*"   First process definition: empty"
    write (u, "(A)")  "*"   Second process definition: two components"
    write (u, "(A)")  "*"     First component: empty"
    write (u, "(A)")  "*"     Second component: test data"
    write (u, "(A)")  "*"   Third process definition:"
    write (u, "(A)")  "*"     Embedded decays and polarization"
    write (u, "(A)")

    allocate (process_core_templates (1))
    allocate (prcdef_2_t :: process_core_templates(1)%core_def)

    allocate (entry)
    call entry%init (var_str ("first"), n_in = 0, n_components = 0)
    call entry%compute_md5sum ()
    call process_def_list%append (entry)

    allocate (entry)
    call entry%init (var_str ("second"), model_name = var_str ("Test"), &

```

```

        n_in = 1, n_components = 2)
allocate (prcdef_2_t :: test_def)
select type (test_def)
type is (prcdef_2_t); test_def%data = 42
end select
call entry%import_component (2, n_out = 2, &
    prt_in = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
    method = var_str ("test"), &
    variant = test_def)
call entry%compute_md5sum ()
call process_def_list%append (entry)

allocate (entry)
call entry%init (var_str ("third"), model_name = var_str ("Test"), &
    n_in = 2, n_components = 1)
allocate (prcdef_2_t :: test_def)
call entry%import_component (1, n_out = 3, &
    prt_in = &
        new_prt_spec ([var_str ("a"), var_str ("b")]), &
    prt_out = &
        [new_prt_spec (var_str ("c")), &
        new_prt_spec (var_str ("d"), .true.), &
        new_prt_spec (var_str ("e"), [var_str ("e_decay")])], &
    method = var_str ("test"), &
    variant = test_def)
call entry%compute_md5sum ()
call process_def_list%append (entry)
call process_def_list%write (u)

write (u, "(A)") ""
write (u, "(A)") "* Write the process definition list to (scratch) file"

scratch_unit = free_unit ()
open (unit = scratch_unit, status="scratch", action = "readwrite")
call process_def_list%write (scratch_unit)
call process_def_list%final ()

write (u, "(A)") "* Reread it"
write (u, "(A)") ""

rewind (scratch_unit)
call process_def_list%read (scratch_unit, process_core_templates)
close (scratch_unit)

call process_def_list%write (u)
call process_def_list%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: process_libraries_2"
end subroutine process_libraries_2

```

Process library object

Test 3: Process library object with several process definitions and library entries. Just construct the object, modify some initial content, and write the result. The modifications are mostly applied directly, so we do not test anything but the contents and the output routine.

```
(Process libraries: execute tests)+≡
    call test (process_libraries_3, "process_libraries_3", &
        "recover process definition list from file", &
        u, results)

(Process libraries: test declarations)+≡
    public :: process_libraries_3

(Process libraries: tests)+≡
    subroutine process_libraries_3 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        type(process_def_entry_t), pointer :: entry
        class(prc_core_driver_t), allocatable :: driver_template

        write (u, "(A)")  "* Test output: process_libraries_3"
        write (u, "(A)")  "* Purpose: Construct a process library object &
            &with entries"
        write (u, "(A)")  ""
        write (u, "(A)")  "* Construct and display a process library object"
        write (u, "(A)")  "*   with 5 entries"
        write (u, "(A)")  "*   associated with 3 matrix element codes"
        write (u, "(A)")  "*   corresponding to 3 process definitions"
        write (u, "(A)")  "*   with 2, 1, 1 components, respectively"
        write (u, "(A)")

        call lib%init (var_str ("testlib"))

        call lib%set_status (STAT_ACTIVE)
        call lib%allocate_entries (5)

        allocate (entry)
        call entry%init (var_str ("test_a"), n_in = 2, n_components = 2)
        allocate (prctest_2_t :: driver_template)
        call lib%init_entry (3, STAT_SOURCE, entry%process_def_t, 2, 2, &
            driver_template)
        call lib%init_entry (4, STAT_COMPILED, entry%process_def_t, 1, 0)
        call lib%append (entry)

        allocate (entry)
        call entry%init (var_str ("test_b"), n_in = 2, n_components = 1)
        call lib%init_entry (2, STAT_CONFIGURED, entry%process_def_t, 1, 1)
        call lib%append (entry)

        allocate (entry)
        call entry%init (var_str ("test_c"), n_in = 2, n_components = 1)
        allocate (prctest_2_t :: driver_template)
        call lib%init_entry (5, STAT_LINKED, entry%process_def_t, 1, 3, &
            driver_template)
```

```

call lib%append (entry)

call lib%write (u)
call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_3"
end subroutine process_libraries_3

```

Process library for test matrix element (no file)

Test 4: We proceed through the library generation and loading phases with a test matrix element type that needs no code written on file.

```

<Process libraries: execute tests>+≡
call test (process_libraries_4, "process_libraries_4", &
  "build and load internal process library", &
  u, results)

<Process libraries: test declarations>+≡
public :: process_libraries_4

<Process libraries: tests>+≡
subroutine process_libraries_4 (u)
  integer, intent(in) :: u
  type(process_library_t) :: lib
  type(process_def_entry_t), pointer :: entry
  class(prc_core_def_t), allocatable :: core_def
  type(os_data_t) :: os_data

  write (u, "(A)")  "* Test output: process_libraries_4"
  write (u, "(A)")  "* Purpose: build a process library with an &
    &internal (pseudo) matrix element"
  write (u, "(A)")  "*          No Makefile or code should be generated"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize a process library with one entry &
    &(no external code)"
  write (u, "(A)")
  call os_data%init ()
  call lib%init (var_str ("proclibs4"))

  allocate (prcdef_2_t :: core_def)

  allocate (entry)
  call entry%init (var_str ("proclibs4_a"), n_in = 1, n_components = 1)
  call entry%import_component (1, n_out = 2, variant = core_def)
  call lib%append (entry)

  write (u, "(A)")  "* Configure library"
  write (u, "(A)")
  call lib%configure (os_data)

  write (u, "(A)")  "* Compute MD5 sum"

```

```

write (u, "(A)")
call lib%compute_md5sum ()

write (u, "(A)")  "* Write makefile (no-op)"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .true.)

write (u, "(A)")  "* Write driver source code (no-op)"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code (no-op)"
write (u, "(A)")
call lib%make_source (os_data)

write (u, "(A)")  "* Compile (no-op)"
write (u, "(A)")
call lib%make_compile (os_data)

write (u, "(A)")  "* Link (no-op)"
write (u, "(A)")
call lib%make_link (os_data)

write (u, "(A)")  "* Load (no-op)"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u)
call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_4"
end subroutine process_libraries_4

```

Build workflow for test matrix element

Test 5: We write source code for a dummy process.

We define another trivial type for the process variant. The test type contains just no variable data, but produces code on file.

```

<Process libraries: test types>+≡
  type, extends (prc_core_def_t) :: prcdef_5_t
  contains
  <Process libraries: prcdef 5: TBP>
end type prcdef_5_t

```

The process variant is named `test_file`.

```

<Process libraries: prcdef 5: TBP>≡
  procedure, nopass :: type_string => prcdef_5_type_string

<Process libraries: test auxiliary>+≡
  function prcdef_5_type_string () result (string)
    type(string_t) :: string

```

```

        string = "test_file"
    end function prcdef_5_type_string

```

We reuse the writer `test_writer_4` from the previous module.

```

<Process libraries: prcdef 5: TBP>+≡
    procedure :: init => prcdef_5_init
<Process libraries: test auxiliary>+≡
    subroutine prcdef_5_init (object)
        class(prcdef_5_t), intent(out) :: object
        allocate (test_writer_4_t :: object%writer)
    end subroutine prcdef_5_init

```

Nothing to write.

```

<Process libraries: prcdef 5: TBP>+≡
    procedure :: write => prcdef_5_write
<Process libraries: test auxiliary>+≡
    subroutine prcdef_5_write (object, unit)
        class(prcdef_5_t), intent(in) :: object
        integer, intent(in) :: unit
    end subroutine prcdef_5_write

```

Nothing to read.

```

<Process libraries: prcdef 5: TBP>+≡
    procedure :: read => prcdef_5_read
<Process libraries: test auxiliary>+≡
    subroutine prcdef_5_read (object, unit)
        class(prcdef_5_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine prcdef_5_read

```

Allocate the driver with the appropriate type.

```

<Process libraries: prcdef 5: TBP>+≡
    procedure :: allocate_driver => prcdef_5_allocate_driver
<Process libraries: test auxiliary>+≡
    subroutine prcdef_5_allocate_driver (object, driver, basename)
        class(prcdef_5_t), intent(in) :: object
        class(prc_core_driver_t), intent(out), allocatable :: driver
        type(string_t), intent(in) :: basename
        allocate (prctest_5_t :: driver)
    end subroutine prcdef_5_allocate_driver

```

This time we need code:

```

<Process libraries: prcdef 5: TBP>+≡
    procedure, nopass :: needs_code => prcdef_5_needs_code
<Process libraries: test auxiliary>+≡
    function prcdef_5_needs_code () result (flag)
        logical :: flag
        flag = .true.
    end function prcdef_5_needs_code

```

For the test case, we implement a single feature `proc1`.

```

<Process libraries: prcdef 5: TBP>+≡
    procedure, nopass :: get_features => prcdef_5_get_features

<Process libraries: test auxiliary>+≡
    subroutine prcdef_5_get_features (features)
        type(string_t), dimension(:), allocatable, intent(out) :: features
        allocate (features (1))
        features = [ var_str ("proc1") ]
    end subroutine prcdef_5_get_features

```

Nothing to connect.

```

<Process libraries: prcdef 5: TBP>+≡
    procedure :: connect => prcdef_5_connect

<Process libraries: test auxiliary>+≡
    subroutine prcdef_5_connect (def, lib_driver, i, proc_driver)
        class(prcdef_5_t), intent(in) :: def
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        class(prc_core_driver_t), intent(inout) :: proc_driver
    end subroutine prcdef_5_connect

```

The driver type.

```

<Process libraries: test types>+≡
    type, extends (prc_core_driver_t) :: prctest_5_t
    contains
    <Process libraries: prctest 5: TBP>
    end type prctest_5_t

```

Return the type name.

```

<Process libraries: prctest 5: TBP>≡
    procedure, nopass :: type_name => prctest_5_type_name

<Process libraries: test auxiliary>+≡
    function prctest_5_type_name () result (type)
        type(string_t) :: type
        type = "test_file"
    end function prctest_5_type_name

```

Here is the actual test:

```

<Process libraries: execute tests>+≡
    call test (process_libraries_5, "process_libraries_5", &
        "build external process library", &
        u, results)

<Process libraries: test declarations>+≡
    public :: process_libraries_5

<Process libraries: tests>+≡
    subroutine process_libraries_5 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        type(process_def_entry_t), pointer :: entry

```



```

class(prc_core_def_t), allocatable :: core_def
type(os_data_t) :: os_data

write (u, "(A)")  "* Test output: process_libraries_5"
write (u, "(A)")  "* Purpose: build a process library with an &
                  &external (pseudo) matrix element"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("proclibs5"))
call os_data%init ()

allocate (prcdef_5_t :: core_def)
select type (core_def)
type is (prcdef_5_t)
    call core_def%init ()
end select

allocate (entry)
call entry%init (var_str ("proclibs5_a"), &
                model_name = var_str ("Test_Model"), &
                n_in = 1, n_components = 1)
call entry%import_component (1, n_out = 2, &
                             prt_in  = new_prt_spec ([var_str ("a")]), &
                             prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
                             method  = var_str ("test"), &
                             variant = core_def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Compute MD5 sum"
write (u, "(A)")
call lib%compute_md5sum ()

write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Write driver source code"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code"
write (u, "(A)")
call lib%make_source (os_data)

write (u, "(A)")  "* Compile"
write (u, "(A)")
call lib%make_compile (os_data)

```

```

write (u, "(A)")  "* Link"
write (u, "(A)")
call lib%make_link (os_data)

call lib%write (u, libpath = .false.)

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_5"
end subroutine process_libraries_5

```

Build and load library with test matrix element

Test 6: We write source code for a dummy process.

This process variant is identical to the previous case, but it supports a driver for the test procedure 'proc1'.

```

<Process libraries: test types>+≡
  type, extends (prc_core_def_t) :: prcdef_6_t
  contains
  <Process libraries: prcdef 6: TBP>
end type prcdef_6_t

```

The process variant is named `test_file`.

```

<Process libraries: prcdef 6: TBP>≡
  procedure, nopass :: type_string => prcdef_6_type_string

<Process libraries: test auxiliary>+≡
  function prcdef_6_type_string () result (string)
    type(string_t) :: string
    string = "test_file"
  end function prcdef_6_type_string

```

We reuse the writer `test_writer_4` from the previous module.

```

<Process libraries: prcdef 6: TBP>+≡
  procedure :: init => prcdef_6_init

<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_init (object)
    class(prcdef_6_t), intent(out) :: object
    allocate (test_writer_4_t :: object%writer)
    call object%writer%init_test ()
  end subroutine prcdef_6_init

```

Nothing to write.

```

<Process libraries: prcdef 6: TBP>+≡
  procedure :: write => prcdef_6_write

```

```

<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_write (object, unit)
    class(prcdef_6_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine prcdef_6_write

```

Nothing to read.

```

<Process libraries: prcdef 6: TBP>+≡
  procedure :: read => prcdef_6_read

<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_read (object, unit)
    class(prcdef_6_t), intent(out) :: object
    integer, intent(in) :: unit
  end subroutine prcdef_6_read

```

Allocate the driver with the appropriate type.

```

<Process libraries: prcdef 6: TBP>+≡
  procedure :: allocate_driver => prcdef_6_allocate_driver

<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_allocate_driver (object, driver, basename)
    class(prcdef_6_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    allocate (prctest_6_t :: driver)
  end subroutine prcdef_6_allocate_driver

```

This time we need code:

```

<Process libraries: prcdef 6: TBP>+≡
  procedure, nopass :: needs_code => prcdef_6_needs_code

<Process libraries: test auxiliary>+≡
  function prcdef_6_needs_code () result (flag)
    logical :: flag
    flag = .true.
  end function prcdef_6_needs_code

```

For the test case, we implement a single feature proc1.

```

<Process libraries: prcdef 6: TBP>+≡
  procedure, nopass :: get_features => prcdef_6_get_features

<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (1))
    features = [ var_str ("proc1") ]
  end subroutine prcdef_6_get_features

```

The interface of the only specific feature.

```

<Process libraries: test types>+≡
  abstract interface
    subroutine proc1_t (n) bind(C)
      import
      integer(c_int), intent(out) :: n
    end subroutine proc1_t
  end interface

```

Connect the feature proc1 with the process driver.

```

<Process libraries: prcdef 6: TBP>+≡
  procedure :: connect => prcdef_6_connect

<Process libraries: test auxiliary>+≡
  subroutine prcdef_6_connect (def, lib_driver, i, proc_driver)
    class(prcdef_6_t), intent(in) :: def
    class(prclib_driver_t), intent(in) :: lib_driver
    integer, intent(in) :: i
    class(prc_core_driver_t), intent(inout) :: proc_driver
    integer(c_int) :: pid, fid
    type(c_funptr) :: fptr
    select type (proc_driver)
    type is (prctest_6_t)
      pid = i
      fid = 1
      call lib_driver%get_fptr (pid, fid, fptr)
      call c_f_procpointer (fptr, proc_driver%proc1)
    end select
  end subroutine prcdef_6_connect

```

The driver type.

```

<Process libraries: test types>+≡
  type, extends (prc_core_driver_t) :: prctest_6_t
    procedure(proc1_t), nopass, pointer :: proc1 => null ()
    contains
    <Process libraries: prctest 6: TBP>
  end type prctest_6_t

```

Return the type name.

```

<Process libraries: prctest 6: TBP>≡
  procedure, nopass :: type_name => prctest_6_type_name

<Process libraries: test auxiliary>+≡
  function prctest_6_type_name () result (type)
    type(string_t) :: type
    type = "test_file"
  end function prctest_6_type_name

```

Here is the actual test:

```

<Process libraries: execute tests>+≡
  call test (process_libraries_6, "process_libraries_6", &
    "build and load external process library", &
    u, results)

```

```

<Process libraries: test declarations>+≡
    public :: process_libraries_6

<Process libraries: tests>+≡
    subroutine process_libraries_6 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        type(process_def_entry_t), pointer :: entry
        class(prc_core_def_t), allocatable :: core_def
        type(os_data_t) :: os_data
        type(string_t), dimension(:), allocatable :: name_list
        type(process_constants_t) :: data
        class(prc_core_driver_t), allocatable :: proc_driver
        integer :: i
        integer(c_int) :: n

        write (u, "(A)")  "* Test output: process_libraries_6"
        write (u, "(A)")  "* Purpose: build and load a process library"
        write (u, "(A)")  "*           with an external (pseudo) matrix element"
        write (u, "(A)")  "*           Check single-call linking"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize a process library with one entry"
        write (u, "(A)")
        call lib%init (var_str ("proclibs6"))
        call os_data%init ()

        allocate (prcdef_6_t :: core_def)
        select type (core_def)
        type is (prcdef_6_t)
            call core_def%init ()
        end select

        allocate (entry)
        call entry%init (var_str ("proclibs6_a"), &
            model_name = var_str ("Test_model"), &
            n_in = 1, n_components = 1)
        call entry%import_component (1, n_out = 2, &
            prt_in = new_prt_spec ([var_str ("a")]), &
            prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
            method = var_str ("test"), &
            variant = core_def)
        call lib%append (entry)

        write (u, "(A)")  "* Configure library"
        write (u, "(A)")
        call lib%configure (os_data)

        write (u, "(A)")  "* Write makefile"
        write (u, "(A)")
        call lib%write_makefile (os_data, force = .true., verbose = .false.)

        write (u, "(A)")  "* Write driver source code"
        write (u, "(A)")
        call lib%write_driver (force = .true.)

```

```

write (u, "(A)")  "* Write process source code, compile, link, load"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u, libpath = .false.)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,A,A)")  "name                = '", &
    char (lib%get_name ()), "'"
write (u, "(1x,A,L1)")  "is active                = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes                = ", &
    lib%get_n_processes ()
write (u, "(1x,A)", advance="no")  "processes                ="
call lib%get_process_id_list (name_list)
do i = 1, size (name_list)
    write (u, "(1x,A)", advance="no")  char (name_list(i))
end do
write (u, *)
write (u, "(1x,A,L1)")  "proclibs6_a is process        = ", &
    lib%contains (var_str ("proclibs6_a"))
write (u, "(1x,A,I0)")  "proclibs6_a has index        = ", &
    lib%get_entry_index (var_str ("proclibs6_a"))
write (u, "(1x,A,L1)")  "foobar is process            = ", &
    lib%contains (var_str ("foobar"))
write (u, "(1x,A,I0)")  "foobar has index            = ", &
    lib%get_entry_index (var_str ("foobar"))
write (u, "(1x,A,I0)")  "n_in(proclibs6_a)            = ", &
    lib%get_n_in (var_str ("proclibs6_a"))
write (u, "(1x,A,A)")  "model_name(proclibs6_a)        = ", &
    char (lib%get_model_name (var_str ("proclibs6_a")))
write (u, "(1x,A)", advance="no")  "components(proclibs6_a) ="
call lib%get_component_list (var_str ("proclibs6_a"), name_list)
do i = 1, size (name_list)
    write (u, "(1x,A)", advance="no")  char (name_list(i))
end do
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Constants of proclibs6_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("proclibs6_a"), 1, data, proc_driver)

write (u, "(1x,A,A)")  "component ID          = ", char (data%id)
write (u, "(1x,A,A)")  "model name            = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum                = '", data%md5sum, "'"
write (u, "(1x,A,L1)")  "openmp supported = ", data%openmp_supported
write (u, "(1x,A,I0)")  "n_in = ", data%n_in
write (u, "(1x,A,I0)")  "n_out = ", data%n_out

```

```

write (u, "(1x,A,I0)") "n_flv = ", data%n_flv
write (u, "(1x,A,I0)") "n_hel = ", data%n_hel
write (u, "(1x,A,I0)") "n_col = ", data%n_col
write (u, "(1x,A,I0)") "n_cin = ", data%n_cin
write (u, "(1x,A,I0)") "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))") "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I0))") "hel state =", data%hel_state
write (u, "(1x,A,10(1x,I0))") "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))") "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))") "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))") "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Call feature of proclibs6_a:"
write (u, "(A)")

select type (proc_driver)
type is (prctest_6_t)
  call proc_driver%proc1 (n)
  write (u, "(1x,A,I0)") "proc1 = ", n
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_6"
end subroutine process_libraries_6

```

MD5 sums

Check MD5 sum calculation.

```

<Process libraries: execute tests>+≡
  call test (process_libraries_7, "process_libraries_7", &
    "process definition list", &
    u, results)

<Process libraries: test declarations>+≡
  public :: process_libraries_7

<Process libraries: tests>+≡
  subroutine process_libraries_7 (u)
    integer, intent(in) :: u
    type(prc_template_t), dimension(:), allocatable :: process_core_templates
    type(process_def_entry_t), target :: entry
    class(prc_core_def_t), allocatable :: test_def
    class(prc_core_def_t), pointer :: def

    write (u, "(A)")  "* Test output: process_libraries_7"
    write (u, "(A)")  "* Purpose: Construct a process definition list &
      &and check MD5 sums"
    write (u, "(A)")
    write (u, "(A)")  "* Construct a process definition list"
    write (u, "(A)")  "* Process: two components"
    write (u, "(A)")

```

```

allocate (process_core_templates (1))
allocate (prcdef_2_t :: process_core_templates(1)%core_def)

call entry%init (var_str ("first"), model_name = var_str ("Test"), &
    n_in = 1, n_components = 2)
allocate (prcdef_2_t :: test_def)
select type (test_def)
type is (prcdef_2_t); test_def%data = 31
end select
call entry%import_component (1, n_out = 3, &
    prt_in = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("c"), &
        var_str ("e")]), &
    method = var_str ("test"), &
    variant = test_def)
allocate (prcdef_2_t :: test_def)
select type (test_def)
type is (prcdef_2_t); test_def%data = 42
end select
call entry%import_component (2, n_out = 2, &
    prt_in = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
    method = var_str ("test"), &
    variant = test_def)
call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute MD5 sums"
write (u, "(A)")

call entry%compute_md5sum ()
call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recalculate MD5 sums (should be identical)"
write (u, "(A)")

call entry%compute_md5sum ()
call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Modify a component and recalculate MD5 sums"
write (u, "(A)")

def => entry%get_core_def_ptr (2)
select type (def)
type is (prcdef_2_t)
    def%data = 54
end select
call entry%compute_md5sum ()
call entry%write (u)

write (u, "(A)")

```



```

write (u, "(A)")  "* Modify the model and recalculate MD5 sums"
write (u, "(A)")

call entry%set_model_name (var_str ("foo"))
call entry%compute_md5sum ()
call entry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_7"
end subroutine process_libraries_7

```

Here is the actual test:

```

<Process libraries: execute tests>+≡
call test (process_libraries_8, "process_libraries_8", &
"library status checks", &
u, results)

<Process libraries: test declarations>+≡
public :: process_libraries_8

<Process libraries: tests>+≡
subroutine process_libraries_8 (u)
integer, intent(in) :: u
type(process_library_t) :: lib
type(process_def_entry_t), pointer :: entry
class(prc_core_def_t), allocatable :: core_def
type(os_data_t) :: os_data

write (u, "(A)")  "* Test output: process_libraries_8"
write (u, "(A)")  "* Purpose: build and load a process library"
write (u, "(A)")  "*           with an external (pseudo) matrix element"
write (u, "(A)")  "*           Check status updates"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("proclibs8"))
call os_data%init ()

allocate (prcdef_6_t :: core_def)
select type (core_def)
type is (prcdef_6_t)
call core_def%init ()
end select

allocate (entry)
call entry%init (var_str ("proclibs8_a"), &
model_name = var_str ("Test_model"), &
n_in = 1, n_components = 1)
call entry%import_component (1, n_out = 2, &
prt_in = new_prt_spec ([var_str ("a")]), &
prt_out = new_prt_spec ([var_str ("b"), var_str ("c")]), &
method = var_str ("test"), &
variant = core_def)
call lib%append (entry)

```

```

write (u, "(A)")  "* Configure library"
write (u, "(A)")

call lib%configure (os_data)
call lib%compute_md5sum ()

call lib%test_transfer_md5sum (1, 1, 1)

write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)

write (u, "(A)")
write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Update status"
write (u, "(A)")

call lib%update_status (os_data)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)

write (u, "(A)")
write (u, "(A)")  "* Write driver source code"
write (u, "(A)")
call lib%write_driver (force = .false.)

write (u, "(A)")  "* Write process source code"
write (u, "(A)")
call lib%make_source (os_data)

write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)

write (u, "(A)")
write (u, "(A)")  "* Compile and load"
write (u, "(A)")

call lib%load (os_data)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status   = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)

write (u, "(A)")
write (u, "(A)")  "* Append process and reconfigure"
write (u, "(A)")

allocate (prcdef_6_t :: core_def)
select type (core_def)

```

```

type is (prcdef_6_t)
    call core_def%init ()
end select

allocate (entry)
call entry%init (var_str ("proclibs8_b"), &
    model_name = var_str ("Test_model"), &
    n_in = 1, n_components = 1)
call entry%import_component (1, n_out = 2, &
    prt_in = new_prt_spec ([var_str ("a")]), &
    prt_out = new_prt_spec ([var_str ("b"), var_str ("d")]), &
    method = var_str ("test"), &
    variant = core_def)
call lib%append (entry)

call lib%configure (os_data)
call lib%compute_md5sum ()
call lib%test_transfer_md5sum (2, 2, 1)
call lib%write_makefile (os_data, force = .false., verbose = .false.)
call lib%write_driver (force = .false.)

write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Update status"
write (u, "(A)")

call lib%update_status (os_data)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Write source code"
write (u, "(A)")

call lib%make_source (os_data)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Reset status"
write (u, "(A)")

call lib%set_status (STAT_CONFIGURED, entries=.true.)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)

```

```

write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Update status"
write (u, "(A)")

call lib%update_status (os_data)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Partial cleanup"
write (u, "(A)")

call lib%clean (os_data, distclean = .false.)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Update status"
write (u, "(A)")

call lib%update_status (os_data)
write (u, "(1x,A,L1)") "library loaded = ", lib%is_loaded ()
write (u, "(1x,A,I0)") "lib status = ", lib%get_status ()
write (u, "(1x,A,I0)") "proc1 status = ", lib%get_status (1)
write (u, "(1x,A,I0)") "proc2 status = ", lib%get_status (2)

write (u, "(A)")
write (u, "(A)")  "* Complete cleanup"

call lib%clean (os_data, distclean = .true.)
call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_libraries_8"
end subroutine process_libraries_8

```

14.5 Process Library Stacks

For storing and handling multiple libraries, we define process library stacks. These are ordinary stacks where new entries are pushed onto the top.

```

<prclib_stacks.f90>≡
  <File header>

```

```

module prclib_stacks

```

```

    <Use strings>
        use io_units
        use format_utils, only: write_separator
        use process_libraries

    <Standard module head>

    <Prclib stacks: public>

    <Prclib stacks: types>

contains

    <Prclib stacks: procedures>

end module prclib_stacks

```

14.5.1 The stack entry type

A stack entry is a process library object, augmented by a pointer to the next entry. We do not need specific methods, all relevant methods are inherited.

On higher level, process libraries should be prepared as process entry objects.

```

    <Prclib stacks: public>≡
        public :: prclib_entry_t

    <Prclib stacks: types>≡
        type, extends (process_library_t) :: prclib_entry_t
            type(prclib_entry_t), pointer :: next => null ()
        end type prclib_entry_t

```

14.5.2 The prclib stack type

For easy conversion and lookup it is useful to store the filling number in the object. The content is stored as a linked list.

```

    <Prclib stacks: public>+≡
        public :: prclib_stack_t

    <Prclib stacks: types>+≡
        type :: prclib_stack_t
            integer :: n = 0
            type(prclib_entry_t), pointer :: first => null ()
        contains
            <Prclib stacks: prclib stack: TBP>
        end type prclib_stack_t

```

Finalizer. Iteratively deallocate the stack entries. The resulting empty stack can be immediately recycled, if necessary.

```

    <Prclib stacks: prclib stack: TBP>≡
        procedure :: final => prclib_stack_final

```

```

<Prclib stacks: procedures>+=
  subroutine prclib_stack_final (object)
    class(prclib_stack_t), intent(inout) :: object
    type(prclib_entry_t), pointer :: lib
    do while (associated (object%first))
      lib => object%first
      object%first => lib%next
      call lib%final ()
      deallocate (lib)
    end do
    object%n = 0
  end subroutine prclib_stack_final

```

Output. The entries on the stack will be ordered LIFO, i.e., backwards.

```

<Prclib stacks: prclib stack: TBP>+=
  procedure :: write => prclib_stack_write

<Prclib stacks: procedures>+=
  subroutine prclib_stack_write (object, unit, libpath)
    class(prclib_stack_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: libpath
    type(prclib_entry_t), pointer :: lib
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    select case (object%n)
    case (0)
      write (u, "(1x,A)") "Process library stack: [empty]"
    case default
      write (u, "(1x,A)") "Process library stack:"
      lib => object%first
      do while (associated (lib))
        call write_separator (u)
        call lib%write (u, libpath)
        lib => lib%next
      end do
    end select
    call write_separator (u, 2)
  end subroutine prclib_stack_write

```

14.5.3 Operating on Stacks

We take a library entry pointer and push it onto the stack. The previous pointer is nullified. Subsequently, the library entry is ‘owned’ by the stack and will be finalized when the stack is deleted.

```

<Prclib stacks: prclib stack: TBP>+=
  procedure :: push => prclib_stack_push

<Prclib stacks: procedures>+=
  subroutine prclib_stack_push (stack, lib)
    class(prclib_stack_t), intent(inout) :: stack

```

```

    type(prclib_entry_t), intent(inout), pointer :: lib
    lib%next => stack%first
    stack%first => lib
    lib => null ()
    stack%n = stack%n + 1
end subroutine prclib_stack_push

```

14.5.4 Accessing Contents

Return a pointer to the topmost stack element. The result type is just the bare `process_library_t`. There is no `target` attribute required since the stack elements are allocated via pointers.

```

<Prclib stacks: prclib stack: TBP>+≡
    procedure :: get_first_ptr => prclib_stack_get_first_ptr

<Prclib stacks: procedures>+≡
    function prclib_stack_get_first_ptr (stack) result (ptr)
        class(prclib_stack_t), intent(in) :: stack
        type(process_library_t), pointer :: ptr
        if (associated (stack%first)) then
            ptr => stack%first%process_library_t
        else
            ptr => null ()
        end if
    end function prclib_stack_get_first_ptr

```

Return a complete list of the libraries (names) in the stack. The list is in the order in which the elements got pushed onto the stack, so the 'first' entry is listed last.

```

<Prclib stacks: prclib stack: TBP>+≡
    procedure :: get_names => prclib_stack_get_names

<Prclib stacks: procedures>+≡
    subroutine prclib_stack_get_names (stack, libname)
        class(prclib_stack_t), intent(in) :: stack
        type(string_t), dimension(:), allocatable, intent(out) :: libname
        type(prclib_entry_t), pointer :: lib
        integer :: i
        allocate (libname (stack%n))
        i = stack%n
        lib => stack%first
        do while (associated (lib))
            libname(i) = lib%get_name ()
            i = i - 1
            lib => lib%next
        end do
    end subroutine prclib_stack_get_names

```

Return a pointer to the library with given name.

```

<Prclib stacks: prclib stack: TBP>+≡
    procedure :: get_library_ptr => prclib_stack_get_library_ptr

```

```

<Prclib stacks: procedures>+≡
  function prclib_stack_get_library_ptr (stack, libname) result (ptr)
    class(prclib_stack_t), intent(in) :: stack
    type(string_t), intent(in) :: libname
    type(process_library_t), pointer :: ptr
    type(prclib_entry_t), pointer :: current
    current => stack%first
    do while (associated (current))
      if (current%get_name () == libname) then
        ptr => current%process_library_t
        return
      end if
      current => current%next
    end do
    ptr => null ()
  end function prclib_stack_get_library_ptr

```

14.5.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<prclib_stacks_ut.f90>≡
  <File header>

  module prclib_stacks_ut
    use unit_tests
    use prclib_stacks_util

    <Standard module head>

    <Prclib stacks: public test>

    contains

    <Prclib stacks: test driver>

  end module prclib_stacks_ut

<prclib_stacks_util.f90>≡
  <File header>

  module prclib_stacks_util

    <Use strings>

    use prclib_stacks

    <Standard module head>

    <Prclib stacks: test declarations>

    contains

    <Prclib stacks: tests>

```



```

    end module prclib_stacks_util
API: driver for the unit tests below.
<Prclib_stacks: public test>≡
    public :: prclib_stacks_test
<Prclib_stacks: test driver>≡
    subroutine prclib_stacks_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Prclib_stacks: execute tests>
    end subroutine prclib_stacks_test

```

Write an empty process library stack

The most trivial test is to write an uninitialized process library stack.

```

<Prclib_stacks: execute tests>≡
    call test (prclib_stacks_1, "prclib_stacks_1", &
        "write an empty process library stack", &
        u, results)
<Prclib_stacks: test declarations>≡
    public :: prclib_stacks_1
<Prclib_stacks: tests>≡
    subroutine prclib_stacks_1 (u)
        integer, intent(in) :: u
        type(prclib_stack_t) :: stack

        write (u, "(A)")  "* Test output: prclib_stacks_1"
        write (u, "(A)")  "* Purpose: display an empty process library stack"
        write (u, "(A)")

        call stack%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: prclib_stacks_1"

    end subroutine prclib_stacks_1

```

Fill a process library stack

Fill a process library stack with two (identical) processes.

```

<Prclib_stacks: execute tests>+≡
    call test (prclib_stacks_2, "prclib_stacks_2", &
        "fill a process library stack", &
        u, results)
<Prclib_stacks: test declarations>+≡
    public :: prclib_stacks_2

```

```

<Prclib stacks: tests>+≡
subroutine prclib_stacks_2 (u)
  integer, intent(in) :: u
  type(prclib_stack_t) :: stack
  type(prclib_entry_t), pointer :: lib

  write (u, "(A)")  "* Test output: prclib_stacks_2"
  write (u, "(A)")  "* Purpose: fill a process library stack"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize two (empty) libraries &
    &and push them on the stack"
  write (u, "(A)")

  allocate (lib)
  call lib%init (var_str ("lib1"))
  call stack%push (lib)

  allocate (lib)
  call lib%init (var_str ("lib2"))
  call stack%push (lib)

  call stack%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

  call stack%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: prclib_stacks_2"

end subroutine prclib_stacks_2

```

14.6 Trivial matrix element for tests

For the purpose of testing the workflow, we implement here two matrix elements with the simplest possible structure.

This matrix element generator can only generate a single scattering process and a single decay process. The scattering process is a quartic interaction of a massless, neutral and colorless scalar s with unit coupling results in a trivial $2 \rightarrow 2$ scattering process. The matrix element is implemented internally, so we do not need the machinery of external process libraries. The decay process is a decay of s into a pair of colored fermions f .

```

<prc_test.f90>≡
<File header>

module prc_test

  use, intrinsic :: iso_c_binding !NODEP!

```

```

<Use kinds>
<Use strings>
  use os_interface
  use process_constants
  use prclib_interfaces
  use prc_core_def
  use particle_specifiers, only: new_prt_spec
  use process_libraries

<Standard module head>

<Test ME: public>

<Test ME: types>

contains

<Test ME: procedures>

end module prc_test

```

14.6.1 Process definition

For the process definition we implement an extension of the `prc_core_def_t` abstract type.

```

<Test ME: public>≡
  public :: prc_test_def_t

<Test ME: types>≡
  type, extends (prc_core_def_t) :: prc_test_def_t
    type(string_t) :: model_name
    type(string_t), dimension(:), allocatable :: prt_in
    type(string_t), dimension(:), allocatable :: prt_out
  contains
    <Test ME: test me def: TBP>
  end type prc_test_def_t

<Test ME: test me def: TBP>≡
  procedure, nopass :: type_string => prc_test_def_type_string

<Test ME: procedures>≡
  function prc_test_def_type_string () result (string)
    type(string_t) :: string
    string = "test_me"
  end function prc_test_def_type_string

```

There is no 'feature' here since there is no external code.

```

<Test ME: test me def: TBP>+≡
  procedure, nopass :: get_features => prc_test_def_get_features

<Test ME: procedures>+≡
  subroutine prc_test_def_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (0))

```

```
end subroutine prc_test_def_get_features
```

Initialization: set some data (not really useful).

```
<Test ME: test me def: TBP>+≡
```

```
procedure :: init => prc_test_def_init
```

```
<Test ME: procedures>+≡
```

```
subroutine prc_test_def_init (object, model_name, prt_in, prt_out)
  class(prc_test_def_t), intent(out) :: object
  type(string_t), intent(in) :: model_name
  type(string_t), dimension(:), intent(in) :: prt_in
  type(string_t), dimension(:), intent(in) :: prt_out
  object%model_name = model_name
  allocate (object%prt_in (size (prt_in)))
  object%prt_in = prt_in
  allocate (object%prt_out (size (prt_out)))
  object%prt_out = prt_out
end subroutine prc_test_def_init
```

Write/read process- and method-specific data. (No-op)

```
<Test ME: test me def: TBP>+≡
```

```
procedure :: write => prc_test_def_write
```

```
<Test ME: procedures>+≡
```

```
subroutine prc_test_def_write (object, unit)
  class(prc_test_def_t), intent(in) :: object
  integer, intent(in) :: unit
end subroutine prc_test_def_write
```

```
<Test ME: test me def: TBP>+≡
```

```
procedure :: read => prc_test_def_read
```

```
<Test ME: procedures>+≡
```

```
subroutine prc_test_def_read (object, unit)
  class(prc_test_def_t), intent(out) :: object
  integer, intent(in) :: unit
end subroutine prc_test_def_read
```

Allocate the driver for test ME matrix elements. We get the actual component ID (basename), and we can transfer all process-specific data from the process definition.

```
<Test ME: test me def: TBP>+≡
```

```
procedure :: allocate_driver => prc_test_def_allocate_driver
```

```
<Test ME: procedures>+≡
```

```
subroutine prc_test_def_allocate_driver (object, driver, basename)
  class(prc_test_def_t), intent(in) :: object
  class(prc_core_driver_t), intent(out), allocatable :: driver
  type(string_t), intent(in) :: basename
  allocate (prc_test_t :: driver)
  select type (driver)
  type is (prc_test_t)
    driver%id = basename
```

```

        driver%model_name = object%model_name
        select case (size (object%prt_in))
        case (1); driver%scattering = .false.
        case (2); driver%scattering = .true.
        end select
    end select
end subroutine prc_test_def_allocate_driver

```

Nothing to connect. This subroutine will not be called.

```

<Test ME: test me def: TBP>+≡
    procedure :: connect => prc_test_def_connect

<Test ME: procedures>+≡
    subroutine prc_test_def_connect (def, lib_driver, i, proc_driver)
        class(prc_test_def_t), intent(in) :: def
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        class(prc_core_driver_t), intent(inout) :: proc_driver
    end subroutine prc_test_def_connect

```

14.6.2 Driver

```

<Test ME: public>+≡
    public :: prc_test_t

<Test ME: types>+≡
    type, extends (process_driver_internal_t) :: prc_test_t
        type(string_t) :: id
        type(string_t) :: model_name
        logical :: scattering = .true.
    contains
        <Test ME: test me driver: TBP>
    end type prc_test_t

```

In contrast to generic matrix-element implementations, we can hard-wire the amplitude method as a type-bound procedure.

```

<Test ME: test me driver: TBP>≡
    procedure, nopass :: get_amplitude => prc_test_get_amplitude

<Test ME: procedures>+≡
    function prc_test_get_amplitude (p) result (amp)
        complex(default) :: amp
        real(default), dimension(:,:), intent(in) :: p
        amp = 1
    end function prc_test_get_amplitude

```

The reported type is the same as for the `prc_test_def_t` type.

```

<Test ME: test me driver: TBP>+≡
    procedure, nopass :: type_name => prc_test_type_name

```

```

<Test ME: procedures>+≡
function prc_test_type_name () result (string)
    type(string_t) :: string
    string = "test_me"
end function prc_test_type_name

```

Fill process constants.

```

<Test ME: test me driver: TBP>+≡
procedure :: fill_constants => prc_test_fill_constants

<Test ME: procedures>+≡
subroutine prc_test_fill_constants (driver, data)
    class(prc_test_t), intent(in) :: driver
    type(process_constants_t), intent(out) :: data
    data%id = driver%id
    data%model_name = driver%model_name
    if (driver%scattering) then
        data%n_in = 2
        data%n_out = 2
        data%n_flv = 1
        data%n_hel = 1
        data%n_col = 1
        data%n_cin = 2
        data%n_cf = 1
        allocate (data%flv_state (4, 1))
        data%flv_state = 25
        allocate (data%hel_state (4, 1))
        data%hel_state = 0
        allocate (data%col_state (2, 4, 1))
        data%col_state = 0
        allocate (data%ghost_flag (4, 1))
        data%ghost_flag = .false.
        allocate (data%color_factors (1))
        data%color_factors = 1
        allocate (data%cf_index (2, 1))
        data%cf_index = 1
    else
        data%n_in = 1
        data%n_out = 2
        data%n_flv = 1
        data%n_hel = 2
        data%n_col = 1
        data%n_cin = 2
        data%n_cf = 1
        allocate (data%flv_state (3, 1))
        data%flv_state(:,1) = [25, 6, -6]
        allocate (data%hel_state (3, 2))
        data%hel_state(:,1) = [0, 1, -1]
        data%hel_state(:,2) = [0, -1, 1]
        allocate (data%col_state (2, 3, 1))
        data%col_state = reshape ([0,0, 1,0, 0,-1], [2,3,1])
        allocate (data%ghost_flag (3, 1))
        data%ghost_flag = .false.
        allocate (data%color_factors (1))
    end if
end subroutine prc_test_fill_constants

```

```

        data%color_factors = 3
        allocate (data%cf_index (2, 1))
        data%cf_index = 1
    end if
end subroutine prc_test_fill_constants

```

14.6.3 Shortcut

Since this module is there for testing purposes, we set up a subroutine that does all the work at once: create a library with the two processes (scattering and decay), configure and load, and set up the driver.

```

<Test ME: public>+≡
    public :: prc_test_create_library
<Test ME: procedures>+≡
    subroutine prc_test_create_library &
        (libname, lib, scattering, decay, procname1, procname2)
        type(string_t), intent(in) :: libname
        type(process_library_t), intent(out) :: lib
        logical, intent(in), optional :: scattering, decay
        type(string_t), intent(in), optional :: procname1, procname2
        type(string_t) :: model_name, procname
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        class(prc_core_def_t), allocatable :: def
        type(process_def_entry_t), pointer :: entry
        type(os_data_t) :: os_data
        logical :: sca, dec
        sca = .true.;   if (present (scattering))   sca = scattering
        dec = .false.;  if (present (decay))        dec = decay

        call os_data%init ()
        call lib%init (libname)
        model_name = "Test"

        if (sca) then
            if (present (procname1)) then
                procname = procname1
            else
                procname = libname
            end if
            allocate (prt_in (2), prt_out (2))
            prt_in  = [var_str ("s"), var_str ("s")]
            prt_out = [var_str ("s"), var_str ("s")]
            allocate (prc_test_def_t :: def)
            select type (def)
            type is (prc_test_def_t)
                call def%init (model_name, prt_in, prt_out)
            end select
            allocate (entry)
            call entry%init (procname, model_name = model_name, &
                n_in = 2, n_components = 1)
            call entry%import_component (1, n_out = size (prt_out), &
                prt_in  = new_prt_spec (prt_in), &

```

```

        prt_out = new_prt_spec (prt_out), &
        method = var_str ("test_me"), &
        variant = def)
    call lib%append (entry)
end if

if (dec) then
    if (present (procname2)) then
        procname = procname2
    else
        procname = libname
    end if
    if (allocated (prt_in)) deallocate (prt_in, prt_out)
    allocate (prt_in (1), prt_out (2))
    prt_in = [var_str ("s")]
    prt_out = [var_str ("f"), var_str ("fbar")]
    allocate (prc_test_def_t :: def)
    select type (def)
    type is (prc_test_def_t)
        call def%init (model_name, prt_in, prt_out)
    end select
    allocate (entry)
    call entry%init (procname, model_name = model_name, &
        n_in = 1, n_components = 1)
    call entry%import_component (1, n_out = size (prt_out), &
        prt_in = new_prt_spec (prt_in), &
        prt_out = new_prt_spec (prt_out), &
        method = var_str ("test_decay"), &
        variant = def)
    call lib%append (entry)
end if

call lib%configure (os_data)
call lib%load (os_data)
end subroutine prc_test_create_library

```

14.6.4 Unit Test

Test module, followed by the corresponding implementation module.

`<prc_test.ut.f90>`≡

<File header>

```

module prc_test_ut
    use unit_tests
    use prc_test_uti

```

<Standard module head>

<Test ME: public test>

contains


```

    <Test ME: test driver>

    end module prc_test_ut
    <prc_test.uti.f90>≡
    <File header>

    module prc_test_uti

    <Use kinds>
    <Use strings>
        use os_interface
        use particle_specifiers, only: new_prt_spec
        use process_constants
        use prc_core_def
        use process_libraries

        use prc_test

    <Standard module head>

    <Test ME: test declarations>

    contains

    <Test ME: tests>

    end module prc_test_uti
    API: driver for the unit tests below.
    <Test ME: public test>≡
        public :: prc_test_test
    <Test ME: test driver>≡
        subroutine prc_test_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
            <Test ME: execute tests>
        end subroutine prc_test_test

```

Generate and load the scattering process

The process is $ss \rightarrow ss$, where s is a trivial scalar particle, for vanishing mass and unit coupling. We initialize the process, build the library, and compute the particular matrix element for momenta of unit energy and right-angle scattering. (The scattering is independent of angle.) The matrix element is equal to unity.

```

    <Test ME: execute tests>≡
        call test (prc_test_1, "prc_test_1", &
            "build and load trivial process", &
            u, results)
    <Test ME: test declarations>≡
        public :: prc_test_1

```

<Test ME: tests>≡

```

subroutine prc_test_1 (u)
  integer, intent(in) :: u
  type(os_data_t) :: os_data
  type(process_library_t) :: lib
  class(prc_core_def_t), allocatable :: def
  type(process_def_entry_t), pointer :: entry
  type(string_t) :: model_name
  type(string_t), dimension(:), allocatable :: prt_in, prt_out
  type(process_constants_t) :: data
  class(prc_core_driver_t), allocatable :: driver
  real(default), dimension(0:3,4) :: p
  integer :: i

  write (u, "(A)")  "* Test output: prc_test_1"
  write (u, "(A)")  "* Purpose: create a trivial process"
  write (u, "(A)")  "*           build a library and &
    &access the matrix element"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize a process library with one entry"
  write (u, "(A)")
  call os_data%init ()
  call lib%init (var_str ("prc_test1"))

  model_name = "Test"
  allocate (prt_in (2), prt_out (2))
  prt_in  = [var_str ("s"), var_str ("s")]
  prt_out = [var_str ("s"), var_str ("s")]

  allocate (prc_test_def_t :: def)
  select type (def)
  type is (prc_test_def_t)
    call def%init (model_name, prt_in, prt_out)
  end select
  allocate (entry)
  call entry%init (var_str ("prc_test1_a"), model_name = model_name, &
    n_in = 2, n_components = 1)
  call entry%import_component (1, n_out = size (prt_out), &
    prt_in  = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method  = var_str ("test_me"), &
    variant = def)
  call lib%append (entry)

  write (u, "(A)")  "* Configure library"
  write (u, "(A)")
  call lib%configure (os_data)

  write (u, "(A)")  "* Load library"
  write (u, "(A)")
  call lib%load (os_data)

  call lib%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active          = ", &
                        lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes        = ", &
                        lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of prc_test1_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("prc_test1_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID      = ", char (data%id)
write (u, "(1x,A,A)")  "model name        = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum          = '", data%md5sum, "'"
write (u, "(1x,A,L1)")  "openmp supported = ", data%openmp_supported
write (u, "(1x,A,I0)")  "n_in = ", data%n_in
write (u, "(1x,A,I0)")  "n_out = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I2))")  "hel state =", data%hel_state(:,1)
write (u, "(1x,A,10(1x,I0))")  "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))")  "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))")  "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))")  "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
             1.0_default, 0.0_default, 0.0_default, 1.0_default, &
             1.0_default, 0.0_default, 0.0_default, -1.0_default, &
             1.0_default, 1.0_default, 0.0_default, 0.0_default, &
             1.0_default, -1.0_default, 0.0_default, 0.0_default &
             ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))")  "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver)
type is (prc_test_t)

```

```

        write (u, "(1x,A,1x,E11.4)") "|amp| =", abs (driver%get_amplitude (p))
    end select

    call lib%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: prc_test_1"

end subroutine prc_test_1

```

Shortcut

This is identical to the previous test, but we create the library be a single command. This is handy for other modules which use the test process.

```

<Test ME: execute tests>+≡
    call test (prc_test_2, "prc_test_2", &
        "build and load trivial process using shortcut", &
        u, results)

<Test ME: test declarations>+≡
    public :: prc_test_2

<Test ME: tests>+≡
    subroutine prc_test_2 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        class(prc_core_driver_t), allocatable :: driver
        type(process_constants_t) :: data
        real(default), dimension(0:3,4) :: p

        write (u, "(A)")  "* Test output: prc_test_2"
        write (u, "(A)")  "*   Purpose: create a trivial process"
        write (u, "(A)")  "*               build a library and &
            &access the matrix element"
        write (u, "(A)")

        write (u, "(A)")  "* Build and load a process library with one entry"

        call prc_test_create_library (var_str ("prc_test2"), lib)
        call lib%connect_process (var_str ("prc_test2"), 1, data, driver)

        p = reshape ([ &
            1.0_default, 0.0_default, 0.0_default, 1.0_default, &
            1.0_default, 0.0_default, 0.0_default,-1.0_default, &
            1.0_default, 1.0_default, 0.0_default, 0.0_default, &
            1.0_default,-1.0_default, 0.0_default, 0.0_default &
            ], [4,4])

        write (u, "(A)")
        write (u, "(A)")  "* Compute matrix element:"
        write (u, "(A)")

        select type (driver)

```

```

type is (prc_test_t)
  write (u, "(1x,A,1x,E11.4)") "|amp| =", abs (driver%get_amplitude (p))
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_test_2"

end subroutine prc_test_2

```

Generate and load the decay process

The process is $s \rightarrow f\bar{f}$, where s is a trivial scalar particle and f is a colored fermion. We initialize the process, build the library, and compute the particular matrix element for a fixed momentum configuration. (The decay is independent of angle.) The matrix element is equal to unity.

```

<Test ME: execute tests>+≡
  call test (prc_test_3, "prc_test_3", &
    "build and load trivial decay", &
    u, results)

<Test ME: test declarations>+≡
  public :: prc_test_3

<Test ME: tests>+≡
  subroutine prc_test_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(process_library_t) :: lib
    class(prc_core_def_t), allocatable :: def
    type(process_def_entry_t), pointer :: entry
    type(string_t) :: model_name
    type(string_t), dimension(:), allocatable :: prt_in, prt_out
    type(process_constants_t) :: data
    class(prc_core_driver_t), allocatable :: driver
    real(default), dimension(0:3,3) :: p
    integer :: i

    write (u, "(A)")  "* Test output: prc_test_3"
    write (u, "(A)")  "* Purpose: create a trivial decay process"
    write (u, "(A)")  "* build a library and &
      &access the matrix element"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize a process library with one entry"
    write (u, "(A)")
    call os_data%init ()
    call lib%init (var_str ("prc_test3"))

    model_name = "Test"
    allocate (prt_in (1), prt_out (2))
    prt_in = [var_str ("s")]

```

```

prt_out = [var_str ("f"), var_str ("F")]

allocate (prc_test_def_t :: def)
select type (def)
type is (prc_test_def_t)
    call def%init (model_name, prt_in, prt_out)
end select
allocate (entry)
call entry%init (var_str ("prc_test3_a"), model_name = model_name, &
    n_in = 1, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("test_me"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Load library"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active" = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes" = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of prc_test3_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("prc_test3_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID" = ", char (data%id)
write (u, "(1x,A,A)")  "model name" = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum" = ', ', data%md5sum, ', '
write (u, "(1x,A,L1)")  "openmp supported = ", data%openmp_supported
write (u, "(1x,A,I0)")  "n_in = ", data%n_in
write (u, "(1x,A,I0)")  "n_out = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =", data%flv_state

```

```

write (u, "(1x,A,10(1x,I2))") "hel state =", data%hel_state(:,1)
write (u, "(1x,A,10(1x,I2))") "hel state =", data%hel_state(:,2)
write (u, "(1x,A,10(1x,I0))") "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))") "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))") "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))") "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    125._default, 0.0_default, 0.0_default, 0.0_default, &
    62.5_default, 0.0_default, 0.0_default, 62.5_default, &
    62.5_default, 0.0_default, 0.0_default,-62.5_default &
    ], [4,3])
do i = 1, 3
    write (u, "(2x,A,I0,A,4(1x,F8.4))")  "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver)
type is (prc_test_t)
    write (u, "(1x,A,1x,E11.4)") "|amp| =", abs (driver%get_amplitude (p))
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_test_3"

end subroutine prc_test_3

```

Shortcut

This is identical to the previous test, but we create the library be a single command. This is handy for other modules which use the test process.

```

<Test ME: execute tests>+≡
    call test (prc_test_4, "prc_test_4", &
        "build and load trivial decay using shortcut", &
        u, results)

<Test ME: test declarations>+≡
    public :: prc_test_4

<Test ME: tests>+≡
    subroutine prc_test_4 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        class(prc_core_driver_t), allocatable :: driver

```

```

type(process_constants_t) :: data
real(default), dimension(0:3,3) :: p

write (u, "(A)")  "* Test output: prc_test_4"
write (u, "(A)")  "* Purpose: create a trivial decay process"
write (u, "(A)")  "*           build a library and &
                    &access the matrix element"
write (u, "(A)")

write (u, "(A)")  "* Build and load a process library with one entry"

call prc_test_create_library (var_str ("prc_test4"), lib, &
                             scattering=.false., decay=.true.)
call lib%connect_process (var_str ("prc_test4"), 1, data, driver)

p = reshape ([ &
              125._default, 0.0_default, 0.0_default, 0.0_default, &
              62.5_default, 0.0_default, 0.0_default, 62.5_default, &
              62.5_default, 0.0_default, 0.0_default, -62.5_default &
              ], [4,3])

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver)
type is (prc_test_t)
    write (u, "(1x,A,1x,E11.4)") "|amp| =", abs (driver%get_amplitude (p))
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_test_4"

end subroutine prc_test_4

```


Chapter 15

Particles

This chapter collects modules that implement particle objects, for use in event records.

While within interactions, all correlations are manifest, a particle array is derived by selecting a particular quantum number set. This involves tracing over all other particles, as far as polarization is concerned. Thus, a particle has definite flavor, color, and a single-particle density matrix for polarization.

su_algebra We make use of $su(N)$ generators as the basis for representing polarization matrices. This module defines the basis and provides the necessary transformation routines.

bloch_vectors This defines polarization objects in Bloch representation. The object describes the spin density matrix of a particle, currently restricted to spin $0 \dots 2$.

polarizations This extends the basic polarization object such that it supports properties of physical particles and appropriate constructors.

particles Particle objects and particle lists, as the base of event records.

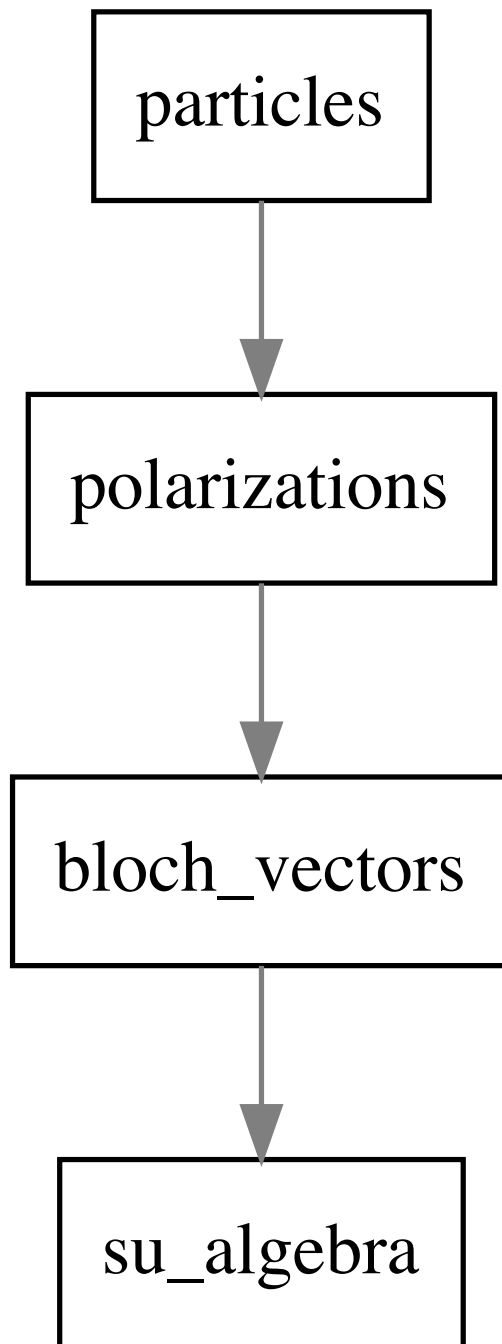


Figure 15.1: Module dependencies in `src/particles`.

15.1 $su(N)$ Algebra

We need a specific choice of basis for a well-defined component representation. The matrix elements of T^a are ordered as $m = \ell, \ell - 1, \dots - \ell$, i.e., from highest down to lowest weight, for both row and column.

We list first the generators of the $su(2)$ subalgebras which leave $|m|$ invariant ($|m| \neq 0$):

$$T^{b+1, b+2, b+3} \equiv \sigma^{1,2,3} \quad (15.1)$$

acting on the respective subspace $|m| = \ell, \ell - 1, \dots$ for $b = 0, 1, \dots$. This defines generators T^a for $a = 1, \dots, 3N/2$ ($\dots 3(N-1)/2$) for N even (odd), respectively.

The following generators successively extend this to $su(4)$, $su(6)$, \dots until $su(N)$ by adding first the missing off-diagonal and then diagonal generators. The phase conventions are analogous.

(It should be possible to code these conventions for generic spin, but in the current implementation we restrict ourselves to $s \leq 2$, i.e., $N \leq 5$.)

```
<su_algebra.f90>≡
  <File header>

  module su_algebra

    <Use kinds>
    use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR

    <Standard module head>

    <su algebra: public>

    contains

    <su algebra: procedures>

  end module su_algebra
```

15.1.1 $su(N)$ fundamental representation

The dimension of the basis for a given spin type. consecutively, starting at SCALAR=1.

```
<su algebra: public>≡
  public :: algebra_dimension

<su algebra: procedures>≡
  function algebra_dimension (s) result (n)
    integer :: n
    integer, intent(in) :: s
    n = fundamental_dimension (s) ** 2 - 1
  end function algebra_dimension
```

The dimension of the fundamental (defining) representation that we use. This implementation assumes that the spin type is numerically equal to the fundamental dimension.

```
<su algebra: public>+≡
  public :: fundamental_dimension
```

```

<su algebra: procedures>+≡
function fundamental_dimension (s) result (d)
  integer :: d
  integer, intent(in) :: s
  d = s
end function fundamental_dimension

```

15.1.2 Mapping between helicity and matrix index

Return the helicity that corresponds to a particular entry in the polarization matrix representation. Helicities are counted downwards, in integers, and zero helicity is included (omitted) for odd (even) spin, respectively.

```

<su algebra: public>+≡
public :: helicity_value

<su algebra: procedures>+≡
function helicity_value (s, i) result (h)
  integer :: h
  integer, intent(in) :: s, i
  integer, dimension(1), parameter :: hh1 = [0]
  integer, dimension(2), parameter :: hh2 = [1, -1]
  integer, dimension(3), parameter :: hh3 = [1, 0, -1]
  integer, dimension(4), parameter :: hh4 = [2, 1, -1, -2]
  integer, dimension(5), parameter :: hh5 = [2, 1, 0, -1, -2]
  h = 0
  select case (s)
  case (SCALAR)
    select case (i)
    case (1:1); h = hh1(i)
    end select
  case (SPINOR)
    select case (i)
    case (1:2); h = hh2(i)
    end select
  case (VECTOR)
    select case (i)
    case (1:3); h = hh3(i)
    end select
  case (VECTORSPINOR)
    select case (i)
    case (1:4); h = hh4(i)
    end select
  case (TENSOR)
    select case (i)
    case (1:5); h = hh5(i)
    end select
  end select
end function helicity_value

```

Inverse: return the index that corresponds to a certain helicity value in the chosen representation.

```

<su algebra: public>+≡

```

```

public :: helicity_index
<su algebra: procedures>+≡
function helicity_index (s, h) result (i)
  integer, intent(in) :: s, h
  integer :: i
  integer, dimension(0:0), parameter :: hi1 = [1]
  integer, dimension(-1:1), parameter :: hi2 = [2, 0, 1]
  integer, dimension(-1:1), parameter :: hi3 = [3, 2, 1]
  integer, dimension(-2:2), parameter :: hi4 = [4, 3, 0, 2, 1]
  integer, dimension(-2:2), parameter :: hi5 = [5, 4, 3, 2, 1]
  select case (s)
  case (SCALAR)
    i = hi1(h)
  case (SPINOR)
    i = hi2(h)
  case (VECTOR)
    i = hi3(h)
  case (VECTORSPINOR)
    i = hi4(h)
  case (TENSOR)
    i = hi5(h)
  end select
end function helicity_index

```

15.1.3 Generator Basis: Cartan Generators

For each supported spin type, we return specific properties of the set of generators via inquiry functions. This is equivalent to using explicit representations of the generators.

For easy access, the properties are hard-coded and selected via case expressions.

Return true if the generator #i is in the Cartan subalgebra, i.e., a diagonal matrix for spin type s.

```

<su algebra: public>+≡
public :: is_cartan_generator
<su algebra: procedures>+≡
elemental function is_cartan_generator (s, i) result (cartan)
  logical :: cartan
  integer, intent(in) :: s, i
  select case (s)
  case (SCALAR)
  case (SPINOR)
    select case (i)
    case (3); cartan = .true.
    case default
      cartan = .false.
    end select
  case (VECTOR)
    select case (i)
    case (3,8); cartan = .true.
    case default

```

```

        cartan = .false.
    end select
case (VECTORSPINOR)
    select case (i)
        case (3,6,15); cartan = .true.
    case default
        cartan = .false.
    end select
case (TENSOR)
    select case (i)
        case (3,6,15,24); cartan = .true.
    case default
        cartan = .false.
    end select
case default
    cartan = .false.
end select
end function is_cartan_generator

```

Return the index of Cartan generator #k in the chosen representation. This has to conform to `cartan` above.

```

<su algebra: public>+≡
    public :: cartan_index

<su algebra: procedures>+≡
    elemental function cartan_index (s, k) result (ci)
        integer :: ci
        integer, intent(in) :: s, k
        integer, dimension(1), parameter :: ci2 = [3]
        integer, dimension(2), parameter :: ci3 = [3,8]
        integer, dimension(3), parameter :: ci4 = [3,6,15]
        integer, dimension(4), parameter :: ci5 = [3,6,15,24]
        select case (s)
            case (SPINOR)
                ci = ci2(k)
            case (VECTOR)
                ci = ci3(k)
            case (VECTORSPINOR)
                ci = ci4(k)
            case (TENSOR)
                ci = ci5(k)
            case default
                ci = 0
        end select
    end function cartan_index

```

The element #k of the result vector `a` is equal to the (h, h) diagonal entry of the generator matrix T^k . That is, evaluating this for all allowed values of `h`, we recover the set of Cartan generator matrices.

```

<su algebra: public>+≡
    public :: cartan_element

<su algebra: procedures>+≡
    function cartan_element (s, h) result (a)

```

```

real(default), dimension(:), allocatable :: a
integer, intent(in) :: s, h
real(default), parameter :: sqrt2 = sqrt (2._default)
real(default), parameter :: sqrt3 = sqrt (3._default)
real(default), parameter :: sqrt10 = sqrt (10._default)
allocate (a (algebra_dimension (s)), source = 0._default)
select case (s)
case (SCALAR)
case (SPINOR)
    select case (h)
    case (1)
        a(3) = 1._default / 2
    case (-1)
        a(3) = -1._default / 2
    end select
case (VECTOR)
    select case (h)
    case (1)
        a(3) = 1._default / 2
        a(8) = 1._default / (2 * sqrt3)
    case (-1)
        a(3) = -1._default / 2
        a(8) = 1._default / (2 * sqrt3)
    case (0)
        a(8) = -1._default / sqrt3
    end select
case (VECTORSPINOR)
    select case (h)
    case (2)
        a(3) = 1._default / 2
        a(15) = 1._default / (2 * sqrt2)
    case (-2)
        a(3) = -1._default / 2
        a(15) = 1._default / (2 * sqrt2)
    case (1)
        a(6) = 1._default / 2
        a(15) = -1._default / (2 * sqrt2)
    case (-1)
        a(6) = -1._default / 2
        a(15) = -1._default / (2 * sqrt2)
    end select
case (TENSOR)
    select case (h)
    case (2)
        a(3) = 1._default / 2
        a(15) = 1._default / (2 * sqrt2)
        a(24) = 1._default / (2 * sqrt10)
    case (-2)
        a(3) = -1._default / 2
        a(15) = 1._default / (2 * sqrt2)
        a(24) = 1._default / (2 * sqrt10)
    case (1)
        a(6) = 1._default / 2
        a(15) = -1._default / (2 * sqrt2)

```

```

        a(24) = 1._default / (2 * sqrt10)
    case (-1)
        a(6) = -1._default / 2
        a(15) = -1._default / (2 * sqrt2)
        a(24) = 1._default / (2 * sqrt10)
    case (0)
        a(24) = -4._default / (2 * sqrt10)
    end select
end select
end function cartan_element

```

Given an array of diagonal matrix elements `rd` of a generator, compute the array `a` of basis coefficients. The array must be ordered as defined by `helicity_value`, i.e., highest weight first. The calculation is organized such that the trace of the generator, i.e., the sum of `rd` values, drops out. The result array `a` has coefficients for all basis generators, but only Cartan generators can get a nonzero coefficient.

```

<su algebra: public>+≡
    public :: cartan_coeff

<su algebra: procedures>+≡
    function cartan_coeff (s, rd) result (a)
        real(default), dimension(:), allocatable :: a
        integer, intent(in) :: s
        real(default), dimension(:), intent(in) :: rd
        real(default), parameter :: sqrt2 = sqrt (2._default)
        real(default), parameter :: sqrt3 = sqrt (3._default)
        real(default), parameter :: sqrt10 = sqrt (10._default)
        integer :: n
        n = algebra_dimension (s)
        allocate (a (n), source = 0._default)
        select case (s)
        case (SPINOR)
            a(3) = rd(1) - rd(2)
        case (VECTOR)
            a(3) = rd(1) - rd(3)
            a(8) = (rd(1) - 2 * rd(2) + rd(3)) / sqrt3
        case (VECTORSPINOR)
            a(3) = rd(1) - rd(4)
            a(6) = rd(2) - rd(3)
            a(15) = (rd(1) - rd(2) - rd(3) + rd(4)) / sqrt2
        case (TENSOR)
            a(3) = rd(1) - rd(5)
            a(6) = rd(2) - rd(4)
            a(15) = (rd(1) - rd(2) - rd(4) + rd(5)) / sqrt2
            a(24) = (rd(1) + rd(2) - 4 * rd(3) + rd(4) + rd(5)) / sqrt10
        end select
    end function cartan_coeff

```


15.1.4 Roots (Off-Diagonal Generators)

Return the appropriate generator index for a given off-diagonal helicity combination. We require $h_1 > h_2$. We return the index of the appropriate real-valued generator if **r** is true, else the complex-valued one.

This is separate from the `cartan_coeff` function above. The reason is that the off-diagonal generators have only a single nonzero matrix element, so there is a one-to-one correspondence of helicity and index.

```
(su algebra: public)+≡
  public :: root_index

(su algebra: procedures)+≡
  function root_index (s, h1, h2, r) result (ai)
    integer :: ai
    integer, intent(in) :: s, h1, h2
    logical :: r
    ai = 0
    select case (s)
    case (SCALAR)
    case (SPINOR)
      select case (h1)
      case (1)
        select case (h2)
        case (-1); ai = 1
        end select
      end select
    case (VECTOR)
      select case (h1)
      case (1)
        select case (h2)
        case (-1); ai = 1
        case (0); ai = 4
        end select
      case (0)
        select case (h2)
        case (-1); ai = 6
        end select
      end select
    case (VECTORSPINOR)
      select case (h1)
      case (2)
        select case (h2)
        case (-2); ai = 1
        case (1); ai = 7
        case (-1); ai = 11
        end select
      case (1)
        select case (h2)
        case (-1); ai = 4
        case (-2); ai = 13
        end select
      case (-1)
        select case (h2)
        case (-2); ai = 9
```

```

        end select
    end select
case (TENSOR)
    select case (h1)
        case (2)
            select case (h2)
                case (-2); ai = 1
                case (1);  ai = 7
                case (-1); ai = 11
                case (0);  ai = 16
            end select
        case (1)
            select case (h2)
                case (-1); ai = 4
                case (-2); ai = 13
                case (0);  ai = 20
            end select
        case (-1)
            select case (h2)
                case (-2); ai = 9
            end select
        case (0)
            select case (h2)
                case (-2); ai = 18
                case (-1); ai = 22
            end select
        end select
    end select
    if (ai /= 0 .and. .not. r) ai = ai + 1
end function root_index

```

Inverse: return the helicity values ($h_2 > h_1$) for an off-diagonal generator. The flag *r* tells whether this is a real or diagonal generator. The others are Cartan generators.

```

<su algebra: public>+≡
    public :: root_helicity

<su algebra: procedures>+≡
    subroutine root_helicity (s, i, h1, h2, r)
        integer, intent(in) :: s, i
        integer, intent(out) :: h1, h2
        logical, intent(out) :: r
        h1 = 0
        h2 = 0
        r = .false.
        select case (s)
        case (SCALAR)
        case (SPINOR)
            select case (i)
            case ( 1, 2); h1 = 1; h2 = -1; r = i == 1
            end select
        case (VECTOR)
            select case (i)
            case ( 1, 2); h1 = 1; h2 = -1; r = i == 1
            end select
        end select
    end subroutine

```

```

        case ( 4, 5); h1 =  1; h2 =  0; r = i == 4
        case ( 6, 7); h1 =  0; h2 = -1; r = i == 6
    end select
case (VECTORSPINOR)
    select case (i)
        case ( 1, 2); h1 =  2; h2 = -2; r = i == 1
        case ( 4, 5); h1 =  1; h2 = -1; r = i == 4
        case ( 7, 8); h1 =  2; h2 =  1; r = i == 7
        case ( 9,10); h1 = -1; h2 = -2; r = i == 9
        case (11,12); h1 =  2; h2 = -1; r = i ==11
        case (13,14); h1 =  1; h2 = -2; r = i ==13
    end select
case (TENSOR)
    select case (i)
        case ( 1, 2); h1 =  2; h2 = -2; r = i == 1
        case ( 4, 5); h1 =  1; h2 = -1; r = i == 4
        case ( 7, 8); h1 =  2; h2 =  1; r = i == 7
        case ( 9,10); h1 = -1; h2 = -2; r = i == 9
        case (11,12); h1 =  2; h2 = -1; r = i ==11
        case (13,14); h1 =  1; h2 = -2; r = i ==13
        case (16,17); h1 =  2; h2 =  0; r = i ==16
        case (18,19); h1 =  0; h2 = -2; r = i ==18
        case (20,21); h1 =  1; h2 =  0; r = i ==20
        case (22,23); h1 =  0; h2 = -1; r = i ==22
    end select
end select
end subroutine root_helicity

```

15.1.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<su_algebra_ut.f90>≡
  <File header>

  module su_algebra_ut
    use unit_tests
    use su_algebra_util

    <Standard module head>

    <su algebra: public test>

    contains

    <su algebra: test driver>

  end module su_algebra_ut
<su_algebra_util.f90>≡
  <File header>

  module su_algebra_util

```

```

    <Use kinds>
    use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
    use su_algebra

    <Standard module head>

    <su algebra: test declarations>

contains

    <su algebra: tests>

end module su_algebra_util
API: driver for the unit tests below.
<su algebra: public test>≡
    public :: su_algebra_test
<su algebra: test driver>≡
    subroutine su_algebra_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <su algebra: execute tests>
    end subroutine su_algebra_test

```

Generator Ordering

Show the position of Cartan generators in the sequence of basis generators.

```

<su algebra: execute tests>≡
    call test (su_algebra_1, "su_algebra_1", &
        "generator ordering", &
        u, results)

<su algebra: test declarations>≡
    public :: su_algebra_1

<su algebra: tests>≡
    subroutine su_algebra_1 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: su_algebra_1"
        write (u, "(A)")  "* Purpose: test su(N) algebra implementation"
        write (u, "(A)")

        write (u, "(A)")  "* su(N) generators: &
            &list and mark Cartan subalgebra"

        write (u, "(A)")
        write (u, "(A)")  "* s = 0"
        call cartan_check (SCALAR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1/2"
    end subroutine su_algebra_1

```

```

call cartan_check (SPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call cartan_check (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call cartan_check (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call cartan_check (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: su_algebra_1"

contains

subroutine cartan_check (s)
  integer, intent(in) :: s
  integer :: i
  write (u, *)
  do i = 1, algebra_dimension (s)
    write (u, "(1x,L1)", advance="no")  is_cartan_generator (s, i)
  end do
  write (u, *)
end subroutine cartan_check

end subroutine su_algebra_1

```

Cartan Generator Basis

Show the explicit matrix representation for all Cartan generators and check their traces and Killing products.

Also test helicity index mappings.

```

<su algebra: execute tests>+≡
  call test (su_algebra_2, "su_algebra_2", &
    "Cartan generator representation", &
    u, results)

<su algebra: test declarations>+≡
  public :: su_algebra_2

<su algebra: tests>+≡
  subroutine su_algebra_2 (u)
    integer, intent(in) :: u

    write (u, "(A)")  "* Test output: su_algebra_2"
    write (u, "(A)")  "* Purpose: test su(N) algebra implementation"
    write (u, "(A)")

```

```

write (u, "(A)")  "* diagonal su(N) generators: &
    &show explicit representation"
write (u, "(A)")  "* and check trace and Killing form"

write (u, "(A)")
write (u, "(A)")  "* s = 1/2"
call cartan_show (SPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call cartan_show (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call cartan_show (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call cartan_show (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: su_algebra_2"

contains

subroutine cartan_show (s)
    integer, intent(in) :: s
    real(default), dimension(:, :), allocatable :: rd
    integer, dimension(:), allocatable :: ci
    integer :: n, d, h, i, j, k, l

    n = algebra_dimension (s)
    d = fundamental_dimension (s)

    write (u, *)
    write (u, "(A2,5X)", advance="no")  "h:"
    do i = 1, d
        j = helicity_index (s, helicity_value (s, i))
        write (u, "(1x,I2,5X)", advance="no")  helicity_value (s, j)
    end do
    write (u, "(8X)", advance="no")
    write (u, "(1X,A)")  "tr"

    allocate (rd (n,d), source = 0._default)
    do i = 1, d
        h = helicity_value (s, i)
        rd(:,i) = cartan_element (s, h)
    end do

    allocate (ci (d-1), source = 0)
    do k = 1, d-1
        ci(k) = cartan_index (s, k)
    end do

```

```

write (u, *)
do k = 1, d-1
  write (u, "('T',I2,':',1X)", advance="no") ci(k)
  do i = 1, d
    write (u, 1, advance="no") rd(ci(k),i)
  end do
  write (u, "(8X)", advance="no")
  write (u, 1) sum (rd(ci(k),:))
end do

write (u, *)
write (u, "(6X)", advance="no")
do k = 1, d-1
  write (u, "(2X,'T',I2,3X)", advance="no") ci(k)
end do
write (u, *)

do k = 1, d-1
  write (u, "('T',I2,2X)", advance="no") ci(k)
  do l = 1, d-1
    write (u, 1, advance="no") dot_product (rd(ci(k),:), rd(ci(l),:))
  end do
  write (u, *)
end do

1    format (1x,F7.4)

end subroutine cartan_show

end subroutine su_algebra_2

```

Bloch Representation: Cartan Generators

Transform from Bloch vectors to matrix and back, considering Cartan generators only.

```

<su algebra: execute tests>+≡
  call test (su_algebra_3, "su_algebra_3", &
    "Cartan generator mapping", &
    u, results)

<su algebra: test declarations>+≡
  public :: su_algebra_3

<su algebra: tests>+≡
  subroutine su_algebra_3 (u)
    integer, intent(in) :: u

    write (u, "(A)")  "* Test output: su_algebra_3"
    write (u, "(A)")  "* Purpose: test su(N) algebra implementation"
    write (u, "(A)")

    write (u, "(A)")  "* diagonal su(N) generators: &
      &transform to matrix and back"

```

```

write (u, "(A)")
write (u, "(A)")  "* s = 1/2"
call cartan_expand (SPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call cartan_expand (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call cartan_expand (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call cartan_expand (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: su_algebra_3"

```

contains

```

subroutine cartan_expand (s)
  integer, intent(in) :: s
  real(default), dimension(:,:), allocatable :: rd
  integer, dimension(:), allocatable :: ci
  real(default), dimension(:), allocatable :: a
  logical, dimension(:), allocatable :: mask
  integer :: n, d, h, i, k, l

  n = algebra_dimension (s)
  d = fundamental_dimension (s)

  allocate (rd (n,d), source = 0._default)
  do i = 1, d
    h = helicity_value (s, i)
    rd(:,i) = cartan_element (s, h)
  end do

  allocate (ci (d-1), source = 0)
  do k = 1, d-1
    ci(k) = cartan_index (s, k)
  end do

  allocate (a (n))

  write (u, *)
  do k = 1, d-1
    a(:) = cartan_coeff (s, rd(ci(k),:))
    write (u, "('T',I2,':',',1X)", advance="no") ci(k)
    do i = 1, n
      if (is_cartan_generator (s, i)) then
        write (u, 1, advance="no") a(i)
      else if (a(i) /= 0) then

```



```

! this should not happen (nonzero non-Cartan entry)
write (u, "(1X,':',I2,':',3X)", advance="no") i
end if
end do
write (u, *)
end do

1    format (1X,F7.4)

end subroutine cartan_expand

end subroutine su_algebra_3

```

Bloch Representation: Roots

List the mapping between helicity transitions and (real) off-diagonal generators.

```

<su algebra: execute tests>+≡
  call test (su_algebra_4, "su_algebra_4", &
    "Root-helicity mapping", &
    u, results)

<su algebra: test declarations>+≡
  public :: su_algebra_4

<su algebra: tests>+≡
  subroutine su_algebra_4 (u)
    integer, intent(in) :: u

    write (u, "(A)")  "* Test output: su_algebra_4"
    write (u, "(A)")  "* Purpose: test su(N) algebra implementation"
    write (u, "(A)")

    write (u, "(A)")  "* off-diagonal su(N) generators: &
      &mapping from/to helicity pair"

    write (u, "(A)")
    write (u, "(A)")  "* s = 1/2"
    call root_expand (SPINOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 1"
    call root_expand (VECTOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 3/2"
    call root_expand (VECTORSPINOR)

    write (u, "(A)")
    write (u, "(A)")  "* s = 2"
    call root_expand (TENSOR)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: su_algebra_4"

```

```

contains

subroutine root_expand (s)
  integer, intent(in) :: s
  integer :: n, d, i, j, h1, h2
  logical :: r

  n = algebra_dimension (s)

  write (u, *)
  do i = 1, n
    if (is_cartan_generator (s, i)) cycle
    call root_helicity (s, i, h1, h2, r)
    j = root_index (s, h1, h2, r)
    write (u, "('T',I2,':')", advance="no") j
    write (u, "(2(Ix,I2))", advance="no") h1, h2
    if (r) then
      write (u, *)
    else
      write (u, "('*')")
    end if
  end do

end subroutine root_expand

end subroutine su_algebra_4

```

15.2 Bloch Representation

Particle polarization is determined by a particular quantum state which has just helicity information. Physically, this is the spin density matrix ρ , where we do not restrict ourselves to pure states.

We adopt the phase convention for a spin-1/2 particle that

$$\rho = \frac{1}{2}(1 + \vec{\alpha} \cdot \vec{\sigma}) \quad (15.2)$$

with the polarization axis $\vec{\alpha}$. For a particle with arbitrary spin s , and thus $N = 2s + 1$ spin states, we extend the above definition to generalized Bloch form

$$\rho = \frac{1}{N} \left(1 + \sqrt{2N(N-1)} \alpha^a T^a \right) \quad (15.3)$$

where the T^a ($a = 1, \dots, N^2 - 1$) are a basis of $su(N)$ algebra generators. These $N \times N$ matrices are hermitean, traceless, and orthogonal via

$$\text{Tr } T^a T^b = \frac{1}{2} \delta^{ab} \quad (15.4)$$

In the spin-1/2 case, this reduces to the above (standard Bloch) representation since $T^a = \sigma^a/2$, $a = 1, 2, 3$. For the spin-1 case, we could use $T^a = \lambda^a/2$ with the Gell-Mann matrices,

$$\rho = \frac{1}{3} \left(1 + \sqrt{3} \alpha^a \lambda^a \right), \quad (15.5)$$

The normalization is chosen that $|\alpha| \leq 1$ for allowed density matrix, where $|\alpha| = 1$ is a necessary, but not sufficient, condition for a pure state.

We need a specific choice of basis for a well-defined component representation. The matrix elements of T^a are ordered as $m = \ell, \ell - 1, \dots, -\ell$, i.e., from highest down to lowest weight, for both row and column.

We list first the generators of the $su(2)$ subalgebras which leave $|m|$ invariant ($|m| \neq 0$):

$$T^{b+1, b+2, b+3} \equiv \sigma^{1, 2, 3} \quad (15.6)$$

acting on the respective subspace $|m| = \ell, \ell - 1, \dots$ for $b = 0, 1, \dots$. This defines generators T^a for $a = 1, \dots, 3N/2$ ($\dots 3(N-1)/2$) for N even (odd), respectively.

The following generators successively extend this to $su(4)$, $su(6)$, \dots until $su(N)$ by adding first the missing off-diagonal and then diagonal generators. The phase conventions are analogous.

(It should be possible to code these conventions for generic spin, but in the current implementation we restrict ourselves to $s \leq 2$, i.e., $N \leq 5$.)

Particle polarization is determined by a particular quantum state which has just helicity information. Physically, this is the spin density matrix ρ , where we do not restrict ourselves to pure states.

We adopt the phase convention for a spin-1/2 particle that

$$\rho = \frac{1}{2}(1 + \vec{\alpha} \cdot \vec{\sigma}) \quad (15.7)$$

with the polarization axis $\vec{\alpha}$. For a particle with arbitrary spin s , and thus $N = 2s + 1$ spin states, we extend the above definition to generalized Bloch form

$$\rho = \frac{1}{N} \left(1 + \sqrt{2N(N-1)} \alpha^a T^a \right) \quad (15.8)$$

where the T^a ($a = 1, \dots, N^2 - 1$) are a basis of $su(N)$ algebra generators. These $N \times N$ matrices are hermitean, traceless, and orthogonal via

$$\text{Tr } T^a T^b = \frac{1}{2} \delta^{ab} \quad (15.9)$$

In the spin-1/2 case, this reduces to the above (standard Bloch) representation since $T^a = \sigma^a/2$, $a = 1, 2, 3$. For the spin-1 case, we could use $T^a = \lambda^a/2$ with the Gell-Mann matrices,

$$\rho = \frac{1}{3} \left(1 + \sqrt{3} \alpha^a \lambda^a \right), \quad (15.10)$$

The normalization is chosen that $|\alpha| \leq 1$ for allowed density matrix, where $|\alpha| = 1$ is a necessary, but not sufficient, condition for a pure state.

`<bloch_vectors.f90>`≡
<File header>

`module bloch_vectors`

<Use kinds>

`use physics_defs, only: UNKNOWN, SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR`
`use su_algebra`

<Standard module head>

<Bloch vectors: public>

<Bloch vectors: types>

`contains`

<Bloch vectors: procedures>

`end module bloch_vectors`

15.2.1 Preliminaries

The normalization factor $\sqrt{2N(N-1)}/N$ that enters the Bloch representation.

<Bloch vectors: procedures>≡

```
function bloch_factor (s) result (f)
  real(default) :: f
  integer, intent(in) :: s
  select case (s)
    case (SCALAR)
      f = 0
    case (SPINOR)
      f = 1
    case (VECTOR)
      f = 2 * sqrt (3._default) / 3
    case (VECTORSPINOR)
      f = 2 * sqrt (6._default) / 4
    case (TENSOR)
      f = 2 * sqrt (10._default) / 5
```

```

    case default
        f = 0
    end select
end function bloch_factor

```

15.2.2 The basic polarization type

The basic polarization object holds just the entries of the Bloch vector as an allocatable array.

Bloch is active whenever the coefficient array is allocated. For convenience, we store the spin type ($2s$) and the multiplicity (N) together with the coefficient array (α). We have to allow for the massless case where s is arbitrary > 0 but $N = 2$, and furthermore the chiral massless case where $N = 1$. In the latter case, the array remains deallocated but the chirality is set to ± 1 .

In the Bloch vector implementation, we do not distinguish between particle and antiparticle. If the distinction applies, it must be made by the caller when transforming between density matrix and Bloch vector.

```

<Bloch vectors: public>≡
    public :: bloch_vector_t
<Bloch vectors: types>≡
    type :: bloch_vector_t
        private
            integer :: spin_type = UNKNOWN
            real(default), dimension(:), allocatable :: a
        contains
            <Bloch vectors: bloch vector: TBP>
    end type bloch_vector_t

```

15.2.3 Direct Access

This basic initializer just sets the spin type, leaving the Bloch vector unallocated. The object therefore does not support nonzero polarization.

```

<Bloch vectors: bloch vector: TBP>≡
    procedure :: init_unpolarized => bloch_vector_init_unpolarized
<Bloch vectors: procedures>+≡
    subroutine bloch_vector_init_unpolarized (pol, spin_type)
        class(bloch_vector_t), intent(out) :: pol
        integer, intent(in) :: spin_type
        pol%spin_type = spin_type
    end subroutine bloch_vector_init_unpolarized

```

The standard initializer allocates the Bloch vector and initializes with zeros, so we can define a polarization later. We make sure that this works only for the supported spin type. Initializing with UNKNOWN spin type resets the Bloch vector to undefined, i.e., unpolarized state.

```

<Bloch vectors: bloch vector: TBP>+≡
    generic :: init => bloch_vector_init
    procedure, private :: bloch_vector_init

```

```

<Bloch vectors: procedures>+≡
subroutine bloch_vector_init (pol, spin_type)
  class(bloch_vector_t), intent(out) :: pol
  integer, intent(in) :: spin_type
  pol%spin_type = spin_type
  select case (spin_type)
  case (SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR)
    allocate (pol%a (algebra_dimension (spin_type)), source = 0._default)
  end select
end subroutine bloch_vector_init

```

Fill the Bloch vector from an array, no change of normalization. No initialization and no check, we assume that the shapes do match.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: from_array => bloch_vector_from_array

<Bloch vectors: procedures>+≡
subroutine bloch_vector_from_array (pol, a)
  class(bloch_vector_t), intent(inout) :: pol
  real(default), dimension(:), allocatable, intent(in) :: a
  pol%a(:) = a
end subroutine bloch_vector_from_array

```

Transform to an array of reals, i.e., extract the Bloch vector as-is.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: to_array => bloch_vector_to_array

<Bloch vectors: procedures>+≡
subroutine bloch_vector_to_array (pol, a)
  class(bloch_vector_t), intent(in) :: pol
  real(default), dimension(:), allocatable, intent(out) :: a
  if (pol%is_defined ()) allocate (a (size (pol%a)), source = pol%a)
end subroutine bloch_vector_to_array

```

15.2.4 Raw I/O

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: write_raw => bloch_vector_write_raw
  procedure :: read_raw => bloch_vector_read_raw

<Bloch vectors: procedures>+≡
subroutine bloch_vector_write_raw (pol, u)
  class(bloch_vector_t), intent(in) :: pol
  integer, intent(in) :: u
  write (u) pol%spin_type
  write (u) allocated (pol%a)
  if (allocated (pol%a)) then
    write (u) pol%a
  end if
end subroutine bloch_vector_write_raw

subroutine bloch_vector_read_raw (pol, u, iostat)
  class(bloch_vector_t), intent(out) :: pol

```

```

integer, intent(in) :: u
integer, intent(out) :: iostat
integer :: s
logical :: polarized
read (u, iostat=iostat) s
read (u, iostat=iostat) polarized
if (iostat /= 0) return
if (polarized) then
  call pol%init (s)
  read (u, iostat=iostat) pol%a
else
  call pol%init_unpolarized (s)
end if
end subroutine bloch_vector_read_raw

```

15.2.5 Properties

Re-export algebra functions that depend on the spin type. These functions do not depend on the Bloch vector being allocated.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: get_n_states
  procedure :: get_length
  procedure :: hel_index => bv_helicity_index
  procedure :: hel_value => bv_helicity_value
  procedure :: bloch_factor => bv_factor

<Bloch vectors: procedures>+≡
  function get_n_states (pol) result (n)
    class(bloch_vector_t), intent(in) :: pol
    integer :: n
    n = fundamental_dimension (pol%spin_type)
  end function get_n_states

  function get_length (pol) result (n)
    class(bloch_vector_t), intent(in) :: pol
    integer :: n
    n = algebra_dimension (pol%spin_type)
  end function get_length

  function bv_helicity_index (pol, h) result (i)
    class(bloch_vector_t), intent(in) :: pol
    integer, intent(in) :: h
    integer :: i
    i = helicity_index (pol%spin_type, h)
  end function bv_helicity_index

  function bv_helicity_value (pol, i) result (h)
    class(bloch_vector_t), intent(in) :: pol
    integer, intent(in) :: i
    integer :: h
    h = helicity_value (pol%spin_type, i)
  end function bv_helicity_value

```

```

function bv_factor (pol) result (f)
  class(bloch_vector_t), intent(in) :: pol
  real(default) :: f
  f = bloch_factor (pol%spin_type)
end function bv_factor

```

If the Bloch vector object is defined, the spin type is anything else but UNKNOWN. This allows us to provide the representation-specific functions above.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: is_defined => bloch_vector_is_defined
<Bloch vectors: procedures>+≡
  function bloch_vector_is_defined (pol) result (flag)
    class(bloch_vector_t), intent(in) :: pol
    logical :: flag
    flag = pol%spin_type /= UNKNOWN
  end function bloch_vector_is_defined

```

If the Bloch vector object is (technically) polarized, it is defined, and the vector coefficient array has been allocated. However, the vector value may be zero.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: is_polarized => bloch_vector_is_polarized
<Bloch vectors: procedures>+≡
  function bloch_vector_is_polarized (pol) result (flag)
    class(bloch_vector_t), intent(in) :: pol
    logical :: flag
    flag = allocated (pol%a)
  end function bloch_vector_is_polarized

```

Return true if the polarization is diagonal, i.e., all entries in the density matrix are on the diagonal. This is equivalent to requiring that only Cartan generator coefficients are nonzero in the Bloch vector.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: is_diagonal => bloch_vector_is_diagonal
<Bloch vectors: procedures>+≡
  function bloch_vector_is_diagonal (pol) result (diagonal)
    class(bloch_vector_t), intent(in) :: pol
    logical :: diagonal
    integer :: s, i
    s = pol%spin_type
    diagonal = .true.
    if (pol%is_polarized ()) then
      do i = 1, size (pol%a)
        if (is_cartan_generator (s, i)) cycle
        if (pol%a(i) /= 0) then
          diagonal = .false.
          return
        end if
      end do
    end if
  end function bloch_vector_is_diagonal

```


Return the Euclidean norm of the Bloch vector. This is equal to the Killing form value of the corresponding algebra generator. We assume that the polarization object has been initialized.

For a pure state, the norm is unity. All other allowed states have a norm less than unity. (For $s \geq 1$, this is a necessary but not sufficient condition.)

```

(Bloch vectors: bloch vector: TBP)+≡
  procedure :: get_norm => bloch_vector_get_norm

(Bloch vectors: procedures)+≡
  function bloch_vector_get_norm (pol) result (norm)
    class(bloch_vector_t), intent(in) :: pol
    real(default) :: norm
    select case (pol%spin_type)
      case (SPINOR, VECTOR, VECTORSPINOR, TENSOR)
        norm = sqrt (dot_product (pol%a, pol%a))
      case default
        norm = 1
    end select
  end function bloch_vector_get_norm

```

15.2.6 Diagonal density matrix

This initializer takes a diagonal density matrix, represented by a real-valued array. We assume that the trace is unity, and that the array has the correct shape for the given `spin_type`.

The `bloch_factor` renormalization is necessary such that a pure state maps to a Bloch vector with unit norm.

```

(Bloch vectors: bloch vector: TBP)+≡
  generic :: init => bloch_vector_init_diagonal
  procedure, private :: bloch_vector_init_diagonal

(Bloch vectors: procedures)+≡
  subroutine bloch_vector_init_diagonal (pol, spin_type, rd)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
    real(default), dimension(:), intent(in) :: rd
    call pol%init (spin_type)
    call pol%set (rd)
  end subroutine bloch_vector_init_diagonal

```

Set a Bloch vector, given a diagonal density matrix as a real array. The Bloch vector must be initialized with correct characteristics.

```

(Bloch vectors: bloch vector: TBP)+≡
  generic :: set => bloch_vector_set_diagonal
  procedure, private :: bloch_vector_set_diagonal

(Bloch vectors: procedures)+≡
  subroutine bloch_vector_set_diagonal (pol, rd)
    class(bloch_vector_t), intent(inout) :: pol
    real(default), dimension(:), intent(in) :: rd
    integer :: s
    s = pol%spin_type

```

```

select case (s)
case (SCALAR,SPINOR,VECTOR,VECTORSPINOR,TENSOR)
  pol%a(:) = cartan_coeff (s, rd) / bloch_factor (s)
end select
end subroutine bloch_vector_set_diagonal

```

15.2.7 Massless density matrix

This is a specific variant which initializes an equipartition for the maximum helicity, corresponding to an unpolarized massless particle.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: init_max_weight => bloch_vector_init_max_weight

<Bloch vectors: procedures>+≡
  subroutine bloch_vector_init_max_weight (pol, spin_type)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
    call pol%init (spin_type)
    select case (spin_type)
    case (VECTOR)
      call pol%set ([0.5_default, 0._default, 0.5_default])
    case (VECTORSPINOR)
      call pol%set ([0.5_default, 0._default, 0._default, 0.5_default])
    case (TENSOR)
      call pol%set ([0.5_default, 0._default, 0._default, 0._default, 0.5_default])
    end select
  end subroutine bloch_vector_init_max_weight

```

Initialize the maximum-weight submatrix with a three-component Bloch vector. This is not as trivial as it seems because we need the above initialization for the generalized Bloch in order to remove the lower weights from the density matrix.

```

<Bloch vectors: bloch vector: TBP>+≡
  procedure :: init_vector => bloch_vector_init_vector
  procedure :: to_vector => bloch_vector_to_vector

<Bloch vectors: procedures>+≡
  subroutine bloch_vector_init_vector (pol, s, a)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: s
    real(default), dimension(3), intent(in) :: a
    call pol%init_max_weight (s)
    select case (s)
    case (SPINOR, VECTOR, VECTORSPINOR, TENSOR)
      pol%a(1:3) = a / bloch_factor (s)
    end select
  end subroutine bloch_vector_init_vector

  subroutine bloch_vector_to_vector (pol, a)
    class(bloch_vector_t), intent(in) :: pol
    real(default), dimension(3), intent(out) :: a
    integer :: s
    s = pol%spin_type

```

```

select case (s)
case (SPINOR, VECTOR, VECTORSPINOR, TENSOR)
  a = pol%a(1:3) * bloch_factor (s)
case default
  a = 0
end select
end subroutine bloch_vector_to_vector

```

15.2.8 Arbitrary density matrix

Initialize the Bloch vector from a density matrix. We assume that the density is valid. In particular, the shape should match, the matrix should be hermitian, and the trace should be unity.

We first fill the diagonal, then add the off-diagonal parts.

```

<Bloch vectors: bloch vector: TBP>+≡
  generic :: init => bloch_vector_init_matrix
  procedure, private :: bloch_vector_init_matrix

<Bloch vectors: procedures>+≡
  subroutine bloch_vector_init_matrix (pol, spin_type, r)
    class(bloch_vector_t), intent(out) :: pol
    integer, intent(in) :: spin_type
    complex(default), dimension(:,:), intent(in) :: r
    select case (spin_type)
    case (SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR)
      call pol%init (spin_type)
      call pol%set (r)
    case default
      call pol%init (UNKNOWN)
    end select
  end subroutine bloch_vector_init_matrix

```

Set a Bloch vector, given an arbitrary density matrix as a real array. The Bloch vector must be initialized with correct characteristics.

```

<Bloch vectors: bloch vector: TBP>+≡
  generic :: set => bloch_vector_set_matrix
  procedure, private :: bloch_vector_set_matrix

<Bloch vectors: procedures>+≡
  subroutine bloch_vector_set_matrix (pol, r)
    class(bloch_vector_t), intent(inout) :: pol
    complex(default), dimension(:,:), intent(in) :: r
    real(default), dimension(:), allocatable :: rd
    integer :: s, d, i, j, h1, h2, ir, ii
    s = pol%spin_type
    select case (s)
    case (SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR)
      d = fundamental_dimension (s)
      allocate (rd (d))
      do i = 1, d
        rd(i) = r(i,i)
      end do

```

```

call pol%set (rd)
do i = 1, d
  h1 = helicity_value (s, i)
  do j = i+1, d
    h2 = helicity_value (s, j)
    ir = root_index (s, h1, h2, .true.)
    ii = root_index (s, h1, h2, .false.)
    pol%a(ir) = real (r(j,i) + r(i,j)) / bloch_factor (s)
    pol%a(ii) = aimag (r(j,i) - r(i,j)) / bloch_factor (s)
  end do
end do
end select
end subroutine bloch_vector_set_matrix

```

Allocate and fill the density matrix r (with the index ordering as defined in `su_algebra`) that corresponds to a given Bloch vector.

If the optional `only_max_weight` is set, the resulting matrix has entries only for $\pm h_{\max}$, as appropriate for a massless particle (for $\text{spin} \geq 1$). Note that we always add the unit matrix, as this is part of the Bloch-vector definition.

(Bloch vectors: bloch vector: TBP)+≡

```

procedure :: to_matrix => bloch_vector_to_matrix

```

(Bloch vectors: procedures)+≡

```

subroutine bloch_vector_to_matrix (pol, r, only_max_weight)
  class(bloch_vector_t), intent(in) :: pol
  complex(default), dimension(:, :), intent(out), allocatable :: r
  logical, intent(in), optional :: only_max_weight
  integer :: d, s, h0, ng, ai, h, h1, h2, i, j
  logical :: is_real, only_max
  complex(default) :: val
  if (.not. pol%is_polarized ()) return
  s = pol%spin_type
  only_max = .false.
  select case (s)
  case (VECTOR, VECTORSPINOR, TENSOR)
    if (present (only_max_weight)) only_max = only_max_weight
  end select
  if (only_max) then
    ng = 2
    h0 = helicity_value (s, 1)
  else
    ng = algebra_dimension (s)
    h0 = 0
  end if
  d = fundamental_dimension (s)
  allocate (r (d, d), source = (0._default, 0._default))
  do i = 1, d
    h = helicity_value (s, i)
    if (abs (h) < h0) cycle
    r(i,i) = 1._default / d &
      + dot_product (cartan_element (s, h), pol%a) * bloch_factor (s)
  end do
  do ai = 1, ng
    if (is_cartan_generator (s, ai)) cycle

```

```

      call root_helicity (s, ai, h1, h2, is_real)
      i = helicity_index (s, h1)
      j = helicity_index (s, h2)
      if (is_real) then
        val = cmplx (pol%a(ai) / 2 * bloch_factor (s), 0._default, &
                     kind=default)
        r(i,j) = r(i,j) + val
        r(j,i) = r(j,i) + val
      else
        val = cmplx (0._default, pol%a(ai) / 2 * bloch_factor (s), &
                     kind=default)
        r(i,j) = r(i,j) - val
        r(j,i) = r(j,i) + val
      end if
    end do
  end subroutine bloch_vector_to_matrix

```

15.2.9 Unit tests

Test module, followed by the corresponding implementation module.

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

```

module bloch_vectors_ut
  use unit_tests
  use bloch_vectors_uti

```

<Standard module head>

<Bloch vectors: public test>

contains

<Bloch vectors: test driver>

```

end module bloch_vectors_ut

```

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

```

module bloch_vectors_uti

```

<Use kinds>

```

  use physics_defs, only: UNKNOWN, SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
  use su_algebra, only: algebra_dimension, fundamental_dimension, helicity_value

```

```

  use bloch_vectors

```

<Standard module head>

<Bloch vectors: test declarations>

contains

⟨Bloch vectors: tests⟩

```
end module bloch_vectors_util
```

API: driver for the unit tests below.

⟨Bloch vectors: public test⟩≡

```
public :: bloch_vectors_test
```

⟨Bloch vectors: test driver⟩≡

```
subroutine bloch_vectors_test (u, results)
```

```
integer, intent(in) :: u
```

```
type(test_results_t), intent(inout) :: results
```

⟨Bloch vectors: execute tests⟩

```
end subroutine bloch_vectors_test
```

Initialization

Initialize the Bloch vector for any spin type. First as unpolarized (no array), then as polarized but with zero polarization.

⟨Bloch vectors: execute tests⟩≡

```
call test (bloch_vectors_1, "bloch_vectors_1", &
```

```
"initialization", &
```

```
u, results)
```

⟨Bloch vectors: test declarations⟩≡

```
public :: bloch_vectors_1
```

⟨Bloch vectors: tests⟩≡

```
subroutine bloch_vectors_1 (u)
```

```
integer, intent(in) :: u
```

```
write (u, "(A)")  "* Test output: bloch_vectors_1"
```

```
write (u, "(A)")  "* Purpose: test Bloch-vector &
```

```
&polarization implementation"
```

```
write (u, "(A)")
```

```
write (u, "(A)")  "* Initialization (unpolarized)"
```

```
write (u, "(A)")
```

```
write (u, "(A)")  "* unknown"
```

```
call bloch_init (UNKNOWN)
```

```
write (u, "(A)")
```

```
write (u, "(A)")  "* s = 0"
```

```
call bloch_init (SCALAR)
```

```
write (u, "(A)")
```

```
write (u, "(A)")  "* s = 1/2"
```

```
call bloch_init (SPINOR)
```

```
write (u, "(A)")
```

```
write (u, "(A)")  "* s = 1"
```

```

call bloch_init (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call bloch_init (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call bloch_init (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_1"

contains

subroutine bloch_init (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  real(default), dimension(:), allocatable :: a
  integer :: i
  write (u, *)
  write (u, "(1X,L1,L1)", advance="no") &
    pol%is_defined (), pol%is_polarized ()
  call pol%init_unpolarized (s)
  write (u, "(1X,L1,L1)", advance="no") &
    pol%is_defined (), pol%is_polarized ()
  call pol%init (s)
  write (u, "(1X,L1,L1)", advance="no") &
    pol%is_defined (), pol%is_polarized ()
  write (u, *)
  call pol%to_array (a)
  if (allocated (a)) then
    write (u, "(*(F7.4))" ) a
    a(:) = [(real (mod (i, 10), kind=default), i = 1, size (a))]
    call pol%from_array (a)
    call pol%to_array (a)
    write (u, "(*(F7.4))" ) a
  else
    write (u, *)
    write (u, *)
  end if
end subroutine bloch_init

end subroutine bloch_vectors_1

```

Pure state (diagonal)

Initialize the Bloch vector with a pure state of definite helicity and check the normalization.

```

<Bloch vectors: execute tests>+=
  call test (bloch_vectors_2, "bloch_vectors_2", &
    "pure state (diagonal)", &

```

```

        u, results)
<Bloch vectors: test declarations>+=
    public :: bloch_vectors_2
<Bloch vectors: tests>+=
    subroutine bloch_vectors_2 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: bloch_vectors_2"
        write (u, "(A)")  "*   Purpose: test Bloch-vector &
            &polarization implementation"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization (polarized, diagonal): &
            &display vector and norm"
        write (u, "(A)")  "*   transform back"

        write (u, "(A)")
        write (u, "(A)")  "* s = 0"
        call bloch_diagonal (SCALAR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1/2"
        call bloch_diagonal (SPINOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1"
        call bloch_diagonal (VECTOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 3/2"
        call bloch_diagonal (VECTORSPINOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 2"
        call bloch_diagonal (TENSOR)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: bloch_vectors_2"

```

contains

```

    subroutine bloch_diagonal (s)
        integer, intent(in) :: s
        type(bloch_vector_t) :: pol
        real(default), dimension(:), allocatable :: a
        real(default), dimension(:), allocatable :: rd
        complex(default), dimension(:,:), allocatable :: r
        integer :: i, j, d
        real(default) :: rj
        real, parameter :: tolerance = 1.E-14_default
        d = fundamental_dimension (s)
        do i = 1, d
            allocate (rd (d), source = 0._default)

```



```

        rd(i) = 1
        call pol%init (s, rd)
        call pol%to_array (a)
        write (u, *)
        write (u, "(A,1X,I2)") "h:", helicity_value (s, i)
        write (u, 1, advance="no") a
        write (u, "(1X,L1)") pol%is_diagonal ()
        write (u, 1) pol%get_norm ()
        call pol%to_matrix (r)
        do j = 1, d
            rj = real (r(j,j))
            if (abs (rj) < tolerance) rj = 0
            write (u, 1, advance="no") rj
        end do
        write (u, "(1X,L1)") matrix_is_diagonal (r)
        deallocate (a, rd, r)
    end do
1    format (99(1X,F7.4,:))
end subroutine bloch_diagonal

function matrix_is_diagonal (r) result (diagonal)
    complex(default), dimension(:,:), intent(in) :: r
    logical :: diagonal
    integer :: i, j
    diagonal = .true.
    do j = 1, size (r, 2)
        do i = 1, size (r, 1)
            if (i == j) cycle
            if (r(i,j) /= 0) then
                diagonal = .false.
                return
            end if
        end do
    end do
end function matrix_is_diagonal

end subroutine bloch_vectors_2

```

Pure state (arbitrary)

Initialize the Bloch vector with an arbitrarily chosen pure state, check the normalization, and transform back to the density matrix.

```

<Bloch vectors: execute tests>+≡
    call test (bloch_vectors_3, "bloch_vectors_3", &
        "pure state (arbitrary)", &
        u, results)

<Bloch vectors: test declarations>+≡
    public :: bloch_vectors_3

<Bloch vectors: tests>+≡
    subroutine bloch_vectors_3 (u)
        integer, intent(in) :: u

```

```

write (u, "(A)")  "* Test output: bloch_vectors_3"
write (u, "(A)")  "* Purpose: test Bloch-vector &
                  &polarization implementation"
write (u, "(A)")

write (u, "(A)")  "* Initialization (pure polarized, arbitrary):"
write (u, "(A)")  "* input matrix, transform, display norm, transform back"

write (u, "(A)")
write (u, "(A)")  "* s = 0"
call bloch_arbitrary (SCALAR)

write (u, "(A)")
write (u, "(A)")  "* s = 1/2"
call bloch_arbitrary (SPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call bloch_arbitrary (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call bloch_arbitrary (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call bloch_arbitrary (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_3"

contains

subroutine bloch_arbitrary (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  complex(default), dimension(:,:), allocatable :: r
  integer :: d
  d = fundamental_dimension (s)
  write (u, *)
  call init_matrix (d, r)
  call write_matrix (d, r)
  call pol%init (s, r)
  write (u, *)
  write (u, 2) pol%get_norm (), pol%is_diagonal ()
  write (u, *)
  call pol%to_matrix (r)
  call write_matrix (d, r)
2  format (1X,F7.4,1X,L1)
end subroutine bloch_arbitrary

subroutine init_matrix (d, r)
  integer, intent(in) :: d

```

```

        complex(default), dimension(:,:), allocatable, intent(out) :: r
        complex(default), dimension(:), allocatable :: a
        real(default) :: norm
        integer :: i, j
        allocate (a (d))
        norm = 0
        do i = 1, d
            a(i) = cmplx (2*i-1, 2*i, kind=default)
            norm = norm + conjg (a(i)) * a(i)
        end do
        a = a / sqrt (norm)
        allocate (r (d,d))
        do i = 1, d
            do j = 1, d
                r(i,j) = conjg (a(i)) * a(j)
            end do
        end do
    end subroutine init_matrix

    subroutine write_matrix (d, r)
        integer, intent(in) :: d
        complex(default), dimension(:,:), intent(in) :: r
        integer :: i, j
        do i = 1, d
            do j = 1, d
                write (u, 1, advance="no") r(i,j)
            end do
            write (u, *)
        end do
1      format (99(1X, '(,F7.4,',',F7.4,')',:))
    end subroutine write_matrix

end subroutine bloch_vectors_3

```

Raw I/O

Check correct input/output in raw format.

```

<Bloch vectors: execute tests>+≡
    call test (bloch_vectors_4, "bloch_vectors_4", &
        "raw I/O", &
        u, results)

<Bloch vectors: test declarations>+≡
    public :: bloch_vectors_4

<Bloch vectors: tests>+≡
    subroutine bloch_vectors_4 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: bloch_vectors_4"
        write (u, "(A)")  "* Purpose: test Bloch-vector &
            &polarization implementation"
        write (u, "(A)")

```

```

write (u, "(A)")  "* Raw I/O"

write (u, "(A)")
write (u, "(A)")  "* s = 0"
call bloch_io (SCALAR)

write (u, "(A)")
write (u, "(A)")  "* s = 1/2"
call bloch_io (SPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call bloch_io (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call bloch_io (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call bloch_io (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_4"

contains

subroutine bloch_io (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  real(default), dimension(:), allocatable :: a
  integer :: n, i, utmp, iostat
  n = algebra_dimension (s)
  allocate (a (n))
  a(:) = [(real (mod (i, 10), kind=default), i = 1, size (a))]
  write (u, *)
  write (u, "(*(F7.4))") a
  call pol%init (s)
  call pol%from_array (a)
  open (newunit = utmp, status = "scratch", action = "readwrite", &
    form = "unformatted")
  call pol%write_raw (utmp)
  rewind (utmp)
  call pol%read_raw (utmp, iostat=iostat)
  close (utmp)
  call pol%to_array (a)
  write (u, "(*(F7.4))") a
end subroutine bloch_io

end subroutine bloch_vectors_4

```

Convenience Methods

Check some further TBP that are called by the polarizations module.

```
(Bloch vectors: execute tests)+≡
    call test (bloch_vectors_5, "bloch_vectors_5", &
        "massless state (unpolarized)", &
        u, results)

(Bloch vectors: test declarations)+≡
    public :: bloch_vectors_5

(Bloch vectors: tests)+≡
    subroutine bloch_vectors_5 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: bloch_vectors_5"
        write (u, "(A)")  "* Purpose: test Bloch-vector &
            &polarization implementation"
        write (u, "(A)")

        write (u, "(A)")  "* Massless states: equipartition"

        write (u, "(A)")
        write (u, "(A)")  "* s = 0"
        call bloch_massless_unpol (SCALAR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1/2"
        call bloch_massless_unpol (SPINOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1"
        call bloch_massless_unpol (VECTOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 3/2"
        call bloch_massless_unpol (VECTORSPINOR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 2"
        call bloch_massless_unpol (TENSOR)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: bloch_vectors_5"

contains

    subroutine bloch_massless_unpol (s)
        integer, intent(in) :: s
        type(bloch_vector_t) :: pol
        complex(default), dimension(:,:), allocatable :: r
        real(default), dimension(:), allocatable :: a
        integer :: d
        d = fundamental_dimension (s)
        call pol%init_max_weight (s)
```

```

        call pol%to_matrix (r, only_max_weight = .false.)
        write (u, *)
        where (abs (r) < 1.e-14_default) r = 0
        call write_matrix (d, r)
        call pol%to_matrix (r, only_max_weight = .true.)
        write (u, *)
        call write_matrix (d, r)
    end subroutine bloch_massless_unpol

    subroutine write_matrix (d, r)
        integer, intent(in) :: d
        complex(default), dimension(:,:), intent(in) :: r
        integer :: i, j
        do i = 1, d
            do j = 1, d
                write (u, 1, advance="no") r(i,j)
            end do
            write (u, *)
        end do
1      format (99(1X,'(',F7.4,',',F7.4,')',:))
    end subroutine write_matrix

end subroutine bloch_vectors_5

```

Massless state (arbitrary)

Initialize the Bloch vector with an arbitrarily chosen pure state which consists only of highest-weight components. Transform back to the density matrix.

```

<Bloch vectors: execute tests>+≡
    call test (bloch_vectors_6, "bloch_vectors_6", &
        "massless state (arbitrary)", &
        u, results)

<Bloch vectors: test declarations>+≡
    public :: bloch_vectors_6

<Bloch vectors: tests>+≡
    subroutine bloch_vectors_6 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: bloch_vectors_6"
        write (u, "(A)")  "* Purpose: test Bloch-vector &
            &polarization implementation"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization (pure polarized massless, arbitrary):"
        write (u, "(A)")  "* input matrix, transform, display norm, transform back"

        write (u, "(A)")
        write (u, "(A)")  "* s = 0"
        call bloch_massless (SCALAR)

        write (u, "(A)")
    end subroutine bloch_vectors_6

```

```

write (u, "(A)")  "* s = 1/2"
call bloch_massless (SPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call bloch_massless (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call bloch_massless (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call bloch_massless (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_6"

contains

subroutine bloch_massless (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  complex(default), dimension(:,:), allocatable :: r
  integer :: d
  d = fundamental_dimension (s)
  write (u, *)
  call init_matrix (d, r)
  call write_matrix (d, r)
  call pol%init (s, r)
  write (u, *)
  write (u, 2)  pol%get_norm (), pol%is_diagonal ()
  write (u, *)
  call pol%to_matrix (r, only_max_weight = .true.)
  call write_matrix (d, r)
2   format (1X,F7.4,1X,L1)
end subroutine bloch_massless

subroutine init_matrix (d, r)
  integer, intent(in) :: d
  complex(default), dimension(:,:), allocatable, intent(out) :: r
  complex(default), dimension(:), allocatable :: a
  real(default) :: norm
  integer :: i, j
  allocate (a (d), source = (0._default, 0._default))
  norm = 0
  do i = 1, d, max (d-1, 1)
    a(i) = cmplx (2*i-1, 2*i, kind=default)
    norm = norm + conjg (a(i)) * a(i)
  end do
  a = a / sqrt (norm)
  allocate (r (d,d), source = (0._default, 0._default))
  do i = 1, d, max (d-1, 1)
    do j = 1, d, max (d-1, 1)

```

```

        r(i,j) = conjg (a(i)) * a(j)
    end do
end do
end subroutine init_matrix

subroutine write_matrix (d, r)
    integer, intent(in) :: d
    complex(default), dimension(:,:), intent(in) :: r
    integer :: i, j
    do i = 1, d
        do j = 1, d
            write (u, 1, advance="no") r(i,j)
        end do
        write (u, *)
    end do
1    format (99(1X,'( ',F7.4,', ',F7.4,')',:))
end subroutine write_matrix

end subroutine bloch_vectors_6

```

Massless state (Bloch vector)

Initialize the (generalized) Bloch vector with an ordinary three-component Bloch vector that applies to the highest-weight part only.

```

<Bloch vectors: execute tests>+≡
    call test (bloch_vectors_7, "bloch_vectors_7", &
        "massless state (vector)", &
        u, results)

<Bloch vectors: test declarations>+≡
    public :: bloch_vectors_7

<Bloch vectors: tests>+≡
    subroutine bloch_vectors_7 (u)
        integer, intent(in) :: u

        write (u, "(A)")  "* Test output: bloch_vectors_7"
        write (u, "(A)")  "* Purpose: test Bloch-vector &
            &polarization implementation"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization &
            &(pure polarized massless, arbitrary Bloch vector):"
        write (u, "(A)")  "* input vector, transform, display norm, &
            &transform back"

        write (u, "(A)")
        write (u, "(A)")  "* s = 0"
        call bloch_massless_vector (SCALAR)

        write (u, "(A)")
        write (u, "(A)")  "* s = 1/2"
        call bloch_massless_vector (SPINOR)
    end subroutine

```



```

write (u, "(A)")
write (u, "(A)")  "* s = 1"
call bloch_massless_vector (VECTOR)

write (u, "(A)")
write (u, "(A)")  "* s = 3/2"
call bloch_massless_vector (VECTORSPINOR)

write (u, "(A)")
write (u, "(A)")  "* s = 2"
call bloch_massless_vector (TENSOR)

write (u, "(A)")
write (u, "(A)")  "* Test output end: bloch_vectors_7"

contains

subroutine bloch_massless_vector (s)
  integer, intent(in) :: s
  type(bloch_vector_t) :: pol
  real(default), dimension(3) :: a
  complex(default), dimension(:,:), allocatable :: r
  write (u, *)
  a = [1._default, 2._default, 4._default]
  a = a / sqrt (sum (a ** 2))
  write (u, 2)  a
  call pol%init_vector (s, a)
  write (u, 2)  pol%get_norm ()
  call pol%to_vector (a)
  write (u, 2)  a
  call pol%to_matrix (r, only_max_weight = .false.)
  write (u, *)
  where (abs (r) < 1.e-14_default) r = 0
  call write_matrix (r)
  call pol%to_matrix (r, only_max_weight = .true.)
  write (u, *)
  call write_matrix (r)
2   format (99(1X,F7.4,:))
end subroutine bloch_massless_vector

subroutine write_matrix (r)
  complex(default), dimension(:,:), intent(in) :: r
  integer :: i, j
  do i = 1, size (r, 1)
    do j = 1, size (r, 2)
      write (u, 1, advance="no") r(i,j)
    end do
    write (u, *)
  end do
1   format (99(1X,'(,F7.4,',',F7.4,')',:))
end subroutine write_matrix

end subroutine bloch_vectors_7

```


15.3 Polarization

Using generalized Bloch vectors and the $su(N)$ algebra (see above) for the internal representation, we can define various modes of polarization. For spin-1/2, and analogously for massless spin- s particles, we introduce

1. Trivial polarization: $\vec{\alpha} = 0$. [This is unpolarized, but distinct from the particular undefined polarization matrix which has the same meaning.]
2. Circular polarization: $\vec{\alpha}$ points in $\pm z$ direction.
3. Transversal polarization: $\vec{\alpha}$ points orthogonal to the z direction, with a phase ϕ that is 0 for the x axis, and $\pi/2 = 90^\circ$ for the y axis. For antiparticles, the phase switches sign, corresponding to complex conjugation.
4. Axis polarization, where we explicitly give $\vec{\alpha}$.

For higher spin, we retain this definition, but apply it to the two components with maximum and minimum weight. In effect, we concentrate on the first three entries in the α^a array. For massless particles, this is sufficient. For massive particles, we then add the possibilities:

5. Longitudinal polarization: Only the 0-component is set. This is possible only for bosons.
6. Diagonal polarization: Explicitly specify all components in the helicity basis. The $su(N)$ representation consists of diagonal generators only, the Cartan subalgebra.

Obviously, this does not exhaust the possible density matrices for higher spin, but it should cover practical applications.

`<polarizations.f90>`≡
<File header>

`module polarizations`

<Use kinds>

```

use io_units
use format_defs, only: FMT_19
use diagnostics
use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
use flavors
use helicities
use quantum_numbers
use state_matrices
use bloch_vectors
```

<Standard module head>

<Polarizations: public>

<Polarizations: types>

<Polarizations: interfaces>

```
contains

<Polarizations: procedures>

end module polarizations
```

15.3.1 The polarization type

Polarization is active whenever the coefficient array is allocated. For convenience, we store the spin type ($2s$) and the multiplicity (N) together with the coefficient array (α). We have to allow for the massless case where s is arbitrary > 0 but $N = 2$, and furthermore the chiral massless case where $N = 1$. In the latter case, the array remains deallocated but the chirality is set to ± 1 .

There is a convention that an antiparticle transforms according to the complex conjugate representation. We apply this only when transforming from/to polarization defined by a three-vector. For antiparticles, the two-component flips sign in that case. When transforming from/to a state matrix or `pmatrix` representation, we do not apply this sign flip.

```
<Polarizations: public>≡
    public :: polarization_t

<Polarizations: types>≡
    type :: polarization_t
        private
        integer :: spin_type = SCALAR
        integer :: multiplicity = 1
        integer :: chirality = 0
        logical :: anti = .false.
        type(bloch_vector_t) :: bv
    contains
    <Polarizations: polarization: TBP>
end type polarization_t
```

15.3.2 Basic initializer and finalizer

We need the particle flavor for determining the allowed helicity values. The Bloch vector is left undefined, so this initializer (in two versions) creates an unpolarized particle. Exception: a chiral particle is always polarized with definite helicity, it doesn't need a Bloch vector.

This is private.

```
<Polarizations: polarization: TBP>≡
    generic, private :: init => polarization_init, polarization_init_flv
    procedure, private :: polarization_init
    procedure, private :: polarization_init_flv

<Polarizations: procedures>≡
    subroutine polarization_init (pol, spin_type, multiplicity, &
        anti, left_handed, right_handed)
        class(polarization_t), intent(out) :: pol
        integer, intent(in) :: spin_type
        integer, intent(in) :: multiplicity
```

```

logical, intent(in) :: anti
logical, intent(in) :: left_handed
logical, intent(in) :: right_handed
pol%spin_type = spin_type
pol%multiplicity = multiplicity
pol%anti = anti
select case (pol%multiplicity)
case (1)
  if (left_handed) then
    pol%chirality = -1
  else if (right_handed) then
    pol%chirality = 1
  end if
end select
select case (pol%chirality)
case (0)
  call pol%bv%init_unpolarized (spin_type)
end select
end subroutine polarization_init

subroutine polarization_init_flv (pol, flv)
class(polarization_t), intent(out) :: pol
type(flavor_t), intent(in) :: flv
call pol%init ( &
  spin_type = flv%get_spin_type (), &
  multiplicity = flv%get_multiplicity (), &
  anti = flv%is_antiparticle (), &
  left_handed = flv%is_left_handed (), &
  right_handed = flv%is_right_handed ())
end subroutine polarization_init_flv

```

Generic polarization: as before, but create a polarized particle (Bloch vector defined) with initial polarization zero.

```

(Polarizations: polarization: TBP)+≡
generic :: init_generic => &
  polarization_init_generic, &
  polarization_init_generic_flv
procedure, private :: polarization_init_generic
procedure, private :: polarization_init_generic_flv

(Polarizations: procedures)+≡
subroutine polarization_init_generic (pol, spin_type, multiplicity, &
  anti, left_handed, right_handed)
class(polarization_t), intent(out) :: pol
integer, intent(in) :: spin_type
integer, intent(in) :: multiplicity
logical, intent(in) :: anti
logical, intent(in) :: left_handed
logical, intent(in) :: right_handed
call pol%init (spin_type, multiplicity, &
  anti, left_handed, right_handed)
select case (pol%chirality)
case (0)
  if (pol%multiplicity == pol%bv%get_n_states ()) then

```

```

        call pol%bv%init (spin_type)
      else
        call pol%bv%init_max_weight (spin_type)
      end if
    end select
  end subroutine polarization_init_generic

  subroutine polarization_init_generic_flv (pol, flv)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    call pol%init_generic ( &
      spin_type = flv%get_spin_type (), &
      multiplicity = flv%get_multiplicity (), &
      anti = flv%is_antiparticle (), &
      left_handed = flv%is_left_handed (), &
      right_handed = flv%is_right_handed ()
    )
  end subroutine polarization_init_generic_flv

```

A finalizer is no longer necessary.

15.3.3 I/O

The default setting produces a tabular output of the polarization vector entries. Optionally, we can create a state matrix and write its contents, emulating the obsolete original implementation.

If `all_states` is true (default), we generate all helicity combinations regardless of the matrix-element value. Otherwise, skip helicities with zero entry, or absolute value less than `tolerance`, if also given.

```

<Polarizations: polarization: TBP>+≡
  procedure :: write => polarization_write

<Polarizations: procedures>+≡
  subroutine polarization_write (pol, unit, state_matrix, all_states, tolerance)
    class(polarization_t), intent(in) :: pol
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: state_matrix, all_states
    real(default), intent(in), optional :: tolerance
    logical :: state_m
    type(state_matrix_t) :: state
    real(default), dimension(:), allocatable :: a
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    state_m = .false.; if (present (state_matrix)) state_m = state_matrix
    if (pol%anti) then
      write (u, "(1x,A,I1,A,I1,A,L1,A)") &
        "Polarization: [spin_type = ", pol%spin_type, &
        ", mult = ", pol%multiplicity, ", anti = ", pol%anti, "]"
    else
      write (u, "(1x,A,I1,A,I1,A)") &
        "Polarization: [spin_type = ", pol%spin_type, &
        ", mult = ", pol%multiplicity, "]"
    end if
    if (state_m) then

```

```

        call pol%to_state (state, all_states, tolerance)
        call state%write (unit=unit)
        call state%final ()
    else if (pol%chirality == 1) then
        write (u, "(1x,A)" "chirality = +"
    else if (pol%chirality == -1) then
        write (u, "(1x,A)" "chirality = -"
    else if (pol%bv%is_polarized ()) then
        call pol%bv%to_array (a)
        do i = 1, size (a)
            write (u, "(1x,I2,':',1x,F10.7)" i, a(i)
        end do
    else
        write (u, "(1x,A)" "[unpolarized]"
    end if
end subroutine polarization_write

```

Binary I/O.

```

(Polarizations: polarization: TBP)+≡
    procedure :: write_raw => polarization_write_raw
    procedure :: read_raw => polarization_read_raw

(Polarizations: procedures)+≡
    subroutine polarization_write_raw (pol, u)
        class(polarization_t), intent(in) :: pol
        integer, intent(in) :: u
        write (u) pol%spin_type
        write (u) pol%multiplicity
        write (u) pol%chirality
        write (u) pol%anti
        call pol%bv%write_raw (u)
    end subroutine polarization_write_raw

    subroutine polarization_read_raw (pol, u, iostat)
        class(polarization_t), intent(out) :: pol
        integer, intent(in) :: u
        integer, intent(out), optional :: iostat
        read (u, iostat=iostat) pol%spin_type
        read (u, iostat=iostat) pol%multiplicity
        read (u, iostat=iostat) pol%chirality
        read (u, iostat=iostat) pol%anti
        call pol%bv%read_raw (u, iostat)
    end subroutine polarization_read_raw

```

15.3.4 Accessing contents

Return true if the particle is technically polarized. The particle is either chiral, or its Bloch vector has been defined. The function returns true even if the Bloch vector is zero or the particle is scalar.

```

(Polarizations: polarization: TBP)+≡
    procedure :: is_polarized => polarization_is_polarized

```

```

(Polarizations: procedures)+≡
function polarization_is_polarized (pol) result (polarized)
  class(polarization_t), intent(in) :: pol
  logical :: polarized
  polarized = pol%chirality /= 0 .or. pol%bv%is_polarized ()
end function polarization_is_polarized

```

Return true if the polarization is diagonal, i.e., all entries in the density matrix are diagonal. For an unpolarized particle, we also return `.true.` since the density matrix is proportional to the unit matrix.

```

(Polarizations: polarization: TBP)+≡
  procedure :: is_diagonal => polarization_is_diagonal

(Polarizations: procedures)+≡
function polarization_is_diagonal (pol) result (diagonal)
  class(polarization_t), intent(in) :: pol
  logical :: diagonal
  select case (pol%chirality)
  case (0)
    diagonal = pol%bv%is_diagonal ()
  case default
    diagonal = .true.
  end select
end function polarization_is_diagonal

```

15.3.5 Mapping between polarization and state matrix

Create the polarization object that corresponds to a state matrix. The state matrix is not necessarily normalized. The result will be either unpolarized, or a generalized Bloch vector that we compute in terms of the appropriate spin generator basis. To this end, we first construct the complete density matrix, then set the Bloch vector with this input.

For a naturally chiral particle (i.e., neutrino), we do not set the polarization vector, it is implied.

Therefore, we cannot account for any sign flip and transform as-is.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_state_matrix => polarization_init_state_matrix

(Polarizations: procedures)+≡
subroutine polarization_init_state_matrix (pol, state)
  class(polarization_t), intent(out) :: pol
  type(state_matrix_t), intent(in), target :: state
  type(state_iterator_t) :: it
  type(flavor_t) :: flv
  type(helicity_t) :: hel
  integer :: d, h1, h2, i, j
  complex(default), dimension(:,,:), allocatable :: r
  complex(default) :: me
  real(default) :: trace
  call it%init (state)
  flv = it%get_flavor (1)
  hel = it%get_helicity (1)

```



```

if (hel%is_defined ()) then
  call pol%init_generic (flv)
  select case (pol%chirality)
  case (0)
    trace = 0
    d = pol%bv%get_n_states ()
    allocate (r (d, d), source = (0._default, 0._default))
    do while (it%is_valid ())
      hel = it%get_helicity (1)
      call hel%get_indices (h1, h2)
      i = pol%bv%hel_index (h1)
      j = pol%bv%hel_index (h2)
      me = it%get_matrix_element ()
      r(i,j) = me
      if (i == j) trace = trace + real (me)
      call it%advance ()
    end do
    if (trace /= 0) call pol%bv%set (r / trace)
  end select
else
  call pol%init (flv)
end if
end subroutine polarization_init_state_matrix

```

Create the state matrix that corresponds to a given polarization. We make use of the polarization iterator as defined below, which should iterate according to the canonical helicity ordering.

(Polarizations: polarization: TBP)+≡

```

procedure :: to_state => polarization_to_state_matrix

```

(Polarizations: procedures)+≡

```

subroutine polarization_to_state_matrix (pol, state, all_states, tolerance)
  class(polarization_t), intent(in), target :: pol
  type(state_matrix_t), intent(out) :: state
  logical, intent(in), optional :: all_states
  real(default), intent(in), optional :: tolerance
  type(polarization_iterator_t) :: it
  type(quantum_numbers_t), dimension(1) :: qn
  complex(default) :: value
  call it%init (pol, all_states, tolerance)
  call state%init (store_values = .true.)
  do while (it%is_valid ())
    value = it%get_value ()
    qn(1) = it%get_quantum_numbers ()
    call state%add_state (qn, value = value)
    call it%advance ()
  end do
  call state%freeze ()
end subroutine polarization_to_state_matrix

```

15.3.6 Specific initializers

Unpolarized particle, no nontrivial entries in the density matrix. This is the default initialization mode.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_unpolarized => polarization_init_unpolarized
(Polarizations: procedures)+≡
  subroutine polarization_init_unpolarized (pol, flv)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    call pol%init (flv)
  end subroutine polarization_init_unpolarized

```

The following three modes are useful mainly for spin-1/2 particle and massless particles of any nonzero spin. Only the highest-weight components are filled.

Circular polarization: The density matrix of the two highest-weight states is

$$\rho(f) = \frac{1 - |f|}{2} \mathbf{1} + |f| \times \begin{cases} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, & f > 0; \\ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, & f < 0, \end{cases}$$

In the generalized Bloch representation, this is an entry for the T^3 generator only, regardless of the spin representation.

A chiral particle is not affected.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_circular => polarization_init_circular
(Polarizations: procedures)+≡
  subroutine polarization_init_circular (pol, flv, f)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: f
    call pol%init (flv)
    select case (pol%chirality)
    case (0)
      call pol%bv%init_vector (pol%spin_type, &
        [0._default, 0._default, f])
    end select
  end subroutine polarization_init_circular

```

Transversal polarization is analogous to circular, but we get a density matrix

$$\rho(f, \phi) = \frac{1 - |f|}{2} \mathbf{1} + \frac{|f|}{2} \begin{pmatrix} 1 & e^{-i\phi} \\ e^{i\phi} & 1 \end{pmatrix}.$$

for the highest-weight subspace. The lower weights are unaffected. The phase is $\phi = 0$ for the x -axis, $\phi = 90^\circ$ for the y axis as polarization vector.

For an antiparticle, the phase switches sign, and for $f < 0$, the off-diagonal elements switch sign.

A chiral particle is not affected.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_transversal => polarization_init_transversal

```

```

(Polarizations: procedures)+≡
subroutine polarization_init_transversal (pol, flv, phi, f)
  class(polarization_t), intent(out) :: pol
  type(flavor_t), intent(in) :: flv
  real(default), intent(in) :: phi, f
  call pol%init (flv)
  select case (pol%chirality)
  case (0)
    if (pol%anti) then
      call pol%bv%init_vector (pol%spin_type, &
        [f * cos (phi), f * sin (phi), 0._default])
    else
      call pol%bv%init_vector (pol%spin_type, &
        [f * cos (phi), -f * sin (phi), 0._default])
    end if
  end select
end subroutine polarization_init_transversal

```

For axis polarization, we again set only the entries with maximum weight, which for spin 1/2 means

$$\rho(f, \phi) = \frac{1}{2} \begin{pmatrix} 1 + \alpha_3 & \alpha_1 - i\alpha_2 \\ \alpha_1 + i\alpha_2 & 1 - \alpha_3 \end{pmatrix}.$$

For an antiparticle, the imaginary part proportional to α_2 switches sign (complex conjugate). A chiral particle is not affected.

In the generalized Bloch representation, this translates into coefficients for $T^{1,2,3}$, all others stay zero.

```

(Polarizations: polarization: TBP)+≡
procedure :: init_axis => polarization_init_axis

(Polarizations: procedures)+≡
subroutine polarization_init_axis (pol, flv, alpha)
  class(polarization_t), intent(out) :: pol
  type(flavor_t), intent(in) :: flv
  real(default), dimension(3), intent(in) :: alpha
  call pol%init (flv)
  select case (pol%chirality)
  case (0)
    if (pol%anti) then
      call pol%bv%init_vector (pol%spin_type, &
        [alpha(1), alpha(2), alpha(3)])
    else
      call pol%bv%init_vector (pol%spin_type, &
        [alpha(1), -alpha(2), alpha(3)])
    end if
  end select
end subroutine polarization_init_axis

```

This version specifies the polarization axis in terms of r (polarization degree) and θ, ϕ (polar and azimuthal angles).

If one of the angles is a nonzero multiple of π , roundoff errors typically will result in tiny contributions to unwanted components. Therefore, include a catch

for small numbers.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_angles => polarization_init_angles

(Polarizations: procedures)+≡
  subroutine polarization_init_angles (pol, flv, r, theta, phi)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: r, theta, phi
    real(default), dimension(3) :: alpha
    real(default), parameter :: eps = 10 * epsilon (1._default)

    alpha(1) = r * sin (theta) * cos (phi)
    alpha(2) = r * sin (theta) * sin (phi)
    alpha(3) = r * cos (theta)
    where (abs (alpha) < eps) alpha = 0
    call pol%init_axis (flv, alpha)
  end subroutine polarization_init_angles

```

Longitudinal polarization is defined only for massive bosons. Only the zero component is filled. Otherwise, unpolarized.

In the generalized Bloch representation, the zero component corresponds to a linear combination of all diagonal (Cartan) generators.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_longitudinal => polarization_init_longitudinal

(Polarizations: procedures)+≡
  subroutine polarization_init_longitudinal (pol, flv, f)
    class(polarization_t), intent(out) :: pol
    type(flavor_t), intent(in) :: flv
    real(default), intent(in) :: f
    real(default), dimension(:), allocatable :: rd
    integer :: s, d
    s = flv%get_spin_type ()
    select case (s)
    case (VECTOR, TENSOR)
      call pol%init_generic (flv)
      if (pol%bv%is_polarized ()) then
        d = pol%bv%get_n_states ()
        allocate (rd (d), source = 0._default)
        rd(pol%bv%hel_index (0)) = f
        call pol%bv%set (rd)
      end if
    case default
      call pol%init_unpolarized (flv)
    end select
  end subroutine polarization_init_longitudinal

```

This is diagonal polarization: we specify all components explicitly. `rd` is the array of diagonal elements of the density matrix. We assume that the length of `rd` is equal to the particle multiplicity.

```

(Polarizations: polarization: TBP)+≡
  procedure :: init_diagonal => polarization_init_diagonal

```

```

<Polarizations: procedures>+≡
subroutine polarization_init_diagonal (pol, flv, rd)
  class(polarization_t), intent(out) :: pol
  type(flavor_t), intent(in) :: flv
  real(default), dimension(:), intent(in) :: rd
  real(default) :: trace
  call pol%init_generic (flv)
  if (pol%bv%is_polarized ()) then
    trace = sum (rd)
    if (trace /= 0) call pol%bv%set (rd / trace)
  end if
end subroutine polarization_init_diagonal

```

15.3.7 Operations

Combine polarization states by computing the outer product of the state matrices.

```

<Polarizations: public>+≡
public :: combine_polarization_states

<Polarizations: procedures>+≡
subroutine combine_polarization_states (pol, state)
  type(polarization_t), dimension(:), intent(in), target :: pol
  type(state_matrix_t), intent(out) :: state
  type(state_matrix_t), dimension(size(pol)), target :: pol_state
  integer :: i
  do i = 1, size (pol)
    call pol(i)%to_state (pol_state(i))
  end do
  call outer_multiply (pol_state, state)
  do i = 1, size (pol)
    call pol_state(i)%final ()
  end do
end subroutine combine_polarization_states

```

Transform a polarization density matrix into a polarization vector. This is possible without information loss only for spin-1/2 and for massless particles. To get a unique answer in all cases, we consider only the components with highest weight. Obviously, this loses the longitudinal component of a massive vector, for instance. The norm of the returned axis is the polarization fraction for the highest-weight subspace. For a scalar particle, we return a zero vector. The same result applies if the highest-weight component vanishes.

This is the inverse operation of `polarization_init_axis` above, where the polarization fraction is set to unity.

For an antiparticle, the `alpha(2)` coefficient flips sign.

```

<Polarizations: polarization: TBP>+≡
procedure :: get_axis => polarization_get_axis

<Polarizations: procedures>+≡
function polarization_get_axis (pol) result (alpha)
  class(polarization_t), intent(in), target :: pol
  real(default), dimension(3) :: alpha

```

```

select case (pol%chirality)
case (0)
  call pol%bv%to_vector (alpha)
  if (.not. pol%anti) alpha(2) = - alpha(2)
case (-1)
  alpha = [0._default, 0._default, -1._default]
case (1)
  alpha = [0._default, 0._default, 1._default]
end select
end function polarization_get_axis

```

This function returns polarization degree and polar and azimuthal angles (θ, ϕ) of the polarization axis. The same restrictions apply as above.

Since we call the `get_axis` method, the phase flips sign for an antiparticle.

```

<Polarizations: polarization: TBP>+≡
  procedure :: to_angles => polarization_to_angles
<Polarizations: procedures>+≡
  subroutine polarization_to_angles (pol, r, theta, phi)
    class(polarization_t), intent(in) :: pol
    real(default), intent(out) :: r, theta, phi
    real(default), dimension(3) :: alpha
    real(default) :: norm, r12
    alpha = pol%get_axis ()
    norm = sum (alpha**2)
    r = sqrt (norm)
    if (norm > 0) then
      r12 = sqrt (alpha(1)**2 + alpha(2)**2)
      theta = atan2 (r12, alpha(3))
      if (any (alpha(1:2) /= 0)) then
        phi = atan2 (alpha(2), alpha(1))
      else
        phi = 0
      end if
    else
      theta = 0
      phi = 0
    end if
  end subroutine polarization_to_angles

```

15.3.8 Polarization Iterator

The iterator acts like a state matrix iterator, i.e., it points to one helicity combination at a time and can return the corresponding helicity object and matrix-element value.

Since the polarization is stored as a Bloch vector, we recover the whole density matrix explicitly upon initialization, store it inside the iterator object, and then just return its elements one at a time.

For an unpolarized particle, the iterator returns a single state with undefined helicity. The value is the value of any diagonal density matrix element, $1/n$ where n is the multiplicity.

```

<Polarizations: public>+≡

```

```

public :: polarization_iterator_t
<Polarizations: types>+≡
type :: polarization_iterator_t
private
type(polarization_t), pointer :: pol => null ()
logical :: polarized = .false.
integer :: h1 = 0
integer :: h2 = 0
integer :: i = 0
integer :: j = 0
complex(default), dimension(:, :), allocatable :: r
complex(default) :: value = 1._default
real(default) :: tolerance = -1._default
logical :: valid = .false.
contains
<Polarizations: polarization iterator: TBP>
end type polarization_iterator_t

```

Output for debugging purposes only, therefore no format for real/complex.

```

<Polarizations: polarization iterator: TBP>≡
procedure :: write => polarization_iterator_write
<Polarizations: procedures>+≡
subroutine polarization_iterator_write (it, unit)
class(polarization_iterator_t), intent(in) :: it
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit)
write (u, "(1X,A)") "Polarization iterator:"
write (u, "(3X,A,L1)") "assigned = ", associated (it%pol)
write (u, "(3X,A,L1)") "valid    = ", it%valid
if (it%valid) then
write (u, "(3X,A,2(1X,I2))") "i, j    = ", it%i, it%j
write (u, "(3X,A,2(1X,I2))") "h1, h2  = ", it%h1, it%h2
write (u, "(3X,A)", advance="no") "value    = "
write (u, *) it%value
if (allocated (it%r)) then
do i = 1, size (it%r, 2)
write (u, *) it%r(i,:)
end do
end if
end if
end subroutine polarization_iterator_write

```

Initialize, i.e., (virtually) point to the first helicity state supported by the polarization object. If the density matrix is nontrivial, we calculate it here.

Following the older state-matrix conventions, the iterator sequence starts at the lowest helicity value. In the current internal representation, this corresponds to the highest index value.

If the current matrix-element value is zero, advance the iterator. Advancing will stop at a nonzero value or if the iterator becomes invalid.

If `tolerance` is given, any state matrix entry less or equal will be treated as zero, causing the iterator to skip an entry. By default, the value is negative, so no entry is skipped.

```

(Polarizations: polarization iterator: TBP)+≡
  procedure :: init => polarization_iterator_init

(Polarizations: procedures)+≡
  subroutine polarization_iterator_init (it, pol, all_states, tolerance)
    class(polarization_iterator_t), intent(out) :: it
    type(polarization_t), intent(in), target :: pol
    logical, intent(in), optional :: all_states
    real(default), intent(in), optional :: tolerance
    integer :: d
    logical :: only_max_weight
    it%pol => pol
    if (present (all_states)) then
      if (.not. all_states) then
        if (present (tolerance)) then
          it%tolerance = tolerance
        else
          it%tolerance = 0
        end if
      end if
    end if
    select case (pol%chirality)
    case (0)
      d = pol%bv%get_n_states ()
      only_max_weight = pol%multiplicity < d
      it%polarized = pol%bv%is_polarized ()
      if (it%polarized) then
        it%i = d
        it%j = it%i
        it%h1 = pol%bv%hel_value (it%i)
        it%h2 = it%h1
        call pol%bv%to_matrix (it%r, only_max_weight)
        it%value = it%r(it%i, it%j)
      else
        it%value = 1._default / d
      end if
      it%valid = .true.
    case (1,-1)
      it%polarized = .true.
      select case (pol%spin_type)
      case (SPINOR)
        it%h1 = pol%chirality
      case (VECTORSPINOR)
        it%h1 = 2 * pol%chirality
      end select
      it%h2 = it%h1
      it%valid = .true.
    end select
    if (it%valid .and. abs (it%value) <= it%tolerance) call it%advance ()
  end subroutine polarization_iterator_init

```


Advance to the next valid helicity state. Repeat if the returned value is zero.

For an unpolarized object, we iterate through the diagonal helicity states with a constant value.

```

(Polarizations: polarization iterator: TBP)+≡
  procedure :: advance => polarization_iterator_advance

(Polarizations: procedures)+≡
  recursive subroutine polarization_iterator_advance (it)
    class(polarization_iterator_t), intent(inout) :: it
    if (it%valid) then
      select case (it%pol%chirality)
      case (0)
        if (it%polarized) then
          if (it%j > 1) then
            it%j = it%j - 1
            it%h2 = it%pol%bv%hel_value (it%j)
            it%value = it%r(it%i, it%j)
          else if (it%i > 1) then
            it%j = it%pol%bv%get_n_states ()
            it%h2 = it%pol%bv%hel_value (it%j)
            it%i = it%i - 1
            it%h1 = it%pol%bv%hel_value (it%i)
            it%value = it%r(it%i, it%j)
          else
            it%valid = .false.
          end if
        else
          it%valid = .false.
        end if
      case default
        it%valid = .false.
      end select
      if (it%valid .and. abs (it%value) <= it%tolerance) call it%advance ()
    end if
  end subroutine polarization_iterator_advance

```

This is true as long as the iterator points to a valid helicity state.

```

(Polarizations: polarization iterator: TBP)+≡
  procedure :: is_valid => polarization_iterator_is_valid

(Polarizations: procedures)+≡
  function polarization_iterator_is_valid (it) result (is_valid)
    logical :: is_valid
    class(polarization_iterator_t), intent(in) :: it
    is_valid = it%valid
  end function polarization_iterator_is_valid

```

Return the matrix element value for the helicity that we are currently pointing at.

```

(Polarizations: polarization iterator: TBP)+≡
  procedure :: get_value => polarization_iterator_get_value

```

```

(Polarizations: procedures)+≡
function polarization_iterator_get_value (it) result (value)
  complex(default) :: value
  class(polarization_iterator_t), intent(in) :: it
  if (it%valid) then
    value = it%value
  else
    value = 0
  end if
end function polarization_iterator_get_value

```

Return a quantum number object for the helicity that we are currently pointing at. This is a single quantum number object, not an array.

Note that the `init` method of the helicity object has the order reversed.

```

(Polarizations: polarization_iterator: TBP)+≡
  procedure :: get_quantum_numbers => polarization_iterator_get_quantum_numbers

(Polarizations: procedures)+≡
function polarization_iterator_get_quantum_numbers (it) result (qn)
  class(polarization_iterator_t), intent(in) :: it
  type(helicity_t) :: hel
  type(quantum_numbers_t) :: qn
  if (it%polarized) then
    call hel%init (it%h2, it%h1)
  end if
  call qn%init (hel)
end function polarization_iterator_get_quantum_numbers

```

15.3.9 Sparse Matrix

We introduce a simple implementation of a sparse matrix that can represent polarization (or similar concepts) for transfer to I/O within the program. It consists of an integer array that represents the index values, and a complex array that represents the nonvanishing entries. The number of nonvanishing entries must be known for initialization, but the entries are filled one at a time.

Here is a base type without the special properties of a spin-density matrix.

```

(Polarizations: public)+≡
  public :: smatrix_t

(Polarizations: types)+≡
  type :: smatrix_t
    private
    integer :: dim = 0
    integer :: n_entry = 0
    integer, dimension(:,:), allocatable :: index
    complex(default), dimension(:), allocatable :: value
  contains
    (Polarizations: smatrix: TBP)
  end type smatrix_t

```

Output.

```

(Polarizations: smatrix: TBP)≡
  procedure :: write => smatrix_write

(Polarizations: procedures)+≡
  subroutine smatrix_write (object, unit, indent)
    class(smatrix_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    integer :: u, i, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    if (allocated (object%value)) then
      if (size (object%value) > 0) then
        do i = 1, object%n_entry
          write (u, "(1x,A,'@(')", advance="no") repeat (" ", ind)
          write (u, "(SP,9999(I2.1,':',1x))", advance="no") &
            object%index(:,i)
          write (u, "('((', " // FMT_19 // ",','," // FMT_19 // &
            ",'))')") object%value(i)
        end do
      else
        write (u, "(1x,A)", advance="no") repeat (" ", ind)
        write (u, "(A)") "[empty matrix]"
      end if
    else
      write (u, "(1x,A)", advance="no") repeat (" ", ind)
      write (u, "(A)") "[undefined matrix]"
    end if
  end subroutine smatrix_write

```

Initialization: allocate arrays to the correct size. We specify both the dimension of the matrix (if different from two, this is rather a generic tensor) and the number of nonvanishing entries.

```

(Polarizations: smatrix: TBP)+≡
  procedure :: init => smatrix_init

(Polarizations: procedures)+≡
  subroutine smatrix_init (smatrix, dim, n_entry)
    class(smatrix_t), intent(out) :: smatrix
    integer, intent(in) :: dim
    integer, intent(in) :: n_entry
    smatrix%dim = dim
    smatrix%n_entry = n_entry
    allocate (smatrix%index (dim, n_entry))
    allocate (smatrix%value (n_entry))
  end subroutine smatrix_init

```

Fill: one entry at a time.

```

(Polarizations: smatrix: TBP)+≡
  procedure :: set_entry => smatrix_set_entry

(Polarizations: procedures)+≡
  subroutine smatrix_set_entry (smatrix, i, index, value)
    class(smatrix_t), intent(inout) :: smatrix

```

```

integer, intent(in) :: i
integer, dimension(:), intent(in) :: index
complex(default), intent(in) :: value
smatrix%index(:,i) = index
smatrix%value(i) = value
end subroutine smatrix_set_entry

```

```

<Polarizations: smatrix: TBP>+≡
  procedure :: exists => smatrix_exists

<Polarizations: procedures>+≡
  elemental function smatrix_exists (smatrix) result (exist)
    logical :: exist
    class(smatrix_t), intent(in) :: smatrix
    exist = .not. all (smatrix%value == 0)
  end function smatrix_exists

```

15.3.10 Polarization Matrix

As an extension of the more generic `smatrix` type, we implement a proper spin-density matrix. After the matrix has been filled, we can fix spin type and multiplicity for a particle, check the matrix for consistency, and normalize it if necessary.

This implementation does not have an antiparticle flag, just like the state matrix object. We therefore cannot account for sign flips when using this object.

TODO: The `pure` flag is for informational purposes only, and it only represents a necessary condition if spin is greater than 1/2. We may either check purity for all spins or drop this.

```

<Polarizations: public>+≡
  public :: pmatrix_t

<Polarizations: types>+≡
  type, extends (smatrix_t) :: pmatrix_t
    private
    integer :: spin_type = 0
    integer :: multiplicity = 0
    logical :: massive = .true.
    integer :: chirality = 0
    real(default) :: degree = 1
    logical :: pure = .false.
  contains
    <Polarizations: pmatrix: TBP>
  end type pmatrix_t

```

Output, including extra data. (The `indent` argument is ignored.)

```

<Polarizations: pmatrix: TBP>≡
  procedure :: write => pmatrix_write

<Polarizations: procedures>+≡
  subroutine pmatrix_write (object, unit, indent)
    class(pmatrix_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent

```

```

integer :: u
u = given_output_unit (unit)
write (u, "(1x,A)") "Polarization: spin density matrix"
write (u, "(3x,A,I0)") "spin type      = ", object%spin_type
write (u, "(3x,A,I0)") "multiplicity = ", object%multiplicity
write (u, "(3x,A,L1)") "massive      = ", object%massive
write (u, "(3x,A,I0)") "chirality    = ", object%chirality
write (u, "(3x,A,F10.7)") "pol.degree  = ", object%degree
write (u, "(3x,A,L1)") "pure state   = ", object%pure
call object%smatrix_t%write (u, 1)
end subroutine pmatrix_write

```

This assignment is trivial, but must be coded explicitly.

```

<Polarizations: pmatrix: TBP>+≡
generic :: assignment(=) => pmatrix_assign_from_smatrix
procedure, private :: pmatrix_assign_from_smatrix

<Polarizations: procedures>+≡
subroutine pmatrix_assign_from_smatrix (pmatrix, smatrix)
  class(pmatrix_t), intent(out) :: pmatrix
  type(smatrix_t), intent(in) :: smatrix
  pmatrix%smatrix_t = smatrix
end subroutine pmatrix_assign_from_smatrix

```

Declare spin, multiplicity, and polarization degree. Check whether all entries fit, and whether this is a valid matrix.

The required properties are:

1. all entries apply to the given spin and mass type
2. the diagonal is real
3. only the upper of corresponding off-diagonal elements is specified, i.e., the row index is less than the column index
4. the trace is nonnegative and equal to the polarization degree (the remainder, proportional to the unit matrix, is understood to be present)
5. the trace of the matrix square is positive and less or equal to the trace of the matrix itself, which is the polarization degree.
6. If the trace of the matrix square and the trace of the matrix are unity, we may have a pure state. (For spin up to $1/2$, this is actually sufficient.)

```

<Polarizations: pmatrix: TBP>+≡
procedure :: normalize => pmatrix_normalize

<Polarizations: procedures>+≡
subroutine pmatrix_normalize (pmatrix, flv, degree, tolerance)
  class(pmatrix_t), intent(inout) :: pmatrix
  type(flavor_t), intent(in) :: flv
  real(default), intent(in), optional :: degree
  real(default), intent(in), optional :: tolerance
  integer :: i, hmax
  logical :: fermion, ok

```

```

real(default) :: trace, trace_sq
real(default) :: tol
tol = 0; if (present (tolerance)) tol = tolerance
pmatrix%spin_type = flv%get_spin_type ()
pmatrix%massive = flv%get_mass () /= 0
if (.not. pmatrix%massive) then
    if (flv%is_left_handed ()) then
        pmatrix%chirality = -1
    else if (flv%is_right_handed ()) then
        pmatrix%chirality = +1
    end if
end if
if (pmatrix%spin_type == SCALAR) then
    pmatrix%multiplicity = 1
else if (pmatrix%massive) then
    pmatrix%multiplicity = pmatrix%spin_type
else if (pmatrix%chirality == 0) then
    pmatrix%multiplicity = 2
else
    pmatrix%multiplicity = 1
end if
if (present (degree)) then
    if (degree < 0 .or. degree > 1) &
        call msg_error ("polarization degree must be between 0 and 1")
    pmatrix%degree = degree
end if
if (size (pmatrix%index, 1) /= 2) call error ("wrong array rank")
fermion = mod (pmatrix%spin_type, 2) == 0
hmax = pmatrix%spin_type / 2
if (pmatrix%n_entry > 0) then
    if (fermion) then
        if (pmatrix%massive) then
            ok = all (pmatrix%index /= 0) &
                .and. all (abs (pmatrix%index) <= hmax)
        else if (pmatrix%chirality == -1) then
            ok = all (pmatrix%index == -hmax)
        else if (pmatrix%chirality == +1) then
            ok = all (pmatrix%index == +hmax)
        else
            ok = all (abs (pmatrix%index) == hmax)
        end if
    else
        if (pmatrix%massive) then
            ok = all (abs (pmatrix%index) <= hmax)
        else
            ok = all (abs (pmatrix%index) == hmax)
        end if
    end if
    if (.not. ok) call error ("illegal index value")
else
    pmatrix%degree = 0
    pmatrix%pure = pmatrix%multiplicity == 1
    return
end if

```

```

trace = 0
do i = 1, pmatrix%n_entry
  associate (index => pmatrix%index(:,i), value => pmatrix%value(i))
    if (index(1) == index(2)) then
      if (abs (aimag (value)) > tol) call error ("diagonal must be real")
      value = real (value, kind=default)
      trace = trace + value

      else if (any (pmatrix%index(1,:) == index(2) &
        .and. pmatrix%index(2,:) == index(1))) then
        call error ("redundant off-diagonal entry")
      else if (index(2) < index (1)) then
        index = index([2,1])
        value = conjg (value)
      end if
    end associate
  end do
  if (abs (trace) <= tol) call error ("trace must not vanish")
  trace = real (trace, kind=default)
  pmatrix%value = pmatrix%value / trace * pmatrix%degree
  trace_sq = (1 - pmatrix%degree ** 2) / pmatrix%multiplicity
  do i = 1, pmatrix%n_entry
    associate (index => pmatrix%index(:,i), value => pmatrix%value(i))
      if (index(1) == index(2)) then
        trace_sq = trace_sq + abs (value) ** 2
      else
        trace_sq = trace_sq + 2 * abs (value) ** 2
      end if
    end associate
  end do
  if (pmatrix%multiplicity == 1) then
    pmatrix%pure = .true.
  else if (abs (trace_sq - 1) <= tol) then
    pmatrix%pure = .true.
  else if (trace_sq - 1 > tol .or. trace_sq < -tol) then
    print *, "Trace of matrix square = ", trace_sq
    call error ("not permissible as density matrix")
  end if
contains
  subroutine error (msg)
    character(*), intent(in) :: msg
    call pmatrix%write ()
    call msg_fatal ("Spin density matrix: " // msg)
  end subroutine error
end subroutine pmatrix_normalize

```

A polarized matrix is defined as one with a positive polarization degree, even if the actual matrix is trivial.

<Polarizations: pmatrix: TBP>+≡

```
procedure :: is_polarized => pmatrix_is_polarized
```

<Polarizations: procedures>+≡

```
elemental function pmatrix_is_polarized (pmatrix) result (flag)
  class(pmatrix_t), intent(in) :: pmatrix
```

```

    logical :: flag
    flag = pmatrix%degree > 0
end function pmatrix_is_polarized

```

Check if there are only diagonal entries.

```

<Polarizations: pmatrix: TBP>+≡
    procedure :: is_diagonal => pmatrix_is_diagonal
<Polarizations: procedures>+≡
    elemental function pmatrix_is_diagonal (pmatrix) result (flag)
        class(pmatrix_t), intent(in) :: pmatrix
        logical :: flag
        flag = all (pmatrix%index(1,:) == pmatrix%index(2,:))
    end function pmatrix_is_diagonal

```

Check if there are only diagonal entries.

```

<Polarizations: pmatrix: TBP>+≡
    procedure :: get_simple_pol => pmatrix_get_simple_pol
<Polarizations: procedures>+≡
    elemental function pmatrix_get_simple_pol (pmatrix) result (pol)
        class(pmatrix_t), intent(in) :: pmatrix
        real(default) :: pol
        if (pmatrix%is_polarized ()) then
            select case (size (pmatrix%value))
            case (0)
                pol = 0
            case (1)
                pol = pmatrix%index (1,1) * pmatrix%degree
            case (2)
                pol = 42
            end select
        else
            pol = 0
        end if
    end function pmatrix_get_simple_pol

```

15.3.11 Data Transformation

Create a `polarization_t` object from the contents of a normalized `pmatrix_t` object. We scan the entries as present in `pmatrix` and transform them into a density matrix, if necessary. The density matrix then initializes the Bloch vector. This is analogous to `polarization_init_state_matrix`.

There is a subtlety associated with massless particles. Since the `pmatrix` doesn't contain the full density matrix but just the nontrivial part, we have to initialize the polarization object with the massless equipartition, which contains nonzero entries for the Cartan generators. The `set` method therefore should not erase those initial contents. This is a constraint for the implementation of `set`, as applied to the Bloch vector.

As mentioned above, `pmatrix_t` does not support an antiparticle flag.

```

<Polarizations: polarization: TBP>+≡
    procedure :: init_pmatrix => polarization_init_pmatrix

```



```

<Polarizations: procedures>+≡
subroutine polarization_init_pmatrix (pol, pmatrix)
  class(polarization_t), intent(out) :: pol
  type(pmatrix_t), intent(in) :: pmatrix
  integer :: d, i, j, k, h1, h2
  complex(default), dimension(:,:), allocatable :: r
  call pol%init_generic ( &
    spin_type = pmatrix%spin_type, &
    multiplicity = pmatrix%multiplicity, &
    anti = .false., &                                     !!! SUFFICIENT?
    left_handed = pmatrix%chirality < 0, &
    right_handed = pmatrix%chirality > 0)
  if (pol%bv%is_polarized ()) then
    d = pol%bv%get_n_states ()
    allocate (r (d, d), source = (0._default, 0._default))
    if (d == pmatrix%multiplicity) then
      do i = 1, d
        r(i,i) = (1 - pmatrix%degree) / d
      end do
    else if (d > pmatrix%multiplicity) then
      r(1,1) = (1 - pmatrix%degree) / 2
      r(d,d) = r(1,1)
    end if
    do k = 1, size (pmatrix%value)
      h1 = pmatrix%index(1,k)
      h2 = pmatrix%index(2,k)
      i = pol%bv%hel_index (h1)
      j = pol%bv%hel_index (h2)
      r(i,j) = r(i,j) + pmatrix%value(k)
      r(j,i) = conjg (r(i,j))
    end do
    call pol%bv%set (r)
  end if
end subroutine polarization_init_pmatrix

```

15.3.12 Unit tests

Test module, followed by the corresponding implementation module.

```

<polarizations_ut.f90>≡
<File header>

module polarizations_ut
  use unit_tests
  use polarizations_uti

<Standard module head>

<Polarizations: public test>

contains

<Polarizations: test driver>

```

```

    end module polarizations_ut
<polarizations.uti.f90>≡
<File header>

module polarizations_uti

<Use kinds>
    use flavors
    use model_data

    use polarizations

<Standard module head>

<Polarizations: test declarations>

contains

<Polarizations: tests>

    end module polarizations_uti
API: driver for the unit tests below.
<Polarizations: public test>≡
    public :: polarizations_test
<Polarizations: test driver>≡
    subroutine polarizations_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Polarizations: execute tests>
    end subroutine polarizations_test

```

Polarization type

Checking the setup for polarization.

```

<Polarizations: execute tests>≡
    call test (polarization_1, "polarization_1", &
        "check polarization setup", &
        u, results)
<Polarizations: test declarations>≡
    public :: polarization_1
<Polarizations: tests>≡
    subroutine polarization_1 (u)
        use os_interface
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(polarization_t) :: pol
        type(flavor_t) :: flv
        real(default), dimension(3) :: alpha

```

```

real(default) :: r, theta, phi
real(default), parameter :: tolerance = 1.E-14_default

write (u, "(A)")  "* Test output: polarization_1"
write (u, "(A)")  "* Purpose: test polarization setup"
write (u, "(A)")

write (u, "(A)")  "* Reading model file"
write (u, "(A)")

call model%init_sm_test ()

write (u, "(A)")  "* Unpolarized fermion"
write (u, "(A)")

call flv%init (1, model)
call pol%init_unpolarized (flv)
call pol%write (u, state_matrix = .true.)
write (u, "(A,L1)") " diagonal =", pol%is_diagonal ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized fermion"
write (u, "(A)")

call pol%init_circular (flv, 0._default)
call pol%write (u, state_matrix = .true., all_states = .false.)

write (u, "(A)")
write (u, "(A)")  "* Transversally polarized fermion, phi=0"
write (u, "(A)")

call pol%init_transversal (flv, 0._default, 1._default)
call pol%write (u, state_matrix = .true.)
write (u, "(A,L1)") " diagonal =", pol%is_diagonal ()

write (u, "(A)")
write (u, "(A)")  "* Transversally polarized fermion, phi=0.9, frac=0.8"
write (u, "(A)")

call pol%init_transversal (flv, 0.9_default, 0.8_default)
call pol%write (u, state_matrix = .true.)
write (u, "(A,L1)") " diagonal =", pol%is_diagonal ()

write (u, "(A)")
write (u, "(A)")  "* All polarization directions of a fermion"
write (u, "(A)")

call pol%init_generic (flv)
call pol%write (u, state_matrix = .true.)

call flv%init (21, model)

write (u, "(A)")

```

```

write (u, "(A)")  "* Circularly polarized gluon, frac=0.3"
write (u, "(A)")

call pol%init_circular (flv, 0.3_default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

call flv%init (23, model)

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized massive vector, frac=-0.7"
write (u, "(A)")

call pol%init_circular (flv, -0.7_default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized massive vector"
write (u, "(A)")

call pol%init_circular (flv, 1._default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* Longitudinally polarized massive vector, frac=0.4"
write (u, "(A)")

call pol%init_longitudinal (flv, 0.4_default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* Longitudinally polarized massive vector"
write (u, "(A)")

call pol%init_longitudinal (flv, 1._default)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* Diagonally polarized massive vector"
write (u, "(A)")

call pol%init_diagonal &
      (flv, [2._default, 1._default, 0._default])
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(A)")  "* All polarization directions of a massive vector"
write (u, "(A)")

```

```

call pol%init_generic (flv)
call pol%write (u, state_matrix = .true.)
call flv%init (21, model)

write (u, "(A)")
write (u, "(A)")  "* Axis polarization (0.2, 0.4, 0.6)"
write (u, "(A)")

alpha = [0.2_default, 0.4_default, 0.6_default]
call pol%init_axis (flv, alpha)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(1X,A)") "Recovered axis:"
alpha = pol%get_axis ()
write (u, "(3(1X,F10.7))") alpha

write (u, "(A)")
write (u, "(A)")  "* Angle polarization (0.5, 0.6, -1)"
r = 0.5_default
theta = 0.6_default
phi = -1._default
call pol%init_angles (flv, r, theta, phi)
write (u, "(A)")
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)

write (u, "(A)")
write (u, "(1X,A)") "Recovered parameters (r, theta, phi):"
call pol%to_angles (r, theta, phi)
write (u, "(3(1X,F10.7))") r, theta, phi

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: polarization_1"

end subroutine polarization_1

```

Sparse-Matrix type

Use a sparse density matrix universally as the input for setting up polarization.

```

<Polarizations: execute tests>+≡
  call test (polarization_2, "polarization_2", &
            "matrix polarization setup", &
            u, results)

<Polarizations: test declarations>+≡
  public :: polarization_2

<Polarizations: tests>+≡
  subroutine polarization_2 (u)

```

```

use os_interface
integer, intent(in) :: u
type(model_data_t), target :: model
type(flavor_t) :: flv
type(polarization_t) :: pol
real(default), dimension(3) :: alpha
type(pmatrix_t) :: pmatrix
real(default), parameter :: tolerance = 1e-8_default

write (u, "(A)")  "* Test output: polarization_2"
write (u, "(A)")  "* Purpose: matrix polarization setup"
write (u, "(A)")

write (u, "(A)")  "* Reading model file"
write (u, "(A)")

call model%init_sm_test ()

write (u, "(A)")  "* Unpolarized fermion"
write (u, "(A)")

call flv%init (1, model)
call pmatrix%init (2, 0)
call pmatrix%normalize (flv, 0._default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)")  "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)")  "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Transversally polarized fermion, phi=0"
write (u, "(A)")

call pmatrix%init (2, 3)
call pmatrix%set_entry (1, [-1,-1], (1._default, 0._default))
call pmatrix%set_entry (2, [+1,+1], (1._default, 0._default))
call pmatrix%set_entry (3, [-1,+1], (1._default, 0._default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)")  "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)")  "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
               all_states = .false., tolerance = tolerance)
! call pol%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Transversally polarized fermion, phi=0.9, frac=0.8"
write (u, "(A)")

call pmatrix%init (2, 3)
call pmatrix%set_entry (1, [-1,-1], (1._default, 0._default))
call pmatrix%set_entry (2, [+1,+1], (1._default, 0._default))
call pmatrix%set_entry (3, [-1,+1], exp ((0._default, -0.9_default)))
call pmatrix%normalize (flv, 0.8_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true.)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Left-handed massive fermion, frac=1"
write (u, "(A)")

call flv%init (11, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [-1,-1], (1._default, 0._default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)")  "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)")  "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Left-handed massive fermion, frac=0.8"
write (u, "(A)")

call flv%init (11, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [-1,-1], (1._default, 0._default))
call pmatrix%normalize (flv, 0.8_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Left-handed massless fermion"

```

```

write (u, "(A)")

call flv%init (12, model)
call pmatrix%init (2, 0)
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true.)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Right-handed massless fermion, frac=0.5"
write (u, "(A)")

call flv%init (-12, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [1,1], (1._default, 0._default))
call pmatrix%normalize (flv, 0.5_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true.)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized gluon, frac=0.3"
write (u, "(A)")

call flv%init (21, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [1,1], (1._default, 0._default))
call pmatrix%normalize (flv, 0.3_default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized massive vector, frac=0.7"
write (u, "(A)")

call flv%init (23, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [1,1], (1._default, 0._default))
call pmatrix%normalize (flv, 0.7_default, tolerance)
call pmatrix%write (u)
write (u, *)

```



```

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Circularly polarized massive vector"
write (u, "(A)")

call flv%init (23, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [1,1], (1._default, 0._default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Longitudinally polarized massive vector, frac=0.4"
write (u, "(A)")

call flv%init (23, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [0,0], (1._default, 0._default))
call pmatrix%normalize (flv, 0.4_default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)")  "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)")  "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Longitudinally polarized massive vector"
write (u, "(A)")

call flv%init (23, model)
call pmatrix%init (2, 1)
call pmatrix%set_entry (1, [0,0], (1._default, 0._default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)
write (u, "(1x,A,L1)")  "polarized = ", pmatrix%is_polarized ()
write (u, "(1x,A,L1)")  "diagonal = ", pmatrix%is_diagonal ()
write (u, *)

```

```

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true., &
    all_states = .false., tolerance = tolerance)
! call pol%final ()

write (u, "(A)")
write (u, "(A)")  "* Axis polarization (0.2, 0.4, 0.6)"
write (u, "(A)")

call flv%init (11, model)
alpha = [0.2_default, 0.4_default, 0.6_default]
alpha = alpha / sqrt (sum (alpha**2))
call pmatrix%init (2, 3)
call pmatrix%set_entry (1, [-1,-1], cmplx (1 - alpha(3), kind=default))
call pmatrix%set_entry (2, [1,-1], &
    cmplx (alpha(1),-alpha(2), kind=default))
call pmatrix%set_entry (3, [1,1], cmplx (1 + alpha(3), kind=default))
call pmatrix%normalize (flv, 1._default, tolerance)
call pmatrix%write (u)
write (u, *)

call pol%init_pmatrix (pmatrix)
call pol%write (u, state_matrix = .true.)
! call pol%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: polarization_2"

end subroutine polarization_2

```

15.4 Particles

This module defines the `particle_t` object type, and the methods and operations that deal with it.

`<particles.f90>`≡
<File header>

`module particles`

<Use kinds with double>

<Use strings>

<Use debug>

`use io_units`

`use format_utils, only: write_compressed_integer_array, write_separator`

`use format_utils, only: pac_fmt`

`use format_defs, only: FMT_16, FMT_19`

`use numeric_utils`

`use diagnostics`

`use lorentz`

`use phs_points, only: phs_point_t, assignment(=)`

`use model_data`

`use flavors`

`use colors`

`use helicities`

`use quantum_numbers`

`use state_matrices`

`use interactions`

`use subevents`

`use polarizations`

`use pdg_arrays, only: is_quark, is_gluon`

<Standard module head>

<Particles: public>

<Particles: parameters>

<Particles: types>

<Particles: interfaces>

`contains`

<Particles: procedures>

`end module particles`

15.4.1 The particle type

Particle status codes

The overall status codes (incoming/outgoing etc.) are inherited from the module `subevents`.

Polarization status:

```

⟨Particles: parameters⟩≡
  integer, parameter, public :: PRT_UNPOLARIZED = 0
  integer, parameter, public :: PRT_DEFINITE_HELICITY = 1
  integer, parameter, public :: PRT_GENERIC_POLARIZATION = 2

```

Definition

The quantum numbers are flavor (from which invariant particle properties can be derived), color, and polarization. The particle may be unpolarized. In this case, **hel** and **pol** are unspecified. If it has a definite helicity, the **hel** component is defined. If it has a generic polarization, the **pol** component is defined. For each particle we store the four-momentum and the invariant mass squared, i.e., the squared norm of the four-momentum. There is also an optional list of parent and child particles, for bookkeeping in physical events. The **vertex** is an optional component that consists of a Lorentz 4-vector, denoting the position and time of the vertex (displaced vertex/time). **lifetime** is an optional component that accounts for the finite lifetime τ of a decaying particle. In case there is no magnetic field etc., the true decay vertex of a particle in the detector would be $\vec{v}' = \vec{v} + \tau \times \vec{p}/p^0$, where p^0 and \vec{p} are the energy and 3-momentum of the particle.

```

⟨Particles: public⟩≡
  public :: particle_t

⟨Particles: types⟩≡
  type :: particle_t
    !private
    integer :: status = PRT_UNDEFIED
    integer :: polarization = PRT_UNPOLARIZED
    type(flavor_t) :: flv
    type(color_t) :: col
    type(helicity_t) :: hel
    type(polarization_t) :: pol
    type(vector4_t) :: p = vector4_null
    real(default) :: p2 = 0
    type(vector4_t), allocatable :: vertex
    real(default), allocatable :: lifetime
    integer, dimension(:), allocatable :: parent
    integer, dimension(:), allocatable :: child
  contains
  ⟨Particles: particle: TBP⟩
end type particle_t

```

Copy a particle. (Deep copy) This excludes the parent-child relations.

```

⟨Particles: particle: TBP⟩≡
  generic :: init => init_particle
  procedure :: init_particle => particle_init_particle

⟨Particles: procedures⟩≡
  subroutine particle_init_particle (prt_out, prt_in)
    class(particle_t), intent(out) :: prt_out

```

```

type(particle_t), intent(in) :: prt_in
prt_out%status = prt_in%status
prt_out%polarization = prt_in%polarization
prt_out%flv = prt_in%flv
prt_out%col = prt_in%col
prt_out%hel = prt_in%hel
prt_out%pol = prt_in%pol
prt_out%p = prt_in%p
prt_out%p2 = prt_in%p2
if (allocated (prt_in%vertex)) &
    allocate (prt_out%vertex, source=prt_in%vertex)
if (allocated (prt_in%lifetime)) &
    allocate (prt_out%lifetime, source=prt_in%lifetime)
end subroutine particle_init_particle

```

Initialize a particle using external information.

```

⟨Particles: particle: TBP⟩+≡
generic :: init => init_external
procedure :: init_external => particle_init_external

⟨Particles: procedures⟩+≡
subroutine particle_init_external &
    (particle, status, pdg, model, col, anti_col, mom)
class(particle_t), intent(out) :: particle
integer, intent(in) :: status, pdg, col, anti_col
class(model_data_t), pointer, intent(in) :: model
type(vector4_t), intent(in) :: mom
type(flavor_t) :: flavor
type(color_t) :: color
call flavor%init (pdg, model)
call particle%set_flavor (flavor)
call color%init_col_acl (col, anti_col)
call particle%set_color (color)
call particle%set_status (status)
call particle%set_momentum (mom)
end subroutine particle_init_external

```

Initialize a particle using a single-particle state matrix which determines flavor, color, and polarization. The state matrix must have unique flavor and color. The factorization mode determines whether the particle is unpolarized, has definite helicity, or generic polarization. This mode is translated into the polarization status.

```

⟨Particles: particle: TBP⟩+≡
generic :: init => init_state
procedure :: init_state => particle_init_state

⟨Particles: procedures⟩+≡
subroutine particle_init_state (prt, state, status, mode)
class(particle_t), intent(out) :: prt
type(state_matrix_t), intent(in), target :: state
integer, intent(in) :: status, mode
type(state_iterator_t) :: it
prt%status = status

```

```

call it%init (state)
prt%flv = it%get_flavor (1)
if (prt%flv%is_radiated ()) prt%status = PRT_BEAM_REMNANT
prt%col = it%get_color (1)
select case (mode)
case (FM_SELECT_HELICITY)
    prt%hel = it%get_helicity (1)
    if (prt%hel%is_defined ()) then
        prt%polarization = PRT_DEFINITE_HELICITY
    end if
case (FM_FACTOR_HELICITY)
    call prt%pol%init_state_matrix (state)
    prt%polarization = PRT_GENERIC_POLARIZATION
end select
end subroutine particle_init_state

```

Finalizer.

```

⟨Particles: particle: TBP⟩+≡
    procedure :: final => particle_final

⟨Particles: procedures⟩+≡
    subroutine particle_final (prt)
        class(particle_t), intent(inout) :: prt
        if (allocated (prt%vertex)) deallocate (prt%vertex)
        if (allocated (prt%lifetime)) deallocate (prt%lifetime)
    end subroutine particle_final

```

I/O

```

⟨Particles: particle: TBP⟩+≡
    procedure :: write => particle_write

⟨Particles: procedures⟩+≡
    subroutine particle_write (prt, unit, testflag, compressed, polarization)
        class(particle_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag, compressed, polarization
        logical :: comp, pacified, pol
        integer :: u, h1, h2
        real(default) :: pp2
        character(len=7) :: fmt
        character(len=20) :: buffer
        comp = .false.; if (present (compressed)) comp = compressed
        pacified = .false.; if (present (testflag)) pacified = testflag
        pol = .true.; if (present (polarization)) pol = polarization
        call pac_fmt (fmt, FMT_19, FMT_16, testflag)
        u = given_output_unit (unit); if (u < 0) return
        pp2 = prt%p2
        if (pacified) call pacify (pp2, tolerance = 1E-10_default)
        select case (prt%status)
        case (PRT_UNDEFINED); write (u, "(1x, A)", advance="no") "[-]"
        case (PRT_BEAM); write (u, "(1x, A)", advance="no") "[b]"
        case (PRT_INCOMING); write (u, "(1x, A)", advance="no") "[i]"

```

```

case (PRT_OUTGOING);      write (u, "(1x, A)", advance="no") "[o]"
case (PRT_VIRTUAL);      write (u, "(1x, A)", advance="no") "[v]"
case (PRT_RESONANT);     write (u, "(1x, A)", advance="no") "[r]"
case (PRT_BEAM_REMNANT); write (u, "(1x, A)", advance="no") "[x]"
end select
write (u, "(1x)", advance="no")
if (comp) then
  write (u, "(A7,1X)", advance="no") char (prt%flv%get_name ())
  if (pol) then
    select case (prt%polarization)
    case (PRT_DEFINITE_HELICITY)
      ! Integer helicity, assumed diagonal
      call prt%hel%get_indices (h1, h2)
      write (u, "(I2,1X)", advance="no") h1
    case (PRT_GENERIC_POLARIZATION)
      ! No space for full density matrix here
      write (u, "(A2,1X)", advance="no") "*"
    case default
      ! Blank entry if helicity is undefined
      write (u, "(A2,1X)", advance="no") " "
    end select
  end if
  write (u, "(2(I4,1X))", advance="no") &
    prt%col%get_col (), prt%col%get_acl ()
  call write_compressed_integer_array (buffer, prt%parent)
  write (u, "(A,1X)", advance="no") buffer
  call write_compressed_integer_array (buffer, prt%child)
  write (u, "(A,1X)", advance="no") buffer
  call prt%p%write(u, testflag = testflag, compressed = comp)
  write (u, "(F12.3)") pp2
else
  call prt%flv%write (unit)
  if (prt%col%is_nonzero ()) then
    call color_write (prt%col, unit)
  end if
  if (pol) then
    select case (prt%polarization)
    case (PRT_DEFINITE_HELICITY)
      call prt%hel%write (unit)
      write (u, *)
    case (PRT_GENERIC_POLARIZATION)
      write (u, *)
      call prt%pol%write (unit, state_matrix = .true.)
    case default
      write (u, *)
    end select
  else
    write (u, *)
  end if
  call prt%p%write (unit, testflag = testflag)
  write (u, "(1x,A,1x," // fmt // ")") "T = ", pp2
  if (allocated (prt%parent)) then
    if (size (prt%parent) /= 0) then
      write (u, "(1x,A,40(1x,I0))") "Parents: ", prt%parent
    end if
  end if
end if

```

```

        end if
    end if
    if (allocated (prt%child)) then
        if (size (prt%child) /= 0) then
            write (u, "(1x,A,40(1x,I0))") "Children:", prt%child
        end if
    end if
    if (allocated (prt%vertex)) then
        write (u, "(1x,A,1x," // fmt // ")") "Vtx t = ", prt%vertex%p(0)
        write (u, "(1x,A,1x," // fmt // ")") "Vtx x = ", prt%vertex%p(1)
        write (u, "(1x,A,1x," // fmt // ")") "Vtx y = ", prt%vertex%p(2)
        write (u, "(1x,A,1x," // fmt // ")") "Vtx z = ", prt%vertex%p(3)
    end if
    if (allocated (prt%lifetime)) then
        write (u, "(1x,A,1x," // fmt // ")") "Lifetime = ", &
            prt%lifetime
    end if
end if
end subroutine particle_write

```

Binary I/O:

```

<Particles: particle: TBP>+≡
    procedure :: write_raw => particle_write_raw
    procedure :: read_raw => particle_read_raw

<Particles: procedures>+≡
    subroutine particle_write_raw (prt, u)
        class(particle_t), intent(in) :: prt
        integer, intent(in) :: u
        write (u) prt%status, prt%polarization
        call prt%flv%write_raw (u)
        call prt%col%write_raw (u)
        select case (prt%polarization)
        case (PRT_DEFINITE_HELICITY)
            call prt%hel%write_raw (u)
        case (PRT_GENERIC_POLARIZATION)
            call prt%pol%write_raw (u)
        end select
        call vector4_write_raw (prt%p, u)
        write (u) prt%p2
        write (u) allocated (prt%parent)
        if (allocated (prt%parent)) then
            write (u) size (prt%parent)
            write (u) prt%parent
        end if
        write (u) allocated (prt%child)
        if (allocated (prt%child)) then
            write (u) size (prt%child)
            write (u) prt%child
        end if
        write (u) allocated (prt%vertex)
        if (allocated (prt%vertex)) then
            call vector4_write_raw (prt%vertex, u)
        end if
    end if

```



```

write (u) allocated (prt%lifetime)
if (allocated (prt%lifetime)) then
    write (u) prt%lifetime
end if
end subroutine particle_write_raw

subroutine particle_read_raw (prt, u, iostat)
    class(particle_t), intent(out) :: prt
    integer, intent(in) :: u
    integer, intent(out) :: iostat
    logical :: allocated_parent, allocated_child
    logical :: allocated_vertex, allocated_lifetime
    integer :: size_parent, size_child
    read (u, iostat=iostat) prt%status, prt%polarization
    call prt%flv%read_raw (u, iostat=iostat)
    call prt%col%read_raw (u, iostat=iostat)
    select case (prt%polarization)
    case (PRT_DEFINITE_HELICITY)
        call prt%hel%read_raw (u, iostat=iostat)
    case (PRT_GENERIC_POLARIZATION)
        call prt%pol%read_raw (u, iostat=iostat)
    end select
    call vector4_read_raw (prt%p, u, iostat=iostat)
    read (u, iostat=iostat) prt%p2
    read (u, iostat=iostat) allocated_parent
    if (allocated_parent) then
        read (u, iostat=iostat) size_parent
        allocate (prt%parent (size_parent))
        read (u, iostat=iostat) prt%parent
    end if
    read (u, iostat=iostat) allocated_child
    if (allocated_child) then
        read (u, iostat=iostat) size_child
        allocate (prt%child (size_child))
        read (u, iostat=iostat) prt%child
    end if
    read (u, iostat=iostat) allocated_vertex
    if (allocated_vertex) then
        allocate (prt%vertex)
        read (u, iostat=iostat) prt%vertex%p
    end if
    read (u, iostat=iostat) allocated_lifetime
    if (allocated_lifetime) then
        allocate (prt%lifetime)
        read (u, iostat=iostat) prt%lifetime
    end if
end subroutine particle_read_raw

```

Setting contents

Reset the status code. Where applicable, set p^2 assuming that the particle is on-shell.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: reset_status => particle_reset_status

⟨Particles: procedures⟩+≡
  elemental subroutine particle_reset_status (prt, status)
    class(particle_t), intent(inout) :: prt
    integer, intent(in) :: status
    prt%status = status
    select case (status)
      case (PRT_BEAM, PRT_INCOMING, PRT_OUTGOING)
        prt%p2 = prt%flv%get_mass () ** 2
      end select
    end subroutine particle_reset_status

```

The color can be given explicitly.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: set_color => particle_set_color

⟨Particles: procedures⟩+≡
  elemental subroutine particle_set_color (prt, col)
    class(particle_t), intent(inout) :: prt
    type(color_t), intent(in) :: col
    prt%col = col
  end subroutine particle_set_color

```

The flavor can be given explicitly.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: set_flavor => particle_set_flavor

⟨Particles: procedures⟩+≡
  subroutine particle_set_flavor (prt, flv)
    class(particle_t), intent(inout) :: prt
    type(flavor_t), intent(in) :: flv
    prt%flv = flv
  end subroutine particle_set_flavor

```

As can the helicity.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: set_helicity => particle_set_helicity

⟨Particles: procedures⟩+≡
  subroutine particle_set_helicity (prt, hel)
    class(particle_t), intent(inout) :: prt
    type(helicity_t), intent(in) :: hel
    prt%hel = hel
  end subroutine particle_set_helicity

```

And the polarization.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: set_pol => particle_set_pol

```

```

<Particles: procedures>+≡
  subroutine particle_set_pol (prt, pol)
    class(particle_t), intent(inout) :: prt
    type(polarization_t), intent(in) :: pol
    prt%pol = pol
  end subroutine particle_set_pol

```

Manually set the model for the particle flavor. This is required, e.g., if the particle has been read from file.

```

<Particles: particle: TBP>+≡
  procedure :: set_model => particle_set_model

<Particles: procedures>+≡
  subroutine particle_set_model (prt, model)
    class(particle_t), intent(inout) :: prt
    class(model_data_t), intent(in), target :: model
    call prt%flv%set_model (model)
  end subroutine particle_set_model

```

The momentum is set independent of the quantum numbers.

```

<Particles: particle: TBP>+≡
  procedure :: set_momentum => particle_set_momentum

<Particles: procedures>+≡
  elemental subroutine particle_set_momentum (prt, p, p2, on_shell)
    class(particle_t), intent(inout) :: prt
    type(vector4_t), intent(in) :: p
    real(default), intent(in), optional :: p2
    logical, intent(in), optional :: on_shell
    prt%p = p
    if (present (on_shell)) then
      if (on_shell) then
        if (prt%flv%is_associated ()) then
          prt%p2 = prt%flv%get_mass () ** 2
          return
        end if
      end if
    end if
    if (present (p2)) then
      prt%p2 = p2
    else
      prt%p2 = p ** 2
    end if
  end subroutine particle_set_momentum

```

Set resonance information. This should be done after momentum assignment, because we need to know whether the particle is spacelike or timelike. The resonance flag is defined only for virtual particles.

```

<Particle: particle: TBP>≡
  procedure :: set_resonance_flag => particle_set_resonance_flag

```

```

(Particles: procedures) +=
  elemental subroutine particle_set_resonance_flag (prt, resonant)
    class(particle_t), intent(inout) :: prt
    logical, intent(in) :: resonant
    select case (prt%status)
    case (PRT_VIRTUAL)
      if (resonant) prt%status = PRT_RESONANT
    end select
  end subroutine particle_set_resonance_flag

```

Set children and parents information.

```

(Particles: particle: TBP) +=
  procedure :: set_children => particle_set_children
  procedure :: set_parents => particle_set_parents

```

```

(Particles: procedures) +=
  subroutine particle_set_children (prt, idx)
    class(particle_t), intent(inout) :: prt
    integer, dimension(:), intent(in) :: idx
    if (allocated (prt%child)) deallocate (prt%child)
    allocate (prt%child (count (idx /= 0)))
    prt%child = pack (idx, idx /= 0)
  end subroutine particle_set_children

  subroutine particle_set_parents (prt, idx)
    class(particle_t), intent(inout) :: prt
    integer, dimension(:), intent(in) :: idx
    if (allocated (prt%parent)) deallocate (prt%parent)
    allocate (prt%parent (count (idx /= 0)))
    prt%parent = pack (idx, idx /= 0)
  end subroutine particle_set_parents

```

```

(Particles: particle: TBP) +=
  procedure :: add_child => particle_add_child

```

```

(Particles: procedures) +=
  subroutine particle_add_child (prt, new_child)
    class(particle_t), intent(inout) :: prt
    integer, intent(in) :: new_child
    integer, dimension(:), allocatable :: idx
    integer :: n, i
    n = prt%get_n_children()
    if (n == 0) then
      call prt%set_children ([new_child])
    else
      do i = 1, n
        if (prt%child(i) == new_child) then
          return
        end if
      end do
      allocate (idx (1:n+1))
      idx(1:n) = prt%get_children ()
      idx(n+1) = new_child
      call prt%set_children (idx)
    end if
  end subroutine particle_add_child

```

```

        end if
    end subroutine particle_add_child

    <Particles: particle: TBP>+≡
    procedure :: add_children => particle_add_children

    <Particles: procedures>+≡
    subroutine particle_add_children (prt, new_child)
        class(particle_t), intent(inout) :: prt
        integer, dimension(:), intent(in) :: new_child
        integer, dimension(:), allocatable :: idx
        integer :: n
        n = prt%get_n_children()
        if (n == 0) then
            call prt%set_children (new_child)
        else
            allocate (idx (1:n+size(new_child)))
            idx(1:n) = prt%get_children ()
            idx(n+1:n+size(new_child)) = new_child
            call prt%set_children (idx)
        end if
    end subroutine particle_add_children

    <Particles: particle: TBP>+≡
    procedure :: set_status => particle_set_status

    <Particles: procedures>+≡
    elemental subroutine particle_set_status (prt, status)
        class(particle_t), intent(inout) :: prt
        integer, intent(in) :: status
        prt%status = status
    end subroutine particle_set_status

    <Particles: particle: TBP>+≡
    procedure :: set_polarization => particle_set_polarization

    <Particles: procedures>+≡
    subroutine particle_set_polarization (prt, polarization)
        class(particle_t), intent(inout) :: prt
        integer, intent(in) :: polarization
        prt%polarization = polarization
    end subroutine particle_set_polarization

    <Particles: particle: TBP>+≡
    generic :: set_vertex => set_vertex_from_vector3, set_vertex_from_xyz, &
        set_vertex_from_vector4, set_vertex_from_xyzt
    procedure :: set_vertex_from_vector4 => particle_set_vertex_from_vector4
    procedure :: set_vertex_from_vector3 => particle_set_vertex_from_vector3
    procedure :: set_vertex_from_xyzt => particle_set_vertex_from_xyzt
    procedure :: set_vertex_from_xyz => particle_set_vertex_from_xyz

```

<Particles: procedures>+≡

```

subroutine particle_set_vertex_from_vector4 (prt, vertex)
  class(particle_t), intent(inout) :: prt
  type(vector4_t), intent(in) :: vertex
  if (allocated (prt%vertex)) deallocate (prt%vertex)
  allocate (prt%vertex, source=vertex)
end subroutine particle_set_vertex_from_vector4

subroutine particle_set_vertex_from_vector3 (prt, vertex)
  class(particle_t), intent(inout) :: prt
  type(vector3_t), intent(in) :: vertex
  type(vector4_t) :: vtx
  vtx = vector4_moving (0._default, vertex)
  if (allocated (prt%vertex)) deallocate (prt%vertex)
  allocate (prt%vertex, source=vtx)
end subroutine particle_set_vertex_from_vector3

subroutine particle_set_vertex_from_xyz_t (prt, vx, vy, vz, t)
  class(particle_t), intent(inout) :: prt
  real(default), intent(in) :: vx, vy, vz, t
  type(vector4_t) :: vertex
  if (allocated (prt%vertex)) deallocate (prt%vertex)
  vertex = vector4_moving (t, vector3_moving ([vx, vy, vz]))
  allocate (prt%vertex, source=vertex)
end subroutine particle_set_vertex_from_xyz_t

subroutine particle_set_vertex_from_xyz (prt, vx, vy, vz)
  class(particle_t), intent(inout) :: prt
  real(default), intent(in) :: vx, vy, vz
  type(vector4_t) :: vertex
  if (allocated (prt%vertex)) deallocate (prt%vertex)
  vertex = vector4_moving (0._default, vector3_moving ([vx, vy, vz]))
  allocate (prt%vertex, source=vertex)
end subroutine particle_set_vertex_from_xyz

```

Set the lifetime of a particle.

<Particles: particle: TBP>+≡

```

procedure :: set_lifetime => particle_set_lifetime

```

<Particles: procedures>+≡

```

elemental subroutine particle_set_lifetime (prt, lifetime)
  class(particle_t), intent(inout) :: prt
  real(default), intent(in) :: lifetime
  if (allocated (prt%lifetime)) deallocate (prt%lifetime)
  allocate (prt%lifetime, source=lifetime)
end subroutine particle_set_lifetime

```

Accessing contents

The status code.

<Particles: particle: TBP>+≡

```

procedure :: get_status => particle_get_status

```

```

<Particles: procedures>+≡
  elemental function particle_get_status (prt) result (status)
    integer :: status
    class(particle_t), intent(in) :: prt
    status = prt%status
  end function particle_get_status

```

Return true if the status is either INCOMING, OUTGOING or RESONANT. BEAM is kept, if keep_beams is set true.

```

<Particles: particle: TBP>+≡
  procedure :: is_real => particle_is_real

<Particles: procedures>+≡
  elemental function particle_is_real (prt, keep_beams) result (flag)
    logical :: flag, kb
    class(particle_t), intent(in) :: prt
    logical, intent(in), optional :: keep_beams
    kb = .false.
    if (present (keep_beams)) kb = keep_beams
    select case (prt%status)
    case (PRT_INCOMING, PRT_OUTGOING, PRT_RESONANT)
      flag = .true.
    case (PRT_BEAM)
      flag = kb
    case default
      flag = .false.
    end select
  end function particle_is_real

```

```

<Particles: particle: TBP>+≡
  procedure :: is_colored => particle_is_colored

```

```

<Particles: procedures>+≡
  elemental function particle_is_colored (particle) result (flag)
    logical :: flag
    class(particle_t), intent(in) :: particle
    flag = particle%col%is_nonzero ()
  end function particle_is_colored

```

[90,100] hopefully catches all of them and not too many.

```

<Particles: particle: TBP>+≡
  procedure :: is_hadronic_beam_remnant => particle_is_hadronic_beam_remnant

<Particles: procedures>+≡
  elemental function particle_is_hadronic_beam_remnant (particle) result (flag)
    class(particle_t), intent(in) :: particle
    logical :: flag
    integer :: pdg
    pdg = particle%flv%get_pdg ()
    flag = particle%status == PRT_BEAM_REMNANT .and. &
      abs(pdg) >= 90 .and. abs(pdg) <= 100
  end function particle_is_hadronic_beam_remnant

```

```

⟨Particles: particle: TBP⟩+≡
  procedure :: is_beam_remnant => particle_is_beam_remnant

⟨Particles: procedures⟩+≡
  elemental function particle_is_beam_remnant (particle) result (flag)
    class(particle_t), intent(in) :: particle
    logical :: flag
    flag = particle%status == PRT_BEAM_REMNANT
  end function particle_is_beam_remnant

```

Polarization status.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: get_polarization_status => particle_get_polarization_status

⟨Particles: procedures⟩+≡
  elemental function particle_get_polarization_status (prt) result (status)
    integer :: status
    class(particle_t), intent(in) :: prt
    status = prt%polarization
  end function particle_get_polarization_status

```

Return the PDG code from the flavor component directly.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: get_pdg => particle_get_pdg

⟨Particles: procedures⟩+≡
  elemental function particle_get_pdg (prt) result (pdg)
    integer :: pdg
    class(particle_t), intent(in) :: prt
    pdg = prt%flv%get_pdg ()
  end function particle_get_pdg

```

Return the color and anticolor quantum numbers.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: get_color => particle_get_color

⟨Particles: procedures⟩+≡
  pure function particle_get_color (prt) result (col)
    integer, dimension(2) :: col
    class(particle_t), intent(in) :: prt
    col(1) = prt%col%get_col ()
    col(2) = prt%col%get_acl ()
  end function particle_get_color

```

Return a copy of the polarization density matrix.

```

⟨Particles: particle: TBP⟩+≡
  procedure :: get_polarization => particle_get_polarization

⟨Particles: procedures⟩+≡
  function particle_get_polarization (prt) result (pol)
    class(particle_t), intent(in) :: prt
    type(polarization_t) :: pol
    pol = prt%pol
  end function particle_get_polarization

```


Return the flavor, color and helicity.

```
(Particles: particle: TBP)+≡  
  procedure :: get_flv => particle_get_flv  
  procedure :: get_col => particle_get_col  
  procedure :: get_hel => particle_get_hel  
  
(Particles: procedures)+≡  
  function particle_get_flv (prt) result (flv)  
    class(particle_t), intent(in) :: prt  
    type(flavor_t) :: flv  
    flv = prt%flv  
  end function particle_get_flv  
  
  function particle_get_col (prt) result (col)  
    class(particle_t), intent(in) :: prt  
    type(color_t) :: col  
    col = prt%col  
  end function particle_get_col  
  
  function particle_get_hel (prt) result (hel)  
    class(particle_t), intent(in) :: prt  
    type(helicity_t) :: hel  
    hel = prt%hel  
  end function particle_get_hel
```

Return the helicity (if defined and diagonal).

```
(Particles: particle: TBP)+≡  
  procedure :: get_helicity => particle_get_helicity  
  
(Particles: procedures)+≡  
  elemental function particle_get_helicity (prt) result (hel)  
    integer :: hel  
    integer, dimension(2) :: hel_arr  
    class(particle_t), intent(in) :: prt  
    hel = 0  
    if (prt%hel%is_defined () .and. prt%hel%is_diagonal ()) then  
      hel_arr = prt%hel%to_pair ()  
      hel = hel_arr (1)  
    end if  
  end function particle_get_helicity
```

Return the number of children/parents

```
(Particles: particle: TBP)+≡  
  procedure :: get_n_parents => particle_get_n_parents  
  procedure :: get_n_children => particle_get_n_children  
  
(Particles: procedures)+≡  
  elemental function particle_get_n_parents (prt) result (n)  
    integer :: n  
    class(particle_t), intent(in) :: prt  
    if (allocated (prt%parent)) then  
      n = size (prt%parent)  
    else  
      n = 0  
    end if  
  end function particle_get_n_parents
```

```

        end if
    end function particle_get_n_parents

    elemental function particle_get_n_children (prt) result (n)
        integer :: n
        class(particle_t), intent(in) :: prt
        if (allocated (prt%child)) then
            n = size (prt%child)
        else
            n = 0
        end if
    end function particle_get_n_children

```

Return the array of parents/children.

(Particles: particle: TBP)+≡

```

    procedure :: get_parents => particle_get_parents
    procedure :: get_children => particle_get_children

```

(Particles: procedures)+≡

```

    function particle_get_parents (prt) result (parent)
        class(particle_t), intent(in) :: prt
        integer, dimension(:), allocatable :: parent
        if (allocated (prt%parent)) then
            allocate (parent (size (prt%parent)))
            parent = prt%parent
        else
            allocate (parent (0))
        end if
    end function particle_get_parents

```

```

    function particle_get_children (prt) result (child)
        class(particle_t), intent(in) :: prt
        integer, dimension(:), allocatable :: child
        if (allocated (prt%child)) then
            allocate (child (size (prt%child)))
            child = prt%child
        else
            allocate (child (0))
        end if
    end function particle_get_children

```

(Particles: particle: TBP)+≡

```

    procedure :: has_children => particle_has_children

```

(Particles: procedures)+≡

```

    elemental function particle_has_children (prt) result (has_children)
        logical :: has_children
        class(particle_t), intent(in) :: prt
        has_children = .false.
        if (allocated (prt%child)) then
            has_children = size (prt%child) > 0
        end if
    end function particle_has_children

```

```

⟨Particles: particle: TBP⟩+=
  procedure :: has_parents => particle_has_parents

⟨Particles: procedures⟩+=
  elemental function particle_has_parents (prt) result (has_parents)
    logical :: has_parents
    class(particle_t), intent(in) :: prt
    has_parents = .false.
    if (allocated (prt%parent)) then
      has_parents = size (prt%parent) > 0
    end if
  end function particle_has_parents

```

Return momentum and momentum squared.

```

⟨Particles: particle: TBP⟩+=
  procedure :: get_momentum => particle_get_momentum
  procedure :: get_p2 => particle_get_p2

⟨Particles: procedures⟩+=
  elemental function particle_get_momentum (prt) result (p)
    type(vector4_t) :: p
    class(particle_t), intent(in) :: prt
    p = prt%p
  end function particle_get_momentum

  elemental function particle_get_p2 (prt) result (p2)
    real(default) :: p2
    class(particle_t), intent(in) :: prt
    p2 = prt%p2
  end function particle_get_p2

```

Return the particle vertex, if allocated.

```

⟨Particles: particle: TBP⟩+=
  procedure :: get_vertex => particle_get_vertex

⟨Particles: procedures⟩+=
  elemental function particle_get_vertex (prt) result (vtx)
    type(vector4_t) :: vtx
    class(particle_t), intent(in) :: prt
    if (allocated (prt%vertex)) then
      vtx = prt%vertex
    else
      vtx = vector4_null
    end if
  end function particle_get_vertex

```

Return the lifetime of a particle.

```

⟨Particles: particle: TBP⟩+=
  procedure :: get_lifetime => particle_get_lifetime

⟨Particles: procedures⟩+=
  elemental function particle_get_lifetime (prt) result (lifetime)
    real(default) :: lifetime
    class(particle_t), intent(in) :: prt

```

```

    if (allocated (prt%lifetime)) then
        lifetime = prt%lifetime
    else
        lifetime = 0
    end if
end function particle_get_lifetime

```

```

⟨Particles: particle: TBP⟩+≡
    procedure :: momentum_to_pythia6 => particle_momentum_to_pythia6

⟨Particles: procedures⟩+≡
    pure function particle_momentum_to_pythia6 (prt) result (p)
        real(double), dimension(1:5) :: p
        class(particle_t), intent(in) :: prt
        p = prt%p%to_pythia6 (sqrt (prt%p2))
    end function particle_momentum_to_pythia6

```

15.4.2 Particle sets

A particle set is what is usually called an event: an array of particles. The individual particle entries carry momentum, quantum numbers, polarization, and optionally connections. There is (also optionally) a correlated state-density matrix that maintains spin correlations that are lost in the individual particle entries.

```

⟨Particles: public⟩+≡
    public :: particle_set_t

⟨Particles: types⟩+≡
    type :: particle_set_t
        ! private !!!
        integer :: n_beam = 0
        integer :: n_in  = 0
        integer :: n_vir = 0
        integer :: n_out = 0
        integer :: n_tot = 0
        integer :: factorization_mode = FM_IGNORE_HELICITY
        type(particle_t), dimension(:), allocatable :: prt
        type(state_matrix_t) :: correlated_state
    contains
        ⟨Particles: particle set: TBP⟩
    end type particle_set_t

```

A particle set can be initialized from an interaction or from a HepMC event record.

```

⟨Particles: particle set: TBP⟩≡
    generic :: init => init_interaction
    procedure :: init_interaction => particle_set_init_interaction

```

When a particle set is initialized from a given interaction, we have to determine the branch within the original state matrix that fixes the particle quantum numbers. This is done with the appropriate probabilities, based on a random number x . The `mode` determines whether the individual particles become unpolarized,

or take a definite (diagonal) helicity, or acquire single-particle polarization matrices. The flag `keep_correlations` tells whether the spin-correlation matrix is to be calculated and stored in addition to the particles. The flag `keep_virtual` tells whether virtual particles should be dropped. Note that if virtual particles are dropped, the spin-correlation matrix makes no sense, and parent-child relations are not set.

For a correct disentangling of color and flavor (in the presence of helicity), we consider two interactions. `int` has no color information, and is used to select a flavor state. Consequently, we trace over helicities here. `int_flows` contains color-flow and potentially helicity information, but is useful only after the flavor combination has been chosen. So this interaction is used to select helicity and color, but restricted to the selected flavor combination.

`int` and `int_flows` may be identical if there is only a single (or no) color flow. If there is just a single flavor combination, `x(1)` can be set to zero.

The current algorithm of evaluator convolution requires that the beam particles are assumed outgoing (in the beam interaction) and become virtual in all derived interactions. In the particle set they should be re-identified as incoming. The optional integer `n_incoming` can be used to perform this correction.

The flag `is_valid` is false if factorization of the state is not possible, in particular if the squared matrix element is zero.

(Particles: procedures)+≡

```

subroutine particle_set_init_interaction &
  (particle_set, is_valid, int, int_flows, mode, x, &
   keep_correlations, keep_virtual, n_incoming, qn_select)
class(particle_set_t), intent(out) :: particle_set
logical, intent(out) :: is_valid
type(interaction_t), intent(in), target :: int, int_flows
integer, intent(in) :: mode
real(default), dimension(2), intent(in) :: x
logical, intent(in) :: keep_correlations, keep_virtual
integer, intent(in), optional :: n_incoming
type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
type(state_matrix_t), dimension(:), allocatable, target :: flavor_state
type(state_matrix_t), dimension(:), allocatable, target :: single_state
integer :: n_in, n_vir, n_out, n_tot
type(quantum_numbers_t), dimension(:,:), allocatable :: qn
logical :: ok
integer :: i, j
if (present (n_incoming)) then
  n_in = n_incoming
  n_vir = int%get_n_vir () - n_incoming
else
  n_in = int%get_n_in ()
  n_vir = int%get_n_vir ()
end if
n_out = int%get_n_out ()
n_tot = int%get_n_tot ()
particle_set%n_in = n_in
particle_set%n_out = n_out
if (keep_virtual) then
  particle_set%n_vir = n_vir
  particle_set%n_tot = n_tot

```

```

else
    particle_set%n_vir = 0
    particle_set%n_tot = n_in + n_out
end if
particle_set%factorization_mode = mode
allocate (qn (n_tot, 1))
if (.not. present (qn_select)) then
    call int%factorize &
        (FM_IGNORE_HELICITY, x(1), is_valid, flavor_state)
    do i = 1, n_tot
        qn(i,:) = flavor_state(i)%get_quantum_number (1)
    end do
else
    do i = 1, n_tot
        qn(i,:) = qn_select(i)
    end do
    is_valid = .true.
end if
if (keep_correlations .and. keep_virtual) then
    call particle_set%correlated_state%final ()
    call int_flows%factorize (mode, x(2), ok, &
        single_state, particle_set%correlated_state, qn(:,1))
else
    call int_flows%factorize (mode, x(2), ok, &
        single_state, qn_in=qn(:,1))
end if
is_valid = is_valid .and. ok
allocate (particle_set%prt (particle_set%n_tot))
j = 1
do i = 1, n_tot
    if (i <= n_in) then
        call particle_set%prt(j)%init (single_state(i), PRT_INCOMING, mode)
        call particle_set%prt(j)%set_momentum (int%get_momentum (i))
    else if (i <= n_in + n_vir) then
        if (.not. keep_virtual) cycle
        call particle_set%prt(j)%init &
            (single_state(i), PRT_VIRTUAL, mode)
        call particle_set%prt(j)%set_momentum (int%get_momentum (i))
    else
        call particle_set%prt(j)%init (single_state(i), PRT_OUTGOING, mode)
        call particle_set%prt(j)%set_momentum &
            (int%get_momentum (i), on_shell = .true.)
    end if
    if (keep_virtual) then
        call particle_set%prt(j)%set_children &
            (interaction_get_children (int, i))
        call particle_set%prt(j)%set_parents &
            (interaction_get_parents (int, i))
    end if
    j = j + 1
end do
if (keep_virtual) then
    call particle_set_resonance_flag &
        (particle_set%prt, int%get_resonance_flags ())

```

```

end if
if (allocated (flavor_state)) then
  do i = 1, size(flavor_state)
    call flavor_state(i)%final ()
  end do
end if
do i = 1, size(single_state)
  call single_state(i)%final ()
end do
end subroutine particle_set_init_interaction

```

Duplicate generic binding, to make sure that assignment works as it should.

```

<Particles: particle set: TBP>+≡
generic :: assignment(=) => init_particle_set
generic :: init => init_particle_set
procedure :: init_particle_set => particle_set_init_particle_set

<Particles: procedures>+≡
subroutine particle_set_init_particle_set (pset_out, pset_in)
  class(particle_set_t), intent(out) :: pset_out
  type(particle_set_t), intent(in) :: pset_in
  integer :: i
  pset_out%n_beam = pset_in%n_beam
  pset_out%n_in = pset_in%n_in
  pset_out%n_vir = pset_in%n_vir
  pset_out%n_out = pset_in%n_out
  pset_out%n_tot = pset_in%n_tot
  pset_out%factorization_mode = pset_in%factorization_mode
  if (allocated (pset_in%prt)) then
    allocate (pset_out%prt (size (pset_in%prt)))
    do i = 1, size (pset_in%prt)
      pset_out%prt(i) = pset_in%prt(i)
    end do
  end if
  pset_out%correlated_state = pset_in%correlated_state
end subroutine particle_set_init_particle_set

```

Manually set the model for the stored particles.

```

<Particles: particle set: TBP>+≡
procedure :: set_model => particle_set_set_model

<Particles: procedures>+≡
subroutine particle_set_set_model (particle_set, model)
  class(particle_set_t), intent(inout) :: particle_set
  class(model_data_t), intent(in), target :: model
  integer :: i
  do i = 1, particle_set%n_tot
    call particle_set%prt(i)%set_model (model)
  end do
  call particle_set%correlated_state%set_model (model)
end subroutine particle_set_set_model

```

Pointer components are hidden inside the particle polarization, and in the correlated state matrix.

```

⟨Particles: particle set: TBP⟩+≡
  procedure :: final => particle_set_final

⟨Particles: procedures⟩+≡
  subroutine particle_set_final (particle_set)
    class(particle_set_t), intent(inout) :: particle_set
    integer :: i
    if (allocated (particle_set%prt)) then
      do i = 1, size(particle_set%prt)
        call particle_set%prt(i)%final ()
      end do
      deallocate (particle_set%prt)
    end if
    call particle_set%correlated_state%final ()
  end subroutine particle_set_final

```

15.4.3 Manual build

Basic initialization. Just allocate with a given number of beam, incoming, virtual, and outgoing particles.

```

⟨Particles: particle set: TBP⟩+≡
  procedure :: basic_init => particle_set_basic_init

⟨Particles: procedures⟩+≡
  subroutine particle_set_basic_init (particle_set, n_beam, n_in, n_vir, n_out)
    class(particle_set_t), intent(out) :: particle_set
    integer, intent(in) :: n_beam, n_in, n_vir, n_out
    particle_set%n_beam = n_beam
    particle_set%n_in = n_in
    particle_set%n_vir = n_vir
    particle_set%n_out = n_out
    particle_set%n_tot = n_beam + n_in + n_vir + n_out
    allocate (particle_set%prt (particle_set%n_tot))
  end subroutine particle_set_basic_init

```

Build a particle set from scratch. This is used for testing purposes. The ordering of particles in the result is beam-incoming-remnant-virtual-outgoing.

Parent-child relations:

- Beams are parents of incoming and beam remnants. The assignment is alternating (first beam, second beam).
- Incoming are parents of virtual and outgoing, collectively.

More specific settings, such as resonance histories, cannot be set this way.

Beam-remnant particles are counted as virtual, but have a different status code.

We assume that the `pdg` array has the correct size.

```

⟨Particles: particle set: TBP⟩+≡
  procedure :: init_direct => particle_set_init_direct

```


(Particles: procedures)+≡

```

subroutine particle_set_init_direct (particle_set, &
    n_beam, n_in, n_rem, n_vir, n_out, pdg, model)
    class(particle_set_t), intent(out) :: particle_set
    integer, intent(in) :: n_beam
    integer, intent(in) :: n_in
    integer, intent(in) :: n_rem
    integer, intent(in) :: n_vir
    integer, intent(in) :: n_out
    integer, dimension(:), intent(in) :: pdg
    class(model_data_t), intent(in), target :: model
    type(flavor_t), dimension(:), allocatable :: flv
    integer :: i, k, n
    call particle_set%basic_init (n_beam, n_in, n_rem+n_vir, n_out)
    n = 0
    call particle_set%prt(n+1:n+n_beam)%reset_status (PRT_BEAM)
    do i = n+1, n+n_beam
        call particle_set%prt(i)%set_children &
            ([[k, k=i+n_beam, n+n_beam+n_in+n_rem, 2]])
    end do
    n = n + n_beam
    call particle_set%prt(n+1:n+n_in)%reset_status (PRT_INCOMING)
    do i = n+1, n+n_in
        if (n_beam > 0) then
            call particle_set%prt(i)%set_parents &
                ([i-n_beam])
        end if
        call particle_set%prt(i)%set_children &
            ([[k, k=n+n_in+n_rem+1, n+n_in+n_rem+n_vir+n_out]])
    end do
    n = n + n_in
    call particle_set%prt(n+1:n+n_rem)%reset_status (PRT_BEAM_REMNANT)
    do i = n+1, n+n_rem
        if (n_beam > 0) then
            call particle_set%prt(i)%set_parents &
                ([i-n_in-n_beam])
        end if
    end do
    n = n + n_rem
    call particle_set%prt(n+1:n+n_vir)%reset_status (PRT_VIRTUAL)
    do i = n+1, n+n_vir
        call particle_set%prt(i)%set_parents &
            ([[k, k=n-n_rem-n_in+1, n-n_rem]])
    end do
    n = n + n_vir
    call particle_set%prt(n+1:n+n_out)%reset_status (PRT_OUTGOING)
    do i = n+1, n+n_out
        call particle_set%prt(i)%set_parents &
            ([[k, k=n-n_vir-n_rem-n_in+1, n-n_vir-n_rem]])
    end do
    allocate (flv (particle_set%n_tot))
    call flv%init (pdg, model)
    do k = n_beam+n_in+1, n_beam+n_in+n_rem
        call flv(k)%tag_radiated ()
    end do
end subroutine

```

```

end do
do i = 1, particle_set%n_tot
  call particle_set%prt(i)%set_flavor (flv(i))
end do
end subroutine particle_set_init_direct

```

Copy a particle set into a new, extended one. Use the mapping array to determine the new positions of particles. The new set contains **n_new** additional entries. Count the new, undefined particles as virtual.

```

⟨Particles: particle set: TBP⟩+≡
  procedure :: transfer => particle_set_transfer

⟨Particles: procedures⟩+≡
  subroutine particle_set_transfer (pset, source, n_new, map)
    class(particle_set_t), intent(out) :: pset
    class(particle_set_t), intent(in) :: source
    integer, intent(in) :: n_new
    integer, dimension(:), intent(in) :: map
    integer :: i
    call pset%basic_init &
      (source%n_beam, source%n_in, source%n_vir + n_new, source%n_out)
    pset%factorization_mode = source%factorization_mode
    do i = 1, source%n_tot
      call pset%prt(map(i))%reset_status (source%prt(i)%get_status ())
      call pset%prt(map(i))%set_flavor (source%prt(i)%get_flv ())
      call pset%prt(map(i))%set_color (source%prt(i)%get_col ())
      call pset%prt(map(i))%set_parents (map (source%prt(i)%get_parents ()))
      call pset%prt(map(i))%set_children (map (source%prt(i)%get_children ()))
      call pset%prt(map(i))%set_polarization &
        (source%prt(i)%get_polarization_status ())
      select case (source%prt(i)%get_polarization_status ())
      case (PRT_DEFINITE_HELICITY)
        call pset%prt(map(i))%set_helicity (source%prt(i)%get_hel ())
      case (PRT_GENERIC_POLARIZATION)
        call pset%prt(map(i))%set_pol (source%prt(i)%get_polarization ())
      end select
    end do
  end subroutine particle_set_transfer

```

Insert a new particle as an intermediate into a previously empty position.

Flavor and status are just set. Color is not set (but see below). The complicated part is reassigning parent-child relations. The inserted particle comes with an array **child** of its children which are supposed to be existing particles.

We first scan all particles that come before the new insertion. Whenever a particle has children that coincide with the children of the new particle, those child entries are removed. (a) If the new particle has no parent entry yet, those child entries are replaced by the index of the new particle and simultaneously, the particle is registered as a parent of the new particle. (b) If the current particle already has a parent entry, those child entries are removed.

When this is done, the new particle is registered as the (only) parent of its children.

```

⟨Particles: particle set: TBP⟩+≡

```

```

    procedure :: insert => particle_set_insert
  <Particles: procedures>+≡
    subroutine particle_set_insert (pset, i, status, flv, child)
      class(particle_set_t), intent(inout) :: pset
      integer, intent(in) :: i
      integer, intent(in) :: status
      type(flavor_t), intent(in) :: flv
      integer, dimension(:), intent(in) :: child
      integer, dimension(:), allocatable :: p_child, parent
      integer :: j, k, c, n_parent
      logical :: no_match
      call pset%prt(i)%reset_status (status)
      call pset%prt(i)%set_flavor (flv)
      call pset%prt(i)%set_children (child)
      n_parent = pset%prt(i)%get_n_parents ()
      do j = 1, i - 1
        p_child = pset%prt(j)%get_children ()
        no_match = .true.
        do k = 1, size (p_child)
          if (any (p_child(k) == child)) then
            if (n_parent == 0 .and. no_match) then
              if (.not. allocated (parent)) then
                parent = [j]
              else
                parent = [parent, j]
              end if
              p_child(k) = i
            else
              p_child(k) = 0
            end if
            no_match = .false.
          end if
        end do
        if (.not. no_match) then
          p_child = pack (p_child, p_child /= 0)
          call pset%prt(j)%set_children (p_child)
        end if
      end do
      if (n_parent == 0) then
        call pset%prt(i)%set_parents (parent)
      end if
      do j = 1, size (child)
        c = child(j)
        call pset%prt(c)%set_parents ([i])
      end do
    end subroutine particle_set_insert

```

This should be done after completing all insertions: recover color assignments for the inserted particles, working backwards from children to parents. A single call to the routine recovers the color and anticolor line indices for a single particle.

```

  <Particles: particle set: TBP>+≡
    procedure :: recover_color => particle_set_recover_color

```

```

(Particles: procedures) +=
  subroutine particle_set_recover_color (pset, i)
    class(particle_set_t), intent(inout) :: pset
    integer, intent(in) :: i
    type(color_t) :: col
    integer, dimension(:), allocatable :: child
    integer :: j
    child = pset%prt(i)%get_children ()
    if (size (child) > 0) then
      col = pset%prt(child(1))%get_col ()
      do j = 2, size (child)
        col = col .fuse. pset%prt(child(j))%get_col ()
      end do
      call pset%prt(i)%set_color (col)
    end if
  end subroutine particle_set_recover_color

```

15.4.4 Extract/modify contents

```

(Particles: particle set: TBP) +=
  generic :: get_color => get_color_all
  generic :: get_color => get_color_indices
  procedure :: get_color_all => particle_set_get_color_all
  procedure :: get_color_indices => particle_set_get_color_indices

```

```

(Particles: procedures) +=
  function particle_set_get_color_all (particle_set) result (col)
    class(particle_set_t), intent(in) :: particle_set
    type(color_t), dimension(:), allocatable :: col
    allocate (col (size (particle_set%prt)))
    col = particle_set%prt%col
  end function particle_set_get_color_all

```

```

(Particles: procedures) +=
  function particle_set_get_color_indices (particle_set, indices) result (col)
    type(color_t), dimension(:), allocatable :: col
    class(particle_set_t), intent(in) :: particle_set
    integer, intent(in), dimension(:), allocatable :: indices
    integer :: i
    allocate (col (size (indices)))
    do i = 1, size (indices)
      col(i) = particle_set%prt(indices(i))%col
    end do
  end function particle_set_get_color_indices

```

Set a single or all color components. This is a wrapper around the corresponding `particle_t` method, with the same options. We assume that the particle array is allocated.

```

(Particles: particle set: TBP) +=
  generic :: set_color => set_color_single
  generic :: set_color => set_color_indices
  generic :: set_color => set_color_all

```

```

procedure :: set_color_single => particle_set_set_color_single
procedure :: set_color_indices => particle_set_set_color_indices
procedure :: set_color_all => particle_set_set_color_all

(Particles: procedures)+=
subroutine particle_set_set_color_single (particle_set, i, col)
  class(particle_set_t), intent(inout) :: particle_set
  integer, intent(in) :: i
  type(color_t), intent(in) :: col
  call particle_set%prt(i)%set_color (col)
end subroutine particle_set_set_color_single

subroutine particle_set_set_color_indices (particle_set, indices, col)
  class(particle_set_t), intent(inout) :: particle_set
  integer, dimension(:), intent(in) :: indices
  type(color_t), dimension(:), intent(in) :: col
  integer :: i
  do i = 1, size (indices)
    call particle_set%prt(indices(i))%set_color (col(i))
  end do
end subroutine particle_set_set_color_indices

subroutine particle_set_set_color_all (particle_set, col)
  class(particle_set_t), intent(inout) :: particle_set
  type(color_t), dimension(:), intent(in) :: col
  call particle_set%prt%set_color (col)
end subroutine particle_set_set_color_all

```

Assigning particles manually may result in color mismatches. This is checked here for all particles in the set. The color object is compared against the color type that belongs to the flavor object. The return value is an allocatable array which consists of the particles with invalid color assignments. If the array size is zero, all is fine.

```

(Particles: particle set: TBP)+=
  procedure :: find_prt_invalid_color => particle_set_find_prt_invalid_color

(Particles: procedures)+=
subroutine particle_set_find_prt_invalid_color (particle_set, index, prt)
  class(particle_set_t), intent(in) :: particle_set
  integer, dimension(:), allocatable, intent(out) :: index
  type(particle_t), dimension(:), allocatable, intent(out), optional :: prt
  type(flavor_t) :: flv
  type(color_t) :: col
  logical, dimension(:), allocatable :: mask
  integer :: i, n, n_invalid
  n = size (particle_set%prt)
  allocate (mask (n))
  do i = 1, n
    associate (prt => particle_set%prt(i))
      flv = prt%get_flv ()
      col = prt%get_col ()
      mask(i) = flv%get_color_type () /= col%get_type ()
    end associate
  end do
end subroutine particle_set_find_prt_invalid_color

```

```

        index = pack ([i, i = 1, n]), mask)
    if (present (prt)) prt = pack (particle_set%prt, mask)
end subroutine particle_set_find_prt_invalid_color

```

(Particles: particle set: TBP)+≡

```

generic :: get_momenta => get_momenta_all
generic :: get_momenta => get_momenta_indices
procedure :: get_momenta_all => particle_set_get_momenta_all
procedure :: get_momenta_indices => particle_set_get_momenta_indices

```

(Particles: procedures)+≡

```

function particle_set_get_momenta_all (particle_set) result (p)
    class(particle_set_t), intent(in) :: particle_set
    type(vector4_t), dimension(:), allocatable :: p
    allocate (p (size (particle_set%prt)))
    p = particle_set%prt%p
end function particle_set_get_momenta_all

```

(Particles: procedures)+≡

```

function particle_set_get_momenta_indices (particle_set, indices) result (p)
    type(vector4_t), dimension(:), allocatable :: p
    class(particle_set_t), intent(in) :: particle_set
    integer, intent(in), dimension(:), allocatable :: indices
    integer :: i
    allocate (p (size (indices)))
    do i = 1, size (indices)
        p(i) = particle_set%prt(indices(i))%p
    end do
end function particle_set_get_momenta_indices

```

Replace a single or all momenta. This is a wrapper around the corresponding `particle_t` method, with the same options. We assume that the particle array is allocated.

(Particles: particle set: TBP)+≡

```

generic :: set_momentum => set_momentum_single
generic :: set_momentum => set_momentum_indices
generic :: set_momentum => set_momentum_all
procedure :: set_momentum_single => particle_set_set_momentum_single
procedure :: set_momentum_indices => particle_set_set_momentum_indices
procedure :: set_momentum_all => particle_set_set_momentum_all

```

(Particles: procedures)+≡

```

subroutine particle_set_set_momentum_single &
    (particle_set, i, p, p2, on_shell)
    class(particle_set_t), intent(inout) :: particle_set
    integer, intent(in) :: i
    type(vector4_t), intent(in) :: p
    real(default), intent(in), optional :: p2
    logical, intent(in), optional :: on_shell
    call particle_set%prt(i)%set_momentum (p, p2, on_shell)
end subroutine particle_set_set_momentum_single

subroutine particle_set_set_momentum_indices &

```

```

        (particle_set, indices, p, p2, on_shell)
class(particle_set_t), intent(inout) :: particle_set
integer, dimension(:), intent(in) :: indices
type(vector4_t), dimension(:), intent(in) :: p
real(default), dimension(:), intent(in), optional :: p2
logical, intent(in), optional :: on_shell
integer :: i
if (present (p2)) then
    do i = 1, size (indices)
        call particle_set%prt(indices(i))%set_momentum (p(i), p2(i), on_shell)
    end do
else
    do i = 1, size (indices)
        call particle_set%prt(indices(i))%set_momentum &
            (p(i), on_shell=on_shell)
    end do
end if
end subroutine particle_set_set_momentum_indices

subroutine particle_set_set_momentum_all (particle_set, p, p2, on_shell)
class(particle_set_t), intent(inout) :: particle_set
type(vector4_t), dimension(:), intent(in) :: p
real(default), dimension(:), intent(in), optional :: p2
logical, intent(in), optional :: on_shell
call particle_set%prt%set_momentum (p, p2, on_shell)
end subroutine particle_set_set_momentum_all

```

Recover a momentum by recombining from children, assuming that this is possible. The reconstructed momentum is not projected on-shell.

(Particles: particle set: TBP)+≡

```

    procedure :: recover_momentum => particle_set_recover_momentum

```

(Particles: procedures)+≡

```

subroutine particle_set_recover_momentum (particle_set, i)
class(particle_set_t), intent(inout) :: particle_set
integer, intent(in) :: i
type(vector4_t), dimension(:), allocatable :: p
integer, dimension(:), allocatable :: index
index = particle_set%prt(i)%get_children ()
p = particle_set%get_momenta (index)
call particle_set%set_momentum (i, sum (p))
end subroutine particle_set_recover_momentum

```

(Particles: particle set: TBP)+≡

```

    procedure :: replace_incoming_momenta => particle_set_replace_incoming_momenta

```

(Particles: procedures)+≡

```

subroutine particle_set_replace_incoming_momenta (particle_set, p)
class(particle_set_t), intent(inout) :: particle_set
type(vector4_t), intent(in), dimension(:) :: p
integer :: i, j
i = 1
do j = 1, particle_set%get_n_tot ()
    if (particle_set%prt(j)%get_status () == PRT_INCOMING) then

```

```

        particle_set%prt(j)%p = p(i)
        i = i + 1
        if (i > particle_set%n_in) exit
    end if
end do
end subroutine particle_set_replace_incoming_momenta

```

<Particles: particle set: TBP>+≡
 procedure :: replace_outgoing_momenta => particle_set_replace_outgoing_momenta

<Particles: procedures>+≡
 subroutine particle_set_replace_outgoing_momenta (particle_set, p)
 class(particle_set_t), intent(inout) :: particle_set
 type(vector4_t), intent(in), dimension(:) :: p
 integer :: i, j
 i = particle_set%n_in + 1
 do j = 1, particle_set%n_tot
 if (particle_set%prt(j)%get_status () == PRT_OUTGOING) then
 particle_set%prt(j)%p = p(i)
 i = i + 1
 end if
 end do
end subroutine particle_set_replace_outgoing_momenta

<Particles: particle set: TBP>+≡
 procedure :: get_outgoing_momenta => particle_set_get_outgoing_momenta

<Particles: procedures>+≡
 function particle_set_get_outgoing_momenta (particle_set) result (p)
 class(particle_set_t), intent(in) :: particle_set
 type(vector4_t), dimension(:), allocatable :: p
 integer :: i, k
 allocate (p (count (particle_set%prt%get_status () == PRT_OUTGOING)))
 k = 0
 do i = 1, size (particle_set%prt)
 if (particle_set%prt(i)%get_status () == PRT_OUTGOING) then
 k = k + 1
 p(k) = particle_set%prt(i)%get_momentum ()
 end if
 end do
end function particle_set_get_outgoing_momenta

<Particles: particle set: TBP>+≡
 procedure :: parent_add_child => particle_set_parent_add_child

<Particles: procedures>+≡
 subroutine particle_set_parent_add_child (particle_set, parent, child)
 class(particle_set_t), intent(inout) :: particle_set
 integer, intent(in) :: parent, child
 call particle_set%prt(child)%set_parents ([parent])
 call particle_set%prt(parent)%add_child (child)
end subroutine particle_set_parent_add_child

Given the `particle_set` before radiation, the new momenta `p_radiated`, the emitter and the `flv_radiated` as well as the model and a random number `r_color` for choosing a color, we update the `particle_set`.

(Particles: particle set: TBP)+≡

```
procedure :: build_radiation => particle_set_build_radiation
```

(Particles: procedures)+≡

```
subroutine particle_set_build_radiation (particle_set, p_radiated, &
    emitter, flv_radiated, model, r_color)
    class(particle_set_t), intent(inout) :: particle_set
    type(vector4_t), intent(in), dimension(:) :: p_radiated
    integer, intent(in) :: emitter
    integer, intent(in), dimension(:) :: flv_radiated
    class(model_data_t), intent(in), target :: model
    real(default), intent(in) :: r_color
    type(particle_set_t) :: new_particle_set
    type(particle_t) :: new_particle
    integer :: i
    integer :: pdg_index_emitter, pdg_index_radiation
    integer, dimension(:), allocatable :: parents, children
    type(flavor_t) :: new_flv
    logical, dimension(:), allocatable :: status_mask
    integer, dimension(:), allocatable :: &
        i_in1, i_beam1, i_remnant1, i_virt1, i_out1
    integer, dimension(:), allocatable :: &
        i_in2, i_beam2, i_remnant2, i_virt2, i_out2
    integer :: n_in1, n_beam1, n_remnant1, n_virt1, n_out1
    integer :: n_in2, n_beam2, n_remnant2, n_virt2, n_out2
    integer :: n, n_tot
    integer :: i_emitter

    n = particle_set%get_n_tot ()
    allocate (status_mask (n))
    do i = 1, n
        status_mask(i) = particle_set%prt(i)%get_status () == PRT_INCOMING
    end do
    n_in1 = count (status_mask)
    allocate (i_in1 (n_in1))
    i_in1 = particle_set%get_indices (status_mask)
    do i = 1, n
        status_mask(i) = particle_set%prt(i)%get_status () == PRT_BEAM
    end do
    n_beam1 = count (status_mask)
    allocate (i_beam1 (n_beam1))
    i_beam1 = particle_set%get_indices (status_mask)
    do i = 1, n
        status_mask(i) = particle_set%prt(i)%get_status () == PRT_BEAM_REMNANT
    end do
    n_remnant1 = count (status_mask)
    allocate (i_remnant1 (n_remnant1))
    i_remnant1 = particle_set%get_indices (status_mask)
    do i = 1, n
        status_mask(i) = particle_set%prt(i)%get_status () == PRT_VIRTUAL
    end do
```

```

n_virt1 = count (status_mask)
allocate (i_virt1 (n_virt1))
i_virt1 = particle_set%get_indices (status_mask)
do i = 1, n
    status_mask(i) = particle_set%prt(i)%get_status () == PRT_OUTGOING
end do
n_out1 = count (status_mask)
allocate (i_out1 (n_out1))
i_out1 = particle_set%get_indices (status_mask)

n_in2 = n_in1; n_beam2 = n_beam1; n_remnant2 = n_remnant1
n_virt2 = n_virt1 + n_out1
n_out2 = n_out1 + 1
n_tot = n_in2 + n_beam2 + n_remnant2 + n_virt2 + n_out2

allocate (i_in2 (n_in2), i_beam2 (n_beam2), i_remnant2 (n_remnant2))
i_in2 = i_in1; i_beam2 = i_beam1; i_remnant2 = i_remnant1

allocate (i_virt2 (n_virt2))
i_virt2(1 : n_virt1) = i_virt1
i_virt2(n_virt1 + 1 : n_virt2) = i_out1

allocate (i_out2 (n_out2))
i_out2(1 : n_out1) = i_out1(1 : n_out1) + n_out1
i_out2(n_out2) = n_tot

new_particle_set%n_beam = n_beam2
new_particle_set%n_in = n_in2
new_particle_set%n_vir = n_virt2
new_particle_set%n_out = n_out2
new_particle_set%n_tot = n_tot
new_particle_set%correlated_state = particle_set%correlated_state
allocate (new_particle_set%prt (n_tot))
if (size (i_beam1) > 0) new_particle_set%prt(i_beam2) = particle_set%prt(i_beam1)
if (size (i_remnant1) > 0) new_particle_set%prt(i_remnant2) = particle_set%prt(i_remnant1)
do i = 1, n_virt1
    new_particle_set%prt(i_virt2(i)) = particle_set%prt(i_virt1(i))
end do

do i = n_virt1 + 1, n_virt2
    new_particle_set%prt(i_virt2(i)) = particle_set%prt(i_out1(i - n_virt1))
    call new_particle_set%prt(i_virt2(i))%reset_status (PRT_VIRTUAL)
end do

do i = 1, n_in2
    new_particle_set%prt(i_in2(i)) = particle_set%prt(i_in1(i))
    new_particle_set%prt(i_in2(i))%p = p_radiated (i)
end do

do i = 1, n_out2 - 1
    new_particle_set%prt(i_out2(i)) = particle_set%prt(i_out1(i))
    new_particle_set%prt(i_out2(i))%p = p_radiated(i + n_in2)
    call new_particle_set%prt(i_out2(i))%reset_status (PRT_OUTGOING)
end do

```

```

call new_particle%reset_status (PRT_OUTGOING)
call new_particle%set_momentum (p_radiated (n_in2 + n_out2))

!!! Helicity and polarization handling is missing at this point
!!! Also, no helicities or polarizations yet
pdg_index_emitter = flv_radiated (emitter)
pdg_index_radiation = flv_radiated (n_in2 + n_out2)
call new_flv%init (pdg_index_radiation, model)
i_emitter = emitter + n_virt2 + n_remnant2 + n_beam2

call reassign_colors (new_particle, new_particle_set%prt(i_emitter), &
    pdg_index_radiation, pdg_index_emitter, r_color)

call new_particle%set_flavor (new_flv)
new_particle_set%prt(n_tot) = new_particle

allocate (children (n_out2))
children = i_out2
do i = n_in2 + n_beam2 + n_remnant2 + n_virt1 + 1, n_in2 + n_beam2 + n_remnant2 + n_virt2
    call new_particle_set%prt(i)%set_children (children)
end do

!!! Set proper parents for outgoing particles
allocate (parents (n_out1))
parents = i_out1
do i = n_in2 + n_beam2 + n_remnant2 + n_virt2 + 1, n_tot
    call new_particle_set%prt(i)%set_parents (parents)
end do
call particle_set%init (new_particle_set)
contains

<build radiation: set color offset>
subroutine reassign_colors (prt_radiated, prt_emitter, i_rad, i_em, r_col)
    type(particle_t), intent(inout) :: prt_radiated, prt_emitter
    integer, intent(in) :: i_rad, i_em
    real(default), intent(in) :: r_col
    type(color_t) :: col_rad, col_em
    if (is_quark (i_em) .and. is_gluon (i_rad)) then
        call reassign_colors_qg (prt_emitter, col_rad, col_em)
    else if (is_gluon (i_em) .and. is_gluon (i_rad)) then
        call reassign_colors_gg (prt_emitter, r_col, col_rad, col_em)
    else if (is_gluon (i_em) .and. is_quark (i_rad)) then
        call reassign_colors_qq (prt_emitter, i_em, col_rad, col_em)
    else
        call msg_fatal ("Invalid splitting")
    end if
    call prt_emitter%set_color (col_em)
    call prt_radiated%set_color (col_rad)
end subroutine reassign_colors

subroutine reassign_colors_qg (prt_emitter, col_rad, col_em)
    type(particle_t), intent(in) :: prt_emitter
    type(color_t), intent(out) :: col_rad, col_em

```

```

integer, dimension(2) :: color_rad, color_em
integer :: i1, i2
integer :: new_color_index
logical :: is_anti_quark

color_em = prt_emitter%get_color ()
i1 = 1; i2 = 2
is_anti_quark = color_em(2) /= 0
if (is_anti_quark) then
    i1 = 2; i2 = 1
end if
new_color_index = color_em(i1)+1
color_rad(i1) = color_em(i1)
color_rad(i2) = new_color_index
color_em(i1) = new_color_index
call col_em%init_col_acl (color_em(1), color_em(2))
call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_qg

subroutine reassign_colors_gg (prt_emitter, random, col_rad, col_em)
    !!! NOT TESTED YET
    type(particle_t), intent(in) :: prt_emitter
    real(default), intent(in) :: random
    type(color_t), intent(out) :: col_rad, col_em
    integer, dimension(2) :: color_rad, color_em
    integer :: i1, i2
    integer :: new_color_index

    color_em = prt_emitter%get_color ()
    new_color_index = maxval (abs (color_em))
    i1 = 1; i2 = 2
    if (random < 0.5) then
        i1 = 2; i2 = 1
    end if
    color_rad(i1) = new_color_index
    color_rad(i2) = color_em(i2)
    color_em(i2) = new_color_index
    call col_em%init_col_acl (color_em(1), color_em(2))
    call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_gg

subroutine reassign_colors_qq (prt_emitter, pdg_emitter, col_rad, col_em)
    !!! NOT TESTED YET
    type(particle_t), intent(in) :: prt_emitter
    integer, intent(in) :: pdg_emitter
    type(color_t), intent(out) :: col_rad, col_em
    integer, dimension(2) :: color_rad, color_em
    integer :: i1, i2
    logical :: is_anti_quark

    color_em = prt_emitter%get_color ()
    i1 = 1; i2 = 2
    is_anti_quark = pdg_emitter < 0
    if (is_anti_quark) then

```

```

        i1 = 2; i1 = 1
    end if
    color_em(i2) = 0
    color_rad(i1) = 0
    color_rad(i2) = color_em(i1)
    call col_em%init_col_acl (color_em(1), color_em(2))
    call col_rad%init_col_acl (color_rad(1), color_rad(2))
end subroutine reassign_colors_qq
end subroutine particle_set_build_radiation

```

Increments the color indices of all particles by their maximal value to distinguish them from the record-keeping Born particles in the LHE-output if the virtual entries are kept.

```

<build radiation: set color offset>≡
subroutine set_color_offset (particle_set)
    type(particle_set_t), intent(inout) :: particle_set
    integer, dimension(2) :: color
    integer :: i, i_color_max
    type(color_t) :: new_color

    i_color_max = 0
    do i = 1, size (particle_set%prt)
        associate (prt => particle_set%prt(i))
            if (prt%get_status () <= PRT_INCOMING) cycle
            color = prt%get_color ()
            i_color_max = maxval([i_color_max, color(1), color(2)])
        end associate
    end do

    do i = 1, size (particle_set%prt)
        associate (prt => particle_set%prt(i))
            if (prt%get_status () /= PRT_OUTGOING) cycle
            color = prt%get_color ()
            where (color /= 0) color = color + i_color_max
            call new_color%init_col_acl (color(1), color(2))
            call prt%set_color (new_color)
        end associate
    end do
end subroutine set_color_offset

```

Output (default format)

```

<Particles: particle set: TBP>+≡
    procedure :: write => particle_set_write

<Particles: procedures>+≡
subroutine particle_set_write &
    (particle_set, unit, testflag, summary, compressed)
class(particle_set_t), intent(in) :: particle_set
integer, intent(in), optional :: unit
logical, intent(in), optional :: testflag, summary, compressed
logical :: summ, comp, pol
type(vector4_t) :: sum_vec

```

```

integer :: u, i
u = given_output_unit (unit); if (u < 0) return
summ = .false.; if (present (summary)) summ = summary
comp = .false.; if (present (compressed)) comp = compressed
pol = particle_set%factorization_mode /= FM_IGNORE_HELICITY
write (u, "(1x,A)") "Particle set:"
call write_separator (u)
if (comp) then
  if (pol) then
    write (u, &
      "((A4,1X),(A6,1X),(A7,1X),(A3),2(A4,1X),2(A20,1X),5(A12,1X)))" &
      "Nr", "Status", "Flavor", "Hel", "Col", "ACol", &
      "Parents", "Children", &
      "P(0)", "P(1)", "P(2)", "P(3)", "P^2"
    )
  else
    write (u, &
      "((A4,1X),(A6,1X),(A7,1X),2(A4,1X),2(A20,1X),5(A12,1X)))" &
      "Nr", "Status", "Flavor", "Col", "ACol", &
      "Parents", "Children", &
      "P(0)", "P(1)", "P(2)", "P(3)", "P^2"
    )
  end if
end if
if (particle_set%n_tot /= 0) then
  do i = 1, particle_set%n_tot
    if (comp) then
      write (u, "(I4,1X,2X)", advance="no") i
    else
      write (u, "(1x,A,1x,I0)", advance="no") "Particle", i
    end if
    call particle_set%prt(i)%write (u, testflag = testflag, &
      compressed = comp, polarization = pol)
  end do
  if (particle_set%correlated_state%is_defined ()) then
    call write_separator (u)
    write (u, *) "Correlated state density matrix:"
    call particle_set%correlated_state%write (u)
  end if
  if (summ) then
    call write_separator (u)
    write (u, "(A)", advance="no") &
      "Sum of incoming momenta: p(0:3) = "
    sum_vec = sum (particle_set%prt%p, &
      mask=particle_set%prt%get_status () == PRT_INCOMING)
    call pacify (sum_vec, tolerance = 1E-3_default)
    call sum_vec%write (u, compressed=.true.)
    write (u, *)
    write (u, "(A)", advance="no") &
      "Sum of beam remnant momenta: p(0:3) = "
    sum_vec = sum (particle_set%prt%p, &
      mask=particle_set%prt%get_status () == PRT_BEAM_REMNANT)
    call pacify (sum_vec, tolerance = 1E-3_default)
    call sum_vec%write (u, compressed=.true.)
    write (u, *)
    write (u, "(A)", advance="no") &

```

```

        "Sum of outgoing momenta: p(0:3) =      "
sum_vec = sum (particle_set%prt%p, &
        mask=particle_set%prt%get_status () == PRT_OUTGOING)
call pacify (sum_vec, tolerance = 1E-3_default)
call sum_vec%write (u, compressed=.true.)
write (u, "(A)") ""
    end if
else
    write (u, "(3x,A)") "[empty]"
end if
end subroutine particle_set_write

```

15.4.5 I/O formats

Here, we define input/output of particle sets in various formats. This is the right place since particle sets contain most of the event information.

All write/read routines take as first argument the object, as second argument the I/O unit which in this case is a mandatory argument. Then follow further event data.

Internal binary format

This format is supposed to contain the complete information, so the particle data set can be fully reconstructed. The exception is the model part of the particle flavors; this is unassigned for the flavor values read from file.

```

<Particles: particle set: TBP>+≡
    procedure :: write_raw => particle_set_write_raw
    procedure :: read_raw => particle_set_read_raw

<Particles: procedures>+≡
    subroutine particle_set_write_raw (particle_set, u)
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in) :: u
        integer :: i
        write (u) &
            particle_set%n_beam, particle_set%n_in, &
            particle_set%n_vir, particle_set%n_out
        write (u) particle_set%factorization_mode
        write (u) particle_set%n_tot
        do i = 1, particle_set%n_tot
            call particle_set%prt(i)%write_raw (u)
        end do
        call particle_set%correlated_state%write_raw (u)
    end subroutine particle_set_write_raw

    subroutine particle_set_read_raw (particle_set, u, iostat)
        class(particle_set_t), intent(out) :: particle_set
        integer, intent(in) :: u
        integer, intent(out) :: iostat
        integer :: i
        read (u, iostat=iostat) &
            particle_set%n_beam, particle_set%n_in, &

```

```

        particle_set%n_vir, particle_set%n_out
    read (u, iostat=iostat) particle_set%factorization_mode
    read (u, iostat=iostat) particle_set%n_tot
    allocate (particle_set%prt (particle_set%n_tot))
    do i = 1, size (particle_set%prt)
        call particle_set%prt(i)%read_raw (u, iostat=iostat)
    end do
    call particle_set%correlated_state%read_raw (u, iostat=iostat)
end subroutine particle_set_read_raw

```

Get contents

Find parents/children of a particular particle recursively; the search terminates if a parent/child has status BEAM, INCOMING, OUTGOING or RESONANT.

(Particles: particle set: TBP)+≡

```

    procedure :: get_real_parents => particle_set_get_real_parents
    procedure :: get_real_children => particle_set_get_real_children

```

(Particles: procedures)+≡

```

function particle_set_get_real_parents (pset, i, keep_beams) result (parent)
    integer, dimension(:), allocatable :: parent
    class(particle_set_t), intent(in) :: pset
    integer, intent(in) :: i
    logical, intent(in), optional :: keep_beams
    logical, dimension(:), allocatable :: is_real
    logical, dimension(:), allocatable :: is_parent, is_real_parent
    logical :: kb
    integer :: j, k
    kb = .false.
    if (present (keep_beams)) kb = keep_beams
    allocate (is_real (pset%n_tot))
    is_real = pset%prt%is_real (kb)
    allocate (is_parent (pset%n_tot), is_real_parent (pset%n_tot))
    is_real_parent = .false.
    is_parent = .false.
    is_parent(pset%prt(i)%get_parents()) = .true.
    do while (any (is_parent))
        where (is_real .and. is_parent)
            is_real_parent = .true.
            is_parent = .false.
        end where
        mark_next_parent: do j = size (is_parent), 1, -1
            if (is_parent(j)) then
                is_parent(pset%prt(j)%get_parents()) = .true.
                is_parent(j) = .false.
                exit mark_next_parent
            end if
        end do mark_next_parent
    end do
    allocate (parent (count (is_real_parent)))
    j = 0
    do k = 1, size (is_real_parent)
        if (is_real_parent(k)) then

```



```

        j = j + 1
        parent(j) = k
    end if
end do
end function particle_set_get_real_parents

function particle_set_get_real_children (pset, i, keep_beams) result (child)
    integer, dimension(:), allocatable :: child
    class(particle_set_t), intent(in) :: pset
    integer, intent(in) :: i
    logical, dimension(:), allocatable :: is_real
    logical, dimension(:), allocatable :: is_child, is_real_child
    logical, intent(in), optional :: keep_beams
    integer :: j, k
    logical :: kb
    kb = .false.
    if (present (keep_beams)) kb = keep_beams
    allocate (is_real (pset%n_tot))
    is_real = pset%prt%is_real (kb)
    is_real = pset%prt%is_real (kb)
    allocate (is_child (pset%n_tot), is_real_child (pset%n_tot))
    is_real_child = .false.
    is_child = .false.
    is_child(pset%prt(i)%get_children()) = .true.
    do while (any (is_child))
        where (is_real .and. is_child)
            is_real_child = .true.
            is_child = .false.
        end where
        mark_next_child: do j = 1, size (is_child)
            if (is_child(j)) then
                is_child(pset%prt(j)%get_children()) = .true.
                is_child(j) = .false.
                exit mark_next_child
            end if
        end do mark_next_child
    end do
    allocate (child (count (is_real_child)))
    j = 0
    do k = 1, size (is_child)
        if (is_real_child(k)) then
            j = j + 1
            child(j) = k
        end if
    end do
end function particle_set_get_real_children

```

Get the n_tot, n_in, and n_out values out of the particle set.

(Particles: particle set: TBP)+≡

```

procedure :: get_n_beam => particle_set_get_n_beam
procedure :: get_n_in => particle_set_get_n_in
procedure :: get_n_vir => particle_set_get_n_vir
procedure :: get_n_out => particle_set_get_n_out

```

```

procedure :: get_n_tot => particle_set_get_n_tot
procedure :: get_n_remnants => particle_set_get_n_remnants

(Particles: procedures) +=
function particle_set_get_n_beam (pset) result (n_beam)
  class(particle_set_t), intent(in) :: pset
  integer :: n_beam
  n_beam = pset%n_beam
end function particle_set_get_n_beam

function particle_set_get_n_in (pset) result (n_in)
  class(particle_set_t), intent(in) :: pset
  integer :: n_in
  n_in = pset%n_in
end function particle_set_get_n_in

function particle_set_get_n_vir (pset) result (n_vir)
  class(particle_set_t), intent(in) :: pset
  integer :: n_vir
  n_vir = pset%n_vir
end function particle_set_get_n_vir

function particle_set_get_n_out (pset) result (n_out)
  class(particle_set_t), intent(in) :: pset
  integer :: n_out
  n_out = pset%n_out
end function particle_set_get_n_out

function particle_set_get_n_tot (pset) result (n_tot)
  class(particle_set_t), intent(in) :: pset
  integer :: n_tot
  n_tot = pset%n_tot
end function particle_set_get_n_tot

function particle_set_get_n_remnants (pset) result (n_remn)
  class(particle_set_t), intent(in) :: pset
  integer :: n_remn
  if (allocated (pset%prt)) then
    n_remn = count (pset%prt%get_status () == PRT_BEAM_REMNANT)
  else
    n_remn = 0
  end if
end function particle_set_get_n_remnants

```

Return a pointer to the particle corresponding to the number

```

(Particles: particle set: TBP) +=
procedure :: get_particle => particle_set_get_particle

(Particles: procedures) +=
function particle_set_get_particle (pset, index) result (particle)
  class(particle_set_t), intent(in) :: pset
  integer, intent(in) :: index
  type(particle_t) :: particle
  particle = pset%prt(index)
end function particle_set_get_particle

```

```

<Particles: particle set: TBP>+≡
  procedure :: get_indices => particle_set_get_indices
<Particles: procedures>+≡
  pure function particle_set_get_indices (pset, mask) result (finals)
    integer, dimension(:), allocatable :: finals
    class(particle_set_t), intent(in) :: pset
    logical, dimension(:), intent(in) :: mask
    integer, dimension(size(mask)) :: indices
    integer :: i
    allocate (finals (count (mask)))
    indices = [(i, i=1, pset%n_tot)]
    finals = pack (indices, mask)
  end function particle_set_get_indices

```

Copy the subset of physical momenta to a phs_point container.

```

<Particles: particle set: TBP>+≡
  procedure :: get_in_and_out_momenta => particle_set_get_in_and_out_momenta
<Particles: procedures>+≡
  function particle_set_get_in_and_out_momenta (pset) result (phs_point)
    type(phs_point_t) :: phs_point
    class(particle_set_t), intent(in) :: pset
    logical, dimension(:), allocatable :: mask
    integer, dimension(:), allocatable :: indices
    type(vector4_t), dimension(:), allocatable :: p
    allocate (mask (pset%get_n_tot ()))
    allocate (p (size (pset%prt)))
    mask = pset%prt%status == PRT_INCOMING .or. &
           pset%prt%status == PRT_OUTGOING
    allocate (indices (count (mask)))
    indices = pset%get_indices (mask)
    phs_point = pset%get_momenta (indices)
  end function particle_set_get_in_and_out_momenta

```

Tools

Build a new particles array without hadronic remnants but with `n_extra` additional spots. We also update the mother-daughter relations assuming the ordering b, i, r, x, o.

```

<Particles: particle set: TBP>+≡
  procedure :: without_hadronic_remnants => &
    particle_set_without_hadronic_remnants
<Particles: procedures>+≡
  subroutine particle_set_without_hadronic_remnants &
    (particle_set, particles, n_particles, n_extra)
    class(particle_set_t), intent(inout) :: particle_set
    type(particle_t), dimension(:), allocatable, intent(out) :: particles
    integer, intent(out) :: n_particles
    integer, intent(in) :: n_extra

```

```

logical, dimension(:), allocatable :: no_hadronic_remnants, &
    no_hadronic_children
integer, dimension(:), allocatable :: children, new_children
integer :: i, j, k, first_remnant
first_remnant = particle_set%n_tot
do i = 1, particle_set%n_tot
    if (particle_set%prt(i)%is_hadronic_beam_remnant ()) then
        first_remnant = i
        exit
    end if
end do
n_particles = count (.not. particle_set%prt%is_hadronic_beam_remnant ())
allocate (no_hadronic_remnants (particle_set%n_tot))
no_hadronic_remnants = .not. particle_set%prt%is_hadronic_beam_remnant ()
allocate (particles (n_particles + n_extra))
k = 1
do i = 1, particle_set%n_tot
    if (no_hadronic_remnants(i)) then
        particles(k) = particle_set%prt(i)
        k = k + 1
    end if
end do
if (n_particles /= particle_set%n_tot) then
    do i = 1, n_particles
        select case (particles(i)%get_status ())
        case (PRT_BEAM)
            if (allocated (children)) deallocate (children)
            allocate (children (particles(i)%get_n_children ()))
            children = particles(i)%get_children ()
            if (allocated (no_hadronic_children)) &
                deallocate (no_hadronic_children)
            allocate (no_hadronic_children (particles(i)%get_n_children ()))
            no_hadronic_children = .not. &
                particle_set%prt(children)%is_hadronic_beam_remnant ()
            if (allocated (new_children)) deallocate (new_children)
            allocate (new_children (count (no_hadronic_children)))
            new_children = pack (children, no_hadronic_children)
            call particles(i)%set_children (new_children)
        case (PRT_INCOMING, PRT_RESONANT)
            <update children after remnant>
        case (PRT_OUTGOING, PRT_BEAM_REMNANT)
        case default
        end select
    end do
end if
end subroutine particle_set_without_hadronic_remnants

```

```

<update children after remnant>≡
    if (allocated (children)) deallocate (children)
    allocate (children (particles(i)%get_n_children ()))
    children = particles(i)%get_children ()
    do j = 1, size (children)
        if (children(j) > first_remnant) then
            children(j) = children (j) - &

```

```

        (particle_set%n_tot - n_particles)
    end if
end do
call particles(i)%set_children (children)

```

Build a new particles array without remnants but with `n_extra` additional spots.
We also update the mother-daughter relations assuming the ordering `b, i, r, x, o`.

```

<Particles: particle set: TBP>+≡
    procedure :: without_remnants => particle_set_without_remnants

<Particles: procedures>+≡
    subroutine particle_set_without_remnants &
        (particle_set, particles, n_particles, n_extra)
        class(particle_set_t), intent(inout) :: particle_set
        type(particle_t), dimension(:), allocatable, intent(out) :: particles
        integer, intent(in) :: n_extra
        integer, intent(out) :: n_particles
        logical, dimension(:), allocatable :: no_remnants, no_children
        integer, dimension(:), allocatable :: children, new_children
        integer :: i,j, k, first_remnant
        first_remnant = particle_set%n_tot
        do i = 1, particle_set%n_tot
            if (particle_set%prt(i)%is_beam_remnant ()) then
                first_remnant = i
                exit
            end if
        end do
        allocate (no_remnants (particle_set%n_tot))
        no_remnants = .not. (particle_set%prt%is_beam_remnant ())
        n_particles = count (no_remnants)
        allocate (particles (n_particles + n_extra))
        k = 1
        do i = 1, particle_set%n_tot
            if (no_remnants(i)) then
                particles(k) = particle_set%prt(i)
                k = k + 1
            end if
        end do
        if (n_particles /= particle_set%n_tot) then
            do i = 1, n_particles
                select case (particles(i)%get_status ())
                case (PRT_BEAM)
                    if (allocated (children)) deallocate (children)
                    allocate (children (particles(i)%get_n_children ()))
                    children = particles(i)%get_children ()
                    if (allocated (no_children)) deallocate (no_children)
                    allocate (no_children (particles(i)%get_n_children ()))
                    no_children = .not. (particle_set%prt(children)%is_beam_remnant ())
                    if (allocated (new_children)) deallocate (new_children)
                    allocate (new_children (count (no_children)))
                    new_children = pack (children, no_children)
                    call particles(i)%set_children (new_children)
                case (PRT_INCOMING, PRT_RESONANT)
                    <update children after remnant>

```

```

        case (PRT_OUTGOING, PRT_BEAM_REMNANT)
        case default
        end select
    end do
end if
end subroutine particle_set_without_remnants

```

(Particles: particle set: TBP)+≡

```

    procedure :: find_particle => particle_set_find_particle

```

(Particles: procedures)+≡

```

    pure function particle_set_find_particle (particle_set, pdg, &
        momentum, abs_smallness, rel_smallness) result (idx)
        integer :: idx
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in) :: pdg
        type(vector4_t), intent(in) :: momentum
        real(default), intent(in), optional :: abs_smallness, rel_smallness
        integer :: i
        logical, dimension(0:3) :: equals
        idx = 0
        do i = 1, size (particle_set%prt)
            if (particle_set%prt(i)%flv%get_pdg () == pdg) then
                equals = nearly_equal (particle_set%prt(i)%p%p, momentum%p, &
                    abs_smallness, rel_smallness)
                if (all (equals)) then
                    idx = i
                    return
                end if
            end if
        end do
    end function particle_set_find_particle

```

(Particles: particle set: TBP)+≡

```

    procedure :: reverse_find_particle => particle_set_reverse_find_particle

```

(Particles: procedures)+≡

```

    pure function particle_set_reverse_find_particle &
        (particle_set, pdg, momentum, abs_smallness, rel_smallness) result (idx)
        integer :: idx
        class(particle_set_t), intent(in) :: particle_set
        integer, intent(in) :: pdg
        type(vector4_t), intent(in) :: momentum
        real(default), intent(in), optional :: abs_smallness, rel_smallness
        integer :: i
        idx = 0
        do i = size (particle_set%prt), 1, -1
            if (particle_set%prt(i)%flv%get_pdg () == pdg) then
                if (all (nearly_equal (particle_set%prt(i)%p%p, momentum%p, &
                    abs_smallness, rel_smallness))) then
                    idx = i
                    return
                end if
            end if
        end do
    end function particle_set_reverse_find_particle

```

```

end do
end function particle_set_reverse_find_particle

```

This connects broken links of the form something $\rightarrow i \rightarrow$ none or j and none $\rightarrow j \rightarrow$ something or none where the particles i and j are *identical*. It also works if $i \rightarrow j$, directly, and thus removes duplicates. We are removing j and connect the possible daughters to i .

```

⟨Particles: particle set: TBP⟩+≡
  procedure :: remove_duplicates => particle_set_remove_duplicates
⟨Particles: procedures⟩+≡
  subroutine particle_set_remove_duplicates (particle_set, smallness)
    class(particle_set_t), intent(inout) :: particle_set
    real(default), intent(in) :: smallness
    integer :: n_removals
    integer, dimension(particle_set%n_tot) :: to_remove
    type(particle_t), dimension(:), allocatable :: particles
    type(vector4_t) :: p_i
    integer, dimension(:), allocatable :: map
    to_remove = 0
    call find_duplicates ()
    n_removals = count (to_remove > 0)
    if (n_removals > 0) then
      call strip_duplicates (particles)
      call particle_set%replace (particles)
    end if

contains

  ⟨Particles: remove duplicates: procedures⟩

end subroutine particle_set_remove_duplicates

```

This does not catch all cases. Missing are splittings of the type $i \rightarrow$ something and j .

```

⟨Particles: remove duplicates: procedures⟩≡
  subroutine find_duplicates ()
    integer :: pdg_i, child_i, i, j
    OUTER: do i = 1, particle_set%n_tot
      if (particle_set%prt(i)%status == PRT_OUTGOING .or. &
        particle_set%prt(i)%status == PRT_VIRTUAL .or. &
        particle_set%prt(i)%status == PRT_RESONANT) then
        if (allocated (particle_set%prt(i)%child)) then
          if (size (particle_set%prt(i)%child) > 1) cycle OUTER
          if (size (particle_set%prt(i)%child) == 1) then
            child_i = particle_set%prt(i)%child(1)
          else
            child_i = 0
          end if
        else
          child_i = 0
        end if
      end if
      pdg_i = particle_set%prt(i)%flv%get_pdg ()
      p_i = particle_set%prt(i)%p
    end do
  end subroutine find_duplicates

```

```

do j = i + 1, particle_set%n_tot
  if (pdg_i == particle_set%prt(j)%flv%get_pdg ()) then
    if (all (nearly_equal (particle_set%prt(j)%p%p, p_i%p, &
      abs_smallness = smallness, &
      rel_smallness = 1E4_default * smallness))) then
      if (child_i == 0 .or. j == child_i) then
        to_remove(j) = i
        if (debug_on) call msg_debug2 (D_PARTICLES, &
          "Particles: Will remove duplicate of i", i)
        if (debug_on) call msg_debug2 (D_PARTICLES, &
          "Particles: j", j)
      end if
    cycle OUTER
  end if
end do
end if
end do OUTER
end subroutine find_duplicates

```

(Particles: remove duplicates: procedures)+≡

```

recursive function get_alive_index (try) result (alive)
  integer :: alive
  integer :: try
  if (map(try) > 0) then
    alive = map(try)
  else
    alive = get_alive_index (to_remove(try))
  end if
end function get_alive_index

```

(Particles: remove duplicates: procedures)+≡

```

subroutine strip_duplicates (particles)
  type(particle_t), dimension(:), allocatable, intent(out) :: particles
  integer :: kept, removed, i, j
  integer, dimension(:), allocatable :: old_children
  logical, dimension(:), allocatable :: parent_set
  if (debug_on) call msg_debug (D_PARTICLES, "Particles: Removing duplicates")
  if (debug_on) call msg_debug (D_PARTICLES, "Particles: n_removals", n_removals)
  if (debug2_active (D_PARTICLES)) then
    call msg_debug2 (D_PARTICLES, "Particles: Given set before removing:")
    call particle_set%write (summary=.true., compressed=.true.)
  end if
  allocate (particles (particle_set%n_tot - n_removals))
  allocate (map (particle_set%n_tot))
  allocate (parent_set (particle_set%n_tot))
  parent_set = .false.
  map = 0
  j = 0
  do i = 1, particle_set%n_tot
    if (to_remove(i) == 0) then
      j = j + 1
      map(i) = j
    end if
  end do
end subroutine strip_duplicates

```



```

        call particles(j)%init (particle_set%prt(i))
    end if
end do
do i = 1, particle_set%n_tot
    if (map(i) /= 0) then
        if (.not. parent_set(map(i))) then
            call particles(map(i))%set_parents &
                (map (particle_set%prt(i)%get_parents ()))
        end if
        call particles(map(i))%set_children &
            (map (particle_set%prt(i)%get_children ()))
    else
        removed = i
        kept = to_remove(i)
        if (particle_set%prt(removed)%has_children ()) then
            old_children = particle_set%prt(removed)%get_children ()
            do j = 1, size (old_children)
                if (map(old_children(j)) > 0) then
                    call particles(map(old_children(j)))%set_parents &
                        ([get_alive_index (kept)])
                    parent_set(map(old_children(j))) = .true.
                    call particles(get_alive_index (kept))%add_child &
                        (map(old_children(j)))
                end if
            end do
            particles(get_alive_index (kept))%status = PRT_RESONANT
        else
            particles(get_alive_index (kept))%status = PRT_OUTGOING
        end if
    end if
end do
end subroutine strip_duplicates

```

Given a subevent, reset status codes. If the new status is beam, incoming, or outgoing, we also make sure that the stored p^2 value is equal to the on-shell mass squared.

```

<Particles: particle set: TBP>+≡
    procedure :: reset_status => particle_set_reset_status

<Particles: procedures>+≡
    subroutine particle_set_reset_status (particle_set, index, status)
        class(particle_set_t), intent(inout) :: particle_set
        integer, dimension(:), intent(in) :: index
        integer, intent(in) :: status
        integer :: i
        if (allocated (particle_set%prt)) then
            do i = 1, size (index)
                call particle_set%prt(index(i))%reset_status (status)
            end do
        end if
        particle_set%n_beam = &
            count (particle_set%prt%get_status () == PRT_BEAM)
        particle_set%n_in = &
            count (particle_set%prt%get_status () == PRT_INCOMING)
    end subroutine

```

```

particle_set%n_out = &
    count (particle_set%prt%get_status () == PRT_OUTGOING)
particle_set%n_vir = particle_set%n_tot &
    - particle_set%n_beam - particle_set%n_in - particle_set%n_out
end subroutine particle_set_reset_status

```

Reduce a particle set to the essential entries. The entries kept are those with status INCOMING, OUTGOING or RESONANT. BEAM is kept if keep_beams is true. Other entries are skipped. The correlated state matrix, if any, is also ignored.

(Particles: particle set: TBP)+≡

```

procedure :: reduce => particle_set_reduce

```

(Particles: procedures)+≡

```

subroutine particle_set_reduce (pset_in, pset_out, keep_beams)
    class(particle_set_t), intent(in) :: pset_in
    type(particle_set_t), intent(out) :: pset_out
    logical, intent(in), optional :: keep_beams
    integer, dimension(:), allocatable :: status, map
    integer :: i, j
    logical :: kb
    kb = .false.; if (present (keep_beams)) kb = keep_beams
    allocate (status (pset_in%n_tot))
    pset_out%factorization_mode = pset_in%factorization_mode
    status = pset_in%prt%get_status ()
    if (kb) pset_out%n_beam = count (status == PRT_BEAM)
    pset_out%n_in = count (status == PRT_INCOMING)
    pset_out%n_vir = count (status == PRT_RESONANT)
    pset_out%n_out = count (status == PRT_OUTGOING)
    pset_out%n_tot = &
        pset_out%n_beam + pset_out%n_in + pset_out%n_vir + pset_out%n_out
    allocate (pset_out%prt (pset_out%n_tot))
    allocate (map (pset_in%n_tot))
    map = 0
    j = 0
    if (kb) call copy_particles (PRT_BEAM)
    call copy_particles (PRT_INCOMING)
    call copy_particles (PRT_RESONANT)
    call copy_particles (PRT_OUTGOING)
    do i = 1, pset_in%n_tot
        if (map(i) == 0) cycle
        call pset_out%prt(map(i))%set_parents &
            (pset_in%get_real_parents (i, kb))
        call pset_out%prt(map(i))%set_parents &
            (map (pset_out%prt(map(i))%parent))
        call pset_out%prt(map(i))%set_children &
            (pset_in%get_real_children (i, kb))
        call pset_out%prt(map(i))%set_children &
            (map (pset_out%prt(map(i))%child))
    end do
contains
    subroutine copy_particles (stat)
        integer, intent(in) :: stat
        integer :: i
        do i = 1, pset_in%n_tot

```

```

        if (status(i) == stat) then
            j = j + 1
            map(i) = j
            call particle_init_particle (pset_out%prt(j), pset_in%prt(i))
        end if
    end do
end subroutine copy_particles
end subroutine particle_set_reduce

```

Remove the beam particles and beam remnants from the particle set if the keep beams flag is false. If keep beams is not given, the beam particles and the beam remnants are removed. The correlated state matrix, if any, is also ignored.

(Particles: particle set: TBP)+≡

```

    procedure :: filter_particles => particle_set_filter_particles

```

(Particles: procedures)+≡

```

subroutine particle_set_filter_particles &
    (pset_in, pset_out, keep_beams, real_parents, keep_virtuals)
class(particle_set_t), intent(in) :: pset_in
type(particle_set_t), intent(out) :: pset_out
logical, intent(in), optional :: keep_beams, real_parents, keep_virtuals
integer, dimension(:), allocatable :: status, map
logical, dimension(:), allocatable :: filter
integer :: i, j
logical :: kb, rp, kv
kb = .false.; if (present (keep_beams)) kb = keep_beams
rp = .false.; if (present (real_parents)) rp = real_parents
kv = .true.; if (present (keep_virtuals)) kv = keep_virtuals
if (debug_on) call msg_debug (D_PARTICLES, "filter_particles")
if (debug2_active (D_PARTICLES)) then
    print *, 'keep_beams = ', kb
    print *, 'real_parents = ', rp
    print *, 'keep_virtuals = ', kv
    print *, '>>> pset_in : '
    call pset_in%write(compressed=.true.)
end if
call count_and_allocate()
map = 0
j = 0
filter = .false.
if (.not. kb) filter = status == PRT_BEAM .or. status == PRT_BEAM_REMNANT
if (.not. kv) filter = filter .or. status == PRT_VIRTUAL
call copy_particles ()
do i = 1, pset_in%n_tot
    if (map(i) == 0) cycle
    if (rp) then
        call pset_out%prt(map(i))%set_parents &
            (map (pset_in%get_real_parents (i, kb)))
        call pset_out%prt(map(i))%set_children &
            (map (pset_in%get_real_children (i, kb)))
    else
        call pset_out%prt(map(i))%set_parents &
            (map (pset_in%prt(i)%get_parents ()))
        call pset_out%prt(map(i))%set_children &

```

```

        (map (pset_in%prt(i)%get_children ()))
    end if
end do
if (debug2_active (D_PARTICLES)) then
    print *, '>>> pset_out : '
    call pset_out%write(compressed=.true.)
end if
contains
    <filter particles: procedures>
end subroutine particle_set_filter_particles

<filter particles: procedures>≡
subroutine copy_particles ()
    integer :: i
    do i = 1, pset_in%n_tot
        if (.not. filter(i)) then
            j = j + 1
            map(i) = j
            call particle_init_particle (pset_out%prt(j), pset_in%prt(i))
        end if
    end do
end subroutine copy_particles

<filter particles: procedures>+≡
subroutine count_and_allocate
    allocate (status (pset_in%n_tot))
    status = particle_get_status (pset_in%prt)
    if (kb) pset_out%n_beam = count (status == PRT_BEAM)
    pset_out%n_in = count (status == PRT_INCOMING)
    if (kb .and. kv) then
        pset_out%n_vir = count (status == PRT_VIRTUAL) + &
            count (status == PRT_RESONANT) + &
            count (status == PRT_BEAM_REMNANT)
    else if (kb .and. .not. kv) then
        pset_out%n_vir = count (status == PRT_RESONANT) + &
            count (status == PRT_BEAM_REMNANT)
    else if (.not. kb .and. kv) then
        pset_out%n_vir = count (status == PRT_VIRTUAL) + &
            count (status == PRT_RESONANT)
    else
        pset_out%n_vir = count (status == PRT_RESONANT)
    end if
    pset_out%n_out = count (status == PRT_OUTGOING)
    pset_out%n_tot = &
        pset_out%n_beam + pset_out%n_in + pset_out%n_vir + pset_out%n_out
    allocate (pset_out%prt (pset_out%n_tot))
    allocate (map (pset_in%n_tot))
    allocate (filter (pset_in%n_tot))
end subroutine count_and_allocate

```

Transform a particle set into HEPEVT-compatible form. In this form, for each particle, the parents and the children are contiguous in the particle array. Usually, this requires to clone some particles.

We do not know in advance how many particles the canonical form will have. To be on the safe side, allocate four times the original size.

(Particles: particle set: TBP)+≡

```
procedure :: to_hepevt_form => particle_set_to_hepevt_form
```

(Particles: procedures)+≡

```
subroutine particle_set_to_hepevt_form (pset_in, pset_out)
  class(particle_set_t), intent(in) :: pset_in
  type(particle_set_t), intent(out) :: pset_out
  type :: particle_entry_t
    integer :: src = 0
    integer :: status = 0
    integer :: orig = 0
    integer :: copy = 0
  end type particle_entry_t
  type(particle_entry_t), dimension(:), allocatable :: prt
  integer, dimension(:), allocatable :: map1, map2
  integer, dimension(:), allocatable :: parent, child
  integer :: n_tot, n_parents, n_children, i, j, c, n

  n_tot = pset_in%n_tot
  allocate (prt (4 * n_tot))
  allocate (map1(4 * n_tot))
  allocate (map2(4 * n_tot))
  map1 = 0
  map2 = 0
  allocate (child (n_tot))
  allocate (parent (n_tot))
  n = 0
  do i = 1, n_tot
    if (pset_in%prt(i)%get_n_parents () == 0) then
      call append (i)
    end if
  end do
  do i = 1, n_tot
    n_children = pset_in%prt(i)%get_n_children ()
    if (n_children > 0) then
      child(1:n_children) = pset_in%prt(i)%get_children ()
      c = child(1)
      if (map1(c) == 0) then
        n_parents = pset_in%prt(c)%get_n_parents ()
        if (n_parents > 1) then
          parent(1:n_parents) = pset_in%prt(c)%get_parents ()
          if (i == parent(1) .and. &
              any( [(map1(i)+j-1, j=1,n_parents)] /= &
                  map1(parent(1:n_parents)))) then
            do j = 1, n_parents
              call append (parent(j))
            end do
          end if
        else if (map1(i) == 0) then
          call append (i)
        end if
      do j = 1, n_children
```

```

        call append (child(j))
    end do
    end if
    else if (map1(i) == 0) then
        call append (i)
    end if
end do
do i = n, 1, -1
    if (prt(i)%status /= PRT_OUTGOING) then
        do j = 1, i-1
            if (prt(j)%status == PRT_OUTGOING) then
                call append(prt(j)%src)
            end if
        end do
    end if
    exit
end if
end do
pset_out%n_beam = count (prt(1:n)%status == PRT_BEAM)
pset_out%n_in   = count (prt(1:n)%status == PRT_INCOMING)
pset_out%n_vir  = count (prt(1:n)%status == PRT_RESONANT)
pset_out%n_out  = count (prt(1:n)%status == PRT_OUTGOING)
pset_out%n_tot = n
allocate (pset_out%prt (n))
do i = 1, n
    call particle_init_particle (pset_out%prt(i), pset_in%prt(prt(i)%src))
    call pset_out%prt(i)%reset_status (prt(i)%status)
    if (prt(i)%orig == 0) then
        call pset_out%prt(i)%set_parents &
            (map2 (pset_in%prt(prt(i)%src)%get_parents ()))
    else
        call pset_out%prt(i)%set_parents ([ prt(i)%orig ])
    end if
    if (prt(i)%copy == 0) then
        call pset_out%prt(i)%set_children &
            (map1 (pset_in%prt(prt(i)%src)%get_children ()))
    else
        call pset_out%prt(i)%set_children ([ prt(i)%copy ])
    end if
end do
contains
subroutine append (i)
    integer, intent(in) :: i
    n = n + 1
    if (n > size (prt)) &
        call msg_bug ("Particle set transform to HEPEVT: insufficient space")
    prt(n)%src = i
    prt(n)%status = pset_in%prt(i)%get_status ()
    if (map1(i) == 0) then
        map1(i) = n
    else
        prt(map2(i))%status = PRT_VIRTUAL
        prt(map2(i))%copy = n
        prt(n)%orig = map2(i)
    end if
end if

```

```

        map2(i) = n
    end subroutine append
end subroutine particle_set_to_hepevt_form

```

This procedure aims at reconstructing the momenta of an interaction, given a particle set. The main task is to find the original hard process, by following the event history.

In-state: take those particles which are flagged as `PRT_INCOMING`

Out-state: try to be smart by checking the immediate children of the incoming particles. If the `state_flg` table is present, check any `PRT_RESONANT` particles that we get this way, whether they are potential out-particles by their PDG codes. If not, replace them by their children, recursively. (Resonances may have been inserted by the corresponding event transform.)

[WK 21-02-16] Revised the algorithm for the case `recover_beams = false`, i.e., the particle set contains beams and radiation. This does not mean that the particle set contains the complete radiation history. To make up for missing information, we follow the history in the interaction one step backwards and do a bit of guesswork to match this to the possibly incomplete history in the particle set. [The current implementation allows only for one stage of radiation; this could be improved by iterating the procedure!]

[WK 21-03-21] Amended the `find_hard_process_in_pset` algorithm as follows: Occasionally, PYTHIA adds a stepchild to the decay of a resonance that WHIZARD has inserted, a shower object that also has other particles in the event as parents. Such objects must not enter the hard-process record. Therefore, resonance child particle objects are ignored if they have more than one parent.

```

(Particles: particle set: TBP) +=
    procedure :: fill_interaction => particle_set_fill_interaction

(Particles: procedures) +=
    subroutine particle_set_fill_interaction &
        (pset, int, n_in, recover_beams, check_match, state_flg, success)
        class(particle_set_t), intent(in) :: pset
        type(interaction_t), intent(inout) :: int
        integer, intent(in) :: n_in
        logical, intent(in), optional :: recover_beams, check_match
        type(state_flg_content_t), intent(in), optional :: state_flg
        logical, intent(out), optional :: success
        integer, dimension(:), allocatable :: map, pdg
        integer, dimension(:), allocatable :: i_in, i_out, p_in, p_out
        logical, dimension(:), allocatable :: i_set
        integer :: n_out, i, p
        logical :: r_beams, check
        r_beams = .false.; if (present (recover_beams)) r_beams = recover_beams
        check = .true.; if (present (check_match)) check = check_match
        if (check) then
            call find_hard_process_in_int (i_in, i_out)
            call find_hard_process_in_pset (p_in, p_out, state_flg, success)
            if (present (success)) then
                if (size (i_in) /= n_in) success = .false.
                if (size (p_in) /= n_in) success = .false.
                if (size (p_out) /= n_out) success = .false.
            end if
        end if
    end subroutine

```

```

        if (.not. success) return
    else
        if (size (i_in) /= n_in) call err_int_n_in
        if (size (p_in) /= n_in) call err_pset_n_in
        if (size (p_out) /= n_out) call err_pset_n_out
    end if
    call extract_hard_process_from_pset (pdg)
    call determine_map_for_hard_process (map, state_flg, success)
    if (present (success)) then
        if (.not. success) return
    end if
    call map_handle_duplicates (map)
    if (.not. r_beams) then
        call determine_map_for_beams (map)
        call map_handle_duplicates (map)
        call determine_map_for_radiation (map, i_in, p_in)
        call map_handle_duplicates (map)
    end if
else
    allocate (map (int%get_n_tot ()))
    map = [(i, i = 1, size (map))]
    r_beams = .false.
end if
allocate (i_set (int%get_n_tot ()), source = .false.)
do p = 1, size (map)
    if (map(p) /= 0) then
        if (.not. i_set(map(p))) then
            call int%set_momentum (pset%prt(p)%get_momentum (), map(p))
            i_set(map(p)) = .true.
        end if
    end if
end do
if (r_beams) then
    do i = 1, n_in
        call reconstruct_beam_and_radiation (i, i_set)
    end do
else
    do i = int%get_n_tot (), 1, -1
        if (.not. i_set(i)) call reconstruct_missing (i, i_set)
    end do
end if
if (any (.not. i_set)) then
    if (present (success)) then
        success = .false.
    else
        call err_map
    end if
end if
contains
subroutine find_hard_process_in_int (i_in, i_out)
    integer, dimension(:), allocatable, intent(out) :: i_in, i_out
    integer :: n_in_i
    integer :: i
    i = int%get_n_tot ()

```



```

n_in_i = interaction_get_n_parents (int, i)
if (n_in_i /= n_in) call err_int_n_in
allocate (i_in (n_in))
i_in = interaction_get_parents (int, i)
i = i_in(1)
n_out = interaction_get_n_children (int, i)
allocate (i_out (n_out))
i_out = interaction_get_children (int, i)
end subroutine find_hard_process_in_int
subroutine find_hard_process_in_pset (p_in, p_out, state_flg, success)
  integer, dimension(:), allocatable, intent(out) :: p_in, p_out
  type(state_flg_content_t), intent(in), optional :: state_flg
  logical, intent(out), optional :: success
  integer, dimension(:), allocatable :: p_status, p_idx, p_child
  integer :: n_out_p, n_child, n_shift
  integer :: i, k, c
  allocate (p_status (pset%n_tot), p_idx (pset%n_tot), p_child (pset%n_tot))
  p_status = pset%prt%get_status ()
  p_idx = [(i, i = 1, pset%n_tot)]
  allocate (p_in (n_in))
  p_in = pack (p_idx, p_status == PRT_INCOMING)
  if (size (p_in) == 0) call err_pset_hard
  i = p_in(1)
  allocate (p_out (n_out))
  n_out_p = particle_get_n_children (pset%prt(i))
  p_out(1:n_out_p) = particle_get_children (pset%prt(i))
  do k = 1, size (p_out)
    i = p_out(k)
    if (present (state_flg)) then
      do while (pset%prt(i)%get_status () == PRT_RESONANT)
        if (state_flg%contains (pset%prt(i)%get_pdg ())) exit
        n_child = particle_get_n_children (pset%prt(i))
        p_child(1:n_child) = particle_get_children (pset%prt(i))
        n_shift = -1
        do c = 1, n_child
          if (particle_get_n_parents (pset%prt(p_child(c))) == 1) then
            n_shift = n_shift + 1
          else
            p_child(c) = 0
          end if
        end do
      end while
      if (n_shift < 0) then
        if (present (success)) then
          success = .false.
          return
        else
          call err_mismatch
        end if
      end if
      p_out(k+1+n_shift:n_out_p+n_shift) = p_out(k+1:n_out_p)
      n_out_p = n_out_p + n_shift
      do c = 1, n_child
        if (p_child(c) /= 0) then
          p_out(k+c-1) = p_child(c)
        end if
      end do
    end do
  end do

```

```

        end if
    end do
    i = p_out(k)
end do
end if
end do
if (present (success)) success = .true.
end subroutine find_hard_process_in_pset
subroutine extract_hard_process_from_pset (pdg)
    integer, dimension(:), allocatable, intent(out) :: pdg
    integer, dimension(:), allocatable :: pdg_p
    logical, dimension(:), allocatable :: mask_p
    integer :: i
    allocate (pdg_p (pset%n_tot))
    pdg_p = pset%prt%get_pdg ()
    allocate (mask_p (pset%n_tot), source = .false.)
    mask_p (p_in) = .true.
    mask_p (p_out) = .true.
    allocate (pdg (n_in + n_out))
    pdg = pack (pdg_p, mask_p)
end subroutine extract_hard_process_from_pset
subroutine determine_map_for_hard_process (map, state_flv, success)
    integer, dimension(:), allocatable, intent(out) :: map
    type(state_flv_content_t), intent(in), optional :: state_flv
    logical, intent(out), optional :: success
    integer, dimension(:), allocatable :: pdg_i, map_i
    integer :: n_tot
    logical, dimension(:), allocatable :: mask_i, mask_p
    logical :: match
    n_tot = int%get_n_tot ()
    if (present (state_flv)) then
        allocate (mask_i (n_tot), source = .false.)
        mask_i (i_in) = .true.
        mask_i (i_out) = .true.
        allocate (pdg_i (n_tot), map_i (n_tot))
        pdg_i = unpack (pdg, mask_i, 0)
        call state_flv%match (pdg_i, match, map_i)
        if (present (success)) then
            success = match
        end if
        if (.not. match) then
            if (present (success)) then
                return
            else
                call err_mismatch
            end if
        end if
        allocate (mask_p (pset%n_tot), source = .false.)
        mask_p (p_in) = .true.
        mask_p (p_out) = .true.
        allocate (map (size (mask_p)), &
            source = unpack (pack (map_i, mask_i), mask_p, 0))
    else
        allocate (map (n_tot), source = 0)
    end if
end subroutine

```

```

        map(p_in) = i_in
        map(p_out) = i_out
    end if
end subroutine determine_map_for_hard_process
subroutine map_handle_duplicates (map)
    integer, dimension(:), intent(inout) :: map
    integer, dimension(1) :: p_parent, p_child
    integer :: p
    do p = 1, pset%n_tot
        if (map(p) == 0) then
            if (pset%prt(p)%get_n_parents () == 1) then
                p_parent = pset%prt(p)%get_parents ()
                if (map(p_parent(1)) /= 0) then
                    if (pset%prt(p_parent(1))%get_n_children () == 1) then
                        map(p) = map(p_parent(1))
                    end if
                end if
            end if
        end if
    end do
    do p = pset%n_tot, 1, -1
        if (map(p) == 0) then
            if (pset%prt(p)%get_n_children () == 1) then
                p_child = pset%prt(p)%get_children ()
                if (map(p_child(1)) /= 0) then
                    if (pset%prt(p_child(1))%get_n_parents () == 1) then
                        map(p) = map(p_child(1))
                    end if
                end if
            end if
        end if
    end do
end subroutine map_handle_duplicates
subroutine determine_map_for_beams (map)
    integer, dimension(:), intent(inout) :: map
    select case (n_in)
    case (1); map(1) = 1
    case (2); map(1:2) = [1,2]
    end select
end subroutine determine_map_for_beams
subroutine determine_map_for_radiation (map, i_in, p_in)
    integer, dimension(:), intent(inout) :: map
    integer, dimension(:), intent(in) :: i_in
    integer, dimension(:), intent(in) :: p_in
    integer, dimension(:), allocatable :: i_cur, p_cur
    integer, dimension(:), allocatable :: i_par, p_par, i_rad, p_rad
    integer :: i, p
    integer :: b, r
    i_cur = i_in
    p_cur = p_in
    do b = 1, n_in
        i = i_cur(b)
        p = p_cur(b)
        i_par = interaction_get_parents (int, i)
    end do
end subroutine

```

```

p_par = pset%prt(p)%get_parents ()
if (size (i_par) == 0 .or. size (p_par) == 0) cycle
if (size (p_par) == 1) then
  if (pset%prt(p_par(1))%get_n_children () == 1) then
    p_par = pset%prt(p_par(1))%get_parents () ! copy of entry
  end if
end if
i_rad = interaction_get_children (int, i_par(1))
p_rad = pset%prt(p_par(1))%get_children ()
do r = 1, size (i_rad)
  if (any (map == i_rad(r))) i_rad(r) = 0
end do
i_rad = pack (i_rad, i_rad /= 0)
do r = 1, size (p_rad)
  if (map(p_rad(r)) /= 0) p_rad(r) = 0
end do
p_rad = pack (p_rad, p_rad /= 0)
do r = 1, min (size (i_rad), size (p_rad))
  map(p_rad(r)) = i_rad(r)
end do
end do
do b = 1, min (size (p_par), size (i_par))
  if (map(p_par(b)) == 0 .and. all (map /= i_par(b))) then
    map(p_par(b)) = i_par(b)
  end if
end do
end subroutine determine_map_for_radiation
subroutine reconstruct_beam_and_radiation (k, i_set)
  integer, intent(in) :: k
  logical, dimension(:), intent(inout) :: i_set
  integer :: k_src, k_pre, k_in, k_rad
  type(interaction_t), pointer :: int_src
  integer, dimension(2) :: i_child
  logical, dimension(2) :: is_final
  integer :: i
  call int%find_source (k, int_src, k_src)
  k_pre = 0
  k_in = k
  do while (.not. i_set (k_in))
    if (k_pre == 0) then
      call int%set_momentum (int_src%get_momentum (k_src), k_in)
    else
      call int%set_momentum (int%get_momentum (k_pre), k_in)
    end if
    i_set(k_in) = .true.
    if (n_in == 2) then
      k_pre = k_in
      i_child = interaction_get_children (int, k_pre)
      do i = 1, 2
        is_final(i) = interaction_get_n_children (int, i_child(i)) == 0
      end do
      if (all (.not. is_final)) then
        k_in = i_child(k); k_rad = 0
      else if (is_final(2)) then

```

```

        k_in = i_child(1); k_rad = i_child(2)
    else if (is_final(1)) then
        k_in = i_child(2); k_rad = i_child(1)
    else
        call err_beams
    end if
    if (k_rad /= 0) then
        if (i_set(k_in)) then
            call int%set_momentum &
                (int%get_momentum(k) - int%get_momentum(k_in), k_rad)
            i_set(k_rad) = .true.
        else
            call err_beams_norad
        end if
    end if
end if
end do
end subroutine reconstruct_beam_and_radiation
subroutine reconstruct_missing(i, i_set)
    integer, intent(in) :: i
    logical, dimension(:), intent(inout) :: i_set
    integer, dimension(:), allocatable :: i_child, i_parent, i_sibling
    integer :: s
    i_child = interaction_get_children(int, i)
    i_parent = interaction_get_parents(int, i)
    if (size(i_child) > 0 .and. all(i_set(i_child))) then
        call int%set_momentum(sum(int%get_momenta(i_child)), i)
    else if (size(i_parent) > 0 .and. all(i_set(i_parent))) then
        i_sibling = interaction_get_children(int, i_parent(1))
        call int%set_momentum(sum(int%get_momenta(i_parent)), i)
        do s = 1, size(i_sibling)
            if (i_sibling(s) == i) cycle
            if (i_set(i_sibling(s))) then
                call int%set_momentum(int%get_momentum(i) &
                    - int%get_momentum(i_sibling(s)), i)
            else
                call err_beams_norad
            end if
        end do
    else
        call err_beams_norad
    end if
    i_set(i) = .true.
end subroutine reconstruct_missing
subroutine err_pset_hard
    call msg_fatal("Reading particle set: no particles marked as incoming")
end subroutine err_pset_hard
subroutine err_int_n_in
    integer :: n
    if (allocated(i_in)) then
        n = size(i_in)
    else
        n = 0
    end if
end if

```

```

        write (msg_buffer, "(A,I0,A,I0)") &
            "Filling hard process from particle set: expect ", n_in, &
            " incoming particle(s), found ", n
        call msg_bug
    end subroutine err_int_n_in
    subroutine err_pset_n_in
        write (msg_buffer, "(A,I0,A,I0)") &
            "Reading hard-process particle set: should contain ", n_in, &
            " incoming particle(s), found ", size (p_in)
        call msg_fatal
    end subroutine err_pset_n_in
    subroutine err_pset_n_out
        write (msg_buffer, "(A,I0,A,I0)") &
            "Reading hard-process particle set: should contain ", n_out, &
            " outgoing particle(s), found ", size (p_out)
        call msg_fatal
    end subroutine err_pset_n_out
    subroutine err_mismatch
        call pset%write ()
        call state_flg%write ()
        call msg_fatal ("Reading particle set: Flavor combination " &
            // "does not match requested process")
    end subroutine err_mismatch
    subroutine err_map
        call pset%write ()
        call int%basic_write ()
        call msg_fatal ("Reading hard-process particle set: " &
            // "Incomplete mapping from particle set to interaction")
    end subroutine err_map
    subroutine err_beams
        call pset%write ()
        call int%basic_write ()
        call msg_fatal ("Reading particle set: Beam structure " &
            // "does not match requested process")
    end subroutine err_beams
    subroutine err_beams_norad
        call pset%write ()
        call int%basic_write ()
        call msg_fatal ("Reading particle set: Beam structure " &
            // "cannot be reconstructed for this configuration")
    end subroutine err_beams_norad
    subroutine err_radiation
        call int%basic_write ()
        call msg_bug ("Reading particle set: Interaction " &
            // "contains inconsistent radiation pattern.")
    end subroutine err_radiation
end subroutine particle_set_fill_interaction

```

This procedure reconstructs an array of vertex indices from the parent-child information in the particle entries, according to the HepMC scheme. For each particle, we determine which vertex it comes from and which vertex it goes to. We return the two arrays and the maximum vertex index.

For each particle in the list, we first check its parents. If for any parent the

vertex where it goes to is already known, this vertex index is assigned as the current 'from' vertex. Otherwise, a new index is created, assigned as the current 'from' vertex, and as the 'to' vertex for all parents.

Then, the analogous procedure is done for the children.

Furthermore, we assign to each vertex the vertex position from the parent(s). We check that these vertex positions coincide, and if not return a null vector.

```

(Particles: particle set: TBP)+≡
  procedure :: assign_vertices => particle_set_assign_vertices

(Particles: procedures)+≡
  subroutine particle_set_assign_vertices &
    (particle_set, v_from, v_to, n_vertices)
    class(particle_set_t), intent(in) :: particle_set
    integer, dimension(:), intent(out) :: v_from, v_to
    integer, intent(out) :: n_vertices
    integer, dimension(:), allocatable :: parent, child
    integer :: n_parents, n_children, vf, vt
    integer :: i, j, v
    v_from = 0
    v_to = 0
    vf = 0
    vt = 0
    do i = 1, particle_set%n_tot
      n_parents = particle_set%prt(i)%get_n_parents ()
      if (n_parents /= 0) then
        allocate (parent (n_parents))
        parent = particle_set%prt(i)%get_parents ()
        SCAN_PARENTS: do j = 1, size (parent)
          v = v_to(parent(j))
          if (v /= 0) then
            v_from(i) = v; exit SCAN_PARENTS
          end if
        end do SCAN_PARENTS
        if (v_from(i) == 0) then
          vf = vf + 1; v_from(i) = vf
          v_to(parent) = vf
        end if
        deallocate (parent)
      end if
      n_children = particle_set%prt(i)%get_n_children ()
      if (n_children /= 0) then
        allocate (child (n_children))
        child = particle_set%prt(i)%get_children ()
        SCAN_CHILDREN: do j = 1, size (child)
          v = v_from(child(j))
          if (v /= 0) then
            v_to(i) = v; exit SCAN_CHILDREN
          end if
        end do SCAN_CHILDREN
        if (v_to(i) == 0) then
          vt = vt + 1; v_to(i) = vt
          v_from(child) = vt
        end if
        deallocate (child)
      end if
    end do
  end subroutine

```

```

        end if
    end do
    n_vertices = max (vf, vt)
end subroutine particle_set_assign_vertices

```

15.4.6 Expression interface

This converts a `particle_set` object as defined here to a more concise `subevt` object that can be used as the event root of an expression. In particular, the latter lacks virtual particles, spin correlations and parent-child relations.

We keep beam particles, incoming partons, and outgoing partons. Furthermore, we keep radiated particles (a.k.a. beam remnants) if they have no children in the current particle set, and mark them as outgoing particles.

If `colorize` is set and true, mark all particles in the subevent as colorized, and set color/anticolor flow indices where they are defined. Colorless particles do not get indices but are still marked as colorized, for consistency.

```

(Particles: particle set: TBP) +=
  procedure :: to_subevt => particle_set_to_subevt

(Particles: procedures) +=
  subroutine particle_set_to_subevt (particle_set, subevt, colorize)
    class(particle_set_t), intent(in) :: particle_set
    type(subevt_t), intent(out) :: subevt
    logical, intent(in), optional :: colorize
    integer :: n_tot, n_beam, n_in, n_out, n_rad
    integer :: i, k, n_active
    integer, dimension(2) :: hel
    logical :: keep
    n_tot = particle_set_get_n_tot      (particle_set)
    n_beam = particle_set_get_n_beam    (particle_set)
    n_in  = particle_set_get_n_in      (particle_set)
    n_out  = particle_set_get_n_out     (particle_set)
    n_rad  = particle_set_get_n_remnants (particle_set)
    call subevt_init (subevt, n_beam + n_rad + n_in + n_out)
    k = 0
    do i = 1, n_tot
      associate (prt => particle_set%prt(i))
        keep = .false.
        select case (particle_get_status (prt))
          case (PRT_BEAM)
            k = k + 1
            call subevt_set_beam (subevt, k, &
              particle_get_pdg (prt), &
              particle_get_momentum (prt), &
              particle_get_p2 (prt))
            keep = .true.
          case (PRT_INCOMING)
            k = k + 1
            call subevt_set_incoming (subevt, k, &
              particle_get_pdg (prt), &
              particle_get_momentum (prt), &
              particle_get_p2 (prt))

```



```

        keep = .true.
    case (PRT_OUTGOING)
        k = k + 1
        call subevt_set_outgoing (subevt, k, &
            particle_get_pdg (prt), &
            particle_get_momentum (prt), &
            particle_get_p2 (prt))
        keep = .true.
    case (PRT_BEAM_REMNANT)
        if (particle_get_n_children (prt) == 0) then
            k = k + 1
            call subevt_set_outgoing (subevt, k, &
                particle_get_pdg (prt), &
                particle_get_momentum (prt), &
                particle_get_p2 (prt))
            keep = .true.
        end if
    end select
    if (keep) then
        if (prt%polarization == PRT_DEFINITE_HELICITY) then
            if (prt%hel%is_diagonal ()) then
                hel = prt%hel%to_pair ()
                call subevt_polarize (subevt, k, hel(1))
            end if
        end if
        if (present (colorize)) then
            if (colorize) then
                call subevt_colorize &
                    (subevt, i, prt%col%get_col (), prt%col%get_acl ())
            end if
        end if
    end associate
    n_active = k
end do
call subevt_reset (subevt, n_active)
end subroutine particle_set_to_subevt

```

This replaces the `particle\set\%prt` array with a given array of particles

(Particles: particle set: TBP)+≡

```

    procedure :: replace => particle_set_replace

```

(Particles: procedures)+≡

```

subroutine particle_set_replace (particle_set, newprt)
    class(particle_set_t), intent(inout) :: particle_set
    type(particle_t), intent(in), dimension(:), allocatable :: newprt
    if (allocated (particle_set%prt)) deallocate (particle_set%prt)
    allocate (particle_set%prt(size (newprt)))
    particle_set%prt = newprt
    particle_set%n_tot = size (newprt)
    particle_set%n_beam = count (particle_get_status (newprt) == PRT_BEAM)
    particle_set%n_in = count (particle_get_status (newprt) == PRT_INCOMING)
    particle_set%n_out = count (particle_get_status (newprt) == PRT_OUTGOING)
    particle_set%n_vir = particle_set%n_tot &

```

```

- particle_set%n_beam - particle_set%n_in - particle_set%n_out
end subroutine particle_set_replace

```

This routines orders the outgoing particles into clusters of colorless particles and such of particles ordered corresponding to the indices of the color lines. All outgoing particles in the ordered set appear as child of the corresponding outgoing particle in the unordered set, including colored beam remnants. We always start continue via the anti-color line, such that color flows within each Lund string system is always continued from the anticolor of one particle to the identical color index of another particle.

(Particles: particle set: TBP)+≡

```

procedure :: order_color_lines => particle_set_order_color_lines

```

(Particles: procedures)+≡

```

subroutine particle_set_order_color_lines (pset_out, pset_in)
  class(particle_set_t), intent(inout) :: pset_out
  type(particle_set_t), intent(in) :: pset_in
  integer :: i, n, n_col_rem
  n_col_rem = 0
  do i = 1, pset_in%n_tot
    if (pset_in%prt(i)%get_status () == PRT_BEAM_REMNANT .and. &
        any (pset_in%prt(i)%get_color () /= 0)) then
      n_col_rem = n_col_rem + 1
    end if
  end do
  pset_out%n_beam = pset_in%n_beam
  pset_out%n_in = pset_in%n_in
  pset_out%n_vir = pset_in%n_vir + pset_in%n_out + n_col_rem
  pset_out%n_out = pset_in%n_out
  pset_out%n_tot = pset_in%n_tot + pset_in%n_out + n_col_rem
  pset_out%correlated_state = pset_in%correlated_state
  pset_out%factorization_mode = pset_in%factorization_mode
  allocate (pset_out%prt (pset_out%n_tot))
  do i = 1, pset_in%n_tot
    call pset_out%prt(i)%init (pset_in%prt(i))
    call pset_out%prt(i)%set_children (pset_in%prt(i)%child)
    call pset_out%prt(i)%set_parents (pset_in%prt(i)%parent)
  end do
  n = pset_in%n_tot
  do i = 1, pset_in%n_tot
    if (pset_out%prt(i)%get_status () == PRT_OUTGOING .and. &
        all (pset_out%prt(i)%get_color () == 0) .and. &
        .not. pset_out%prt(i)%has_children ()) then
      n = n + 1
      call pset_out%prt(n)%init (pset_out%prt(i))
      call pset_out%prt(i)%reset_status (PRT_VIRTUAL)
      call pset_out%prt(i)%add_child (n)
      call pset_out%prt(i)%set_parents ([i])
    end if
  end do
  if (n_col_rem > 0) then
    do i = 1, n_col_rem
    end do
  end if
end if

```

```

end subroutine particle_set_order_color_lines

Eliminate numerical noise
<Particles: public>+≡
  public :: pacify
<Particles: interfaces>≡
  interface pacify
    module procedure pacify_particle
    module procedure pacify_particle_set
  end interface pacify

<Particles: procedures>+≡
  subroutine pacify_particle (prt)
    class(particle_t), intent(inout) :: prt
    real(default) :: e
    e = epsilon (1._default) * energy (prt%p)
    call pacify (prt%p, 10 * e)
    call pacify (prt%p2, 1e4 * e)
  end subroutine pacify_particle

  subroutine pacify_particle_set (pset)
    class(particle_set_t), intent(inout) :: pset
    integer :: i
    do i = 1, pset%n_tot
      call pacify (pset%prt(i))
    end do
  end subroutine pacify_particle_set

```

15.4.7 Unit tests

Test module, followed by the corresponding implementation module.

```

<particles_ut.f90>≡
  <File header>

  module particles_ut
    use unit_tests
    use particles_ut_i

    <Standard module head>

    <Particles: public test>

    contains

    <Particles: test driver>

  end module particles_ut

<particles_ut_i.f90>≡
  <File header>

```

```

module particles_util

  <Use kinds>
    use io_units
    use numeric_utils
    use constants, only: one, tiny_07
    use lorentz
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices
    use interactions
    use evaluators
    use model_data
    use subevents

    use particles

  <Standard module head>

  <Particles: test declarations>

contains

  <Particles: tests>

  <Particles: test auxiliary>

end module particles_util
API: driver for the unit tests below.
<Particles: public test>≡
  public :: particles_test
<Particles: test driver>≡
  subroutine particles_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Particles: execute tests>
  end subroutine particles_test

```

Check the basic setup of the `particle_set_t` type: Set up a chain of production and decay and factorize the result into particles. The process is $d\bar{d} \rightarrow Z \rightarrow q\bar{q}$.

```

<Particles: execute tests>≡
  call test (particles_1, "particles_1", &
    "check particle_set routines", &
    u, results)

<Particles: test declarations>≡
  public :: particles_1

<Particles: tests>≡
  subroutine particles_1 (u)
    use os_interface

```

```

integer, intent(in) :: u
type(model_data_t), target :: model
type(flavor_t), dimension(3) :: flv
type(color_t), dimension(3) :: col
type(helicity_t), dimension(3) :: hel
type(quantum_numbers_t), dimension(3) :: qn
type(vector4_t), dimension(3) :: p
type(interaction_t), target :: int1, int2
type(quantum_numbers_mask_t) :: qn_mask_conn
type(evaluator_t), target :: eval
type(interaction_t) :: int
type(particle_set_t) :: particle_set1, particle_set2
type(particle_set_t) :: particle_set3, particle_set4
type(subevt_t) :: subevt
logical :: ok
integer :: unit, iostat

write (u, "(A)")  "* Test output: Particles"
write (u, "(A)")  "* Purpose: test particle_set routines"
write (u, "(A)")

write (u, "(A)")  "* Reading model file"

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* Initializing production process"

call int1%basic_init (2, 0, 1, set_relations=.true.)
call flv%init ([1, -1, 23], model)
call col%init_col_acl ([0, 0, 0], [0, 0, 0])
call hel(3)%init (1, 1)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0.25_default, 0._default))
call hel(3)%init (1,-1)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0._default, 0.25_default))
call hel(3)%init (-1, 1)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0._default,-0.25_default))
call hel(3)%init (-1,-1)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0.25_default, 0._default))
call hel(3)%init (0, 0)
call qn%init (flv, col, hel)
call int1%add_state (qn, value=(0.5_default, 0._default))
call int1%freeze ()
p(1) = vector4_moving (45._default, 45._default, 3)
p(2) = vector4_moving (45._default,-45._default, 3)
p(3) = p(1) + p(2)
call int1%set_momenta (p)

write (u, "(A)")
write (u, "(A)")  "* Setup decay process"

```

```

call int2%basic_init (1, 0, 2, set_relations=.true.)
call flv%init ([23, 1, -1], model)
call col%init_col_acl ([0, 501, 0], [0, 0, 501])
call hel%init ([1, 1, 1], [1, 1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(1._default, 0._default))
call hel%init ([1, 1, 1], [-1,-1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0._default, 0.1_default))
call hel%init ([-1,-1,-1], [1, 1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0._default,-0.1_default))
call hel%init ([-1,-1,-1], [-1,-1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(1._default, 0._default))
call hel%init ([0, 1,-1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(4._default, 0._default))
call hel%init ([0,-1, 1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(2._default, 0._default))
call hel%init ([0, 1,-1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(2._default, 0._default))
call hel%init ([0,-1, 1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(4._default, 0._default))
call flv%init ([23, 2, -2], model)
call hel%init ([0, 1,-1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0.5_default, 0._default))
call hel%init ([0,-1, 1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0.5_default, 0._default))
call int2%freeze ()
p(2) = vector4_moving (45._default, 45._default, 2)
p(3) = vector4_moving (45._default,-45._default, 2)
call int2%set_momenta (p)
call int2%set_source_link (1, int1, 3)
call int1%basic_write (u)
call int2%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Concatenate production and decay"

call eval%init_product (int1, int2, qn_mask_conn, &
    connections_are_resonant=.true.)
call eval%receive_momenta ()
call eval%evaluate ()
call eval%write (u)

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (complete, polarized)"

```

```

write (u, "(A)")

int = eval%interaction_t
call particle_set1%init &
    (ok, int, int, FM_FACTOR_HELICITY, &
    [0.2_default, 0.2_default], .false., .true.)
call particle_set1%write (u)

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (in/out only, selected helicity)"
write (u, "(A)")

int = eval%interaction_t
call particle_set2%init &
    (ok, int, int, FM_SELECT_HELICITY, &
    [0.9_default, 0.9_default], .false., .false.)
call particle_set2%write (u)
call particle_set2%final ()

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (complete, selected helicity)"
write (u, "(A)")

int = eval%interaction_t
call particle_set2%init &
    (ok, int, int, FM_SELECT_HELICITY, &
    [0.7_default, 0.7_default], .false., .true.)
call particle_set2%write (u)

write (u, "(A)")
write (u, "(A)") &
    "* Factorize (complete, polarized, correlated); write and read again"
write (u, "(A)")

int = eval%interaction_t
call particle_set3%init &
    (ok, int, int, FM_FACTOR_HELICITY, &
    [0.7_default, 0.7_default], .true., .true.)
call particle_set3%write (u)

unit = free_unit ()
open (unit, action="readwrite", form="unformatted", status="scratch")
call particle_set3%write_raw (unit)
rewind (unit)
call particle_set4%read_raw (unit, iostat=iostat)
call particle_set4%set_model (model)
close (unit)

write (u, "(A)")
write (u, "(A)")  "* Result from reading"
write (u, "(A)")

call particle_set4%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Transform to a subevt object"
write (u, "(A)")

call particle_set4%to_subevt (subevt)
call subevt_write (subevt, u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call particle_set1%final ()
call particle_set2%final ()
call particle_set3%final ()
call particle_set4%final ()
call eval%final ()
call int1%final ()
call int2%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_1"

end subroutine particles_1

```

Reconstruct a hard interaction from a particle set.

```

<Particles: execute tests>+≡
  call test (particles_2, "particles_2", &
    "reconstruct hard interaction", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_2

<Particles: tests>+≡
  subroutine particles_2 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(flavor_t), dimension(:), allocatable :: flv
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "* Test output: Particles"
    write (u, "(A)")  "*   Purpose: reconstruct simple interaction"
    write (u, "(A)")

    write (u, "(A)")  "* Set up a 2 -> 3 interaction"
    write (u, "(A)")  "    + incoming partons marked as virtual"
    write (u, "(A)")  "    + no quantum numbers"
    write (u, "(A)")

    call reset_interaction_counter ()

```



```

call int%basic_init (0, 2, 3)
do i = 1, 2
  do j = 3, 5
    call int%relate (i, j)
  end do
end do

allocate (qn (5))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
  mask = [.false., .false., .true., .true., .true.])
call state_flv%set_entry (1, &
  pdg = [11, 12, 3, 4, 5], &
  map = [1, 2, 3, 4, 5])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 0
pset%n_in   = 2
pset%n_vir  = 0
pset%n_out  = 3
pset%n_tot  = 5
allocate (pset%prt (pset%n_tot))
do i = 1, 2
  call pset%prt(i)%reset_status (PRT_INCOMING)
  call pset%prt(i)%set_children ([3,4,5])
end do
do i = 3, 5
  call pset%prt(i)%reset_status (PRT_OUTGOING)
  call pset%prt(i)%set_parents ([1,2])
end do
call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (2._default))
call pset%prt(3)%set_momentum (vector4_at_rest (5._default))
call pset%prt(4)%set_momentum (vector4_at_rest (4._default))
call pset%prt(5)%set_momentum (vector4_at_rest (3._default))

allocate (flv (5))
call flv%init ([11,12,5,4,3])
do i = 1, 5
  call pset%prt(i)%set_flavor (flv(i))
end do

```

```

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*"   Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "*" Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "*" Test output end: particles_2"

end subroutine particles_2

```

Reconstruct an interaction with beam structure, e.g., a hadronic interaction, from a particle set.

```

<Particles: execute tests>+≡
  call test (particles_3, "particles_3", &
    "reconstruct interaction with beam structure", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_3

<Particles: tests>+≡
  subroutine particles_3 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "*" Test output: Particles"
    write (u, "(A)")  "*"   Purpose: reconstruct simple interaction"
    write (u, "(A)")

    write (u, "(A)")  "*" Set up a 2 -> 2 -> 3 interaction with radiation"
    write (u, "(A)")  "    + no quantum numbers"
    write (u, "(A)")

    call reset_interaction_counter ()
    call int%basic_init (0, 6, 3)
    call int%relate (1, 3)
    call int%relate (1, 4)
    call int%relate (2, 5)
    call int%relate (2, 6)

```

```

do i = 4, 6, 2
  do j = 7, 9
    call int%relate (i, j)
  end do
end do

allocate (qn (9))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
  mask = [.false., .false., .false., .false., .false., .false., &
    .true., .true., .true.])
call state_flv%set_entry (1, &
  pdg = [2011, 2012, 91, 11, 92, 12, 3, 4, 5], &
  map = [1, 2, 3, 4, 5, 6, 7, 8, 9])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

call create_test_particle_set_1 (pset)

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_3"

end subroutine particles_3

```

```

(Particles: test auxiliary)≡
subroutine create_test_particle_set_1 (pset)
  type(particle_set_t), intent(out) :: pset

```

```

type(flavor_t), dimension(:), allocatable :: flv
integer :: i
pset%n_beam = 2
pset%n_in   = 2
pset%n_vir  = 2
pset%n_out  = 3
pset%n_tot  = 9

allocate (pset%prt (pset%n_tot))
call pset%prt(1)%reset_status (PRT_BEAM)
call pset%prt(2)%reset_status (PRT_BEAM)
call pset%prt(3)%reset_status (PRT_INCOMING)
call pset%prt(4)%reset_status (PRT_INCOMING)
call pset%prt(5)%reset_status (PRT_BEAM_REMNANT)
call pset%prt(6)%reset_status (PRT_BEAM_REMNANT)
call pset%prt(7)%reset_status (PRT_OUTGOING)
call pset%prt(8)%reset_status (PRT_OUTGOING)
call pset%prt(9)%reset_status (PRT_OUTGOING)

call pset%prt(1)%set_children ([3,5])
call pset%prt(2)%set_children ([4,6])
call pset%prt(3)%set_children ([7,8,9])
call pset%prt(4)%set_children ([7,8,9])

call pset%prt(3)%set_parents ([1])
call pset%prt(4)%set_parents ([2])
call pset%prt(5)%set_parents ([1])
call pset%prt(6)%set_parents ([2])
call pset%prt(7)%set_parents ([3,4])
call pset%prt(8)%set_parents ([3,4])
call pset%prt(9)%set_parents ([3,4])

call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (2._default))
call pset%prt(3)%set_momentum (vector4_at_rest (4._default))
call pset%prt(4)%set_momentum (vector4_at_rest (6._default))
call pset%prt(5)%set_momentum (vector4_at_rest (3._default))
call pset%prt(6)%set_momentum (vector4_at_rest (5._default))
call pset%prt(7)%set_momentum (vector4_at_rest (7._default))
call pset%prt(8)%set_momentum (vector4_at_rest (8._default))
call pset%prt(9)%set_momentum (vector4_at_rest (9._default))

allocate (flv (9))
call flv%init ([2011, 2012, 11, 12, 91, 92, 3, 4, 5])
do i = 1, 9
    call pset%prt(i)%set_flavor (flv(i))
end do
end subroutine create_test_particle_set_1

```

Reconstruct an interaction with beam structure, e.g., a hadronic interaction, from a particle set that is missing the beam information.

```

⟨Particles: execute tests⟩+=
    call test (particles_4, "particles_4", &

```

```

        "reconstruct interaction with missing beams", &
        u, results)
<Particles: test declarations>+≡
    public :: particles_4
<Particles: tests>+≡
    subroutine particles_4 (u)

        integer, intent(in) :: u
        type(interaction_t) :: int
        type(interaction_t), target :: int_beams
        type(state_flv_content_t) :: state_flv
        type(particle_set_t) :: pset
        type(flavor_t), dimension(:), allocatable :: flv
        type(quantum_numbers_t), dimension(:), allocatable :: qn
        integer :: i, j

        write (u, "(A)")  "* Test output: Particles"
        write (u, "(A)")  "* Purpose: reconstruct beams"
        write (u, "(A)")

        call reset_interaction_counter ()

        write (u, "(A)")  "* Set up an interaction that contains beams only"
        write (u, "(A)")

        call int_beams%basic_init (0, 0, 2)
        call int_beams%set_momentum (vector4_at_rest (1._default), 1)
        call int_beams%set_momentum (vector4_at_rest (2._default), 2)
        allocate (qn (2))
        call int_beams%add_state (qn)
        call int_beams%freeze ()

        call int_beams%basic_write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Set up a 2 -> 2 -> 3 interaction with radiation"
        write (u, "(A)")  "    + no quantum numbers"
        write (u, "(A)")

        call int%basic_init (0, 6, 3)
        call int%relate (1, 3)
        call int%relate (1, 4)
        call int%relate (2, 5)
        call int%relate (2, 6)
        do i = 4, 6, 2
            do j = 7, 9
                call int%relate (i, j)
            end do
        end do
        do i = 1, 2
            call int%set_source_link (i, int_beams, i)
        end do
    end subroutine particles_4

```

```

deallocate (qn)
allocate (qn (9))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
    mask = [.false., .false., .false., .false., .false., .false., &
    .true., .true., .true.])
call state_flv%set_entry (1, &
    pdg = [2011, 2012, 91, 11, 92, 12, 3, 4, 5], &
    map = [1, 2, 3, 4, 5, 6, 7, 8, 9])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 0
pset%n_in   = 2
pset%n_vir  = 0
pset%n_out  = 3
pset%n_tot  = 5

allocate (pset%prt (pset%n_tot))
call pset%prt(1)%reset_status (PRT_INCOMING)
call pset%prt(2)%reset_status (PRT_INCOMING)
call pset%prt(3)%reset_status (PRT_OUTGOING)
call pset%prt(4)%reset_status (PRT_OUTGOING)
call pset%prt(5)%reset_status (PRT_OUTGOING)

call pset%prt(1)%set_children ([3,4,5])
call pset%prt(2)%set_children ([3,4,5])

call pset%prt(3)%set_parents ([1,2])
call pset%prt(4)%set_parents ([1,2])
call pset%prt(5)%set_parents ([1,2])

call pset%prt(1)%set_momentum (vector4_at_rest (6._default))
call pset%prt(2)%set_momentum (vector4_at_rest (6._default))
call pset%prt(3)%set_momentum (vector4_at_rest (3._default))
call pset%prt(4)%set_momentum (vector4_at_rest (4._default))
call pset%prt(5)%set_momentum (vector4_at_rest (5._default))

allocate (flv (5))
call flv%init ([11, 12, 3, 4, 5])
do i = 1, 5
    call pset%prt(i)%set_flavor (flv(i))

```

```

end do

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*"   Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv, &
    recover_beams = .true.)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "*" Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "*" Test output end: particles_4"

end subroutine particles_4

```

Reconstruct an interaction with beam structure and cloned particles (radiated particles repeated in the event record, to maintain some canonical ordering).

```

<Particles: execute tests>+≡
    call test (particles_5, "particles_5", &
        "reconstruct interaction with beams and duplicate entries", &
        u, results)

<Particles: test declarations>+≡
    public :: particles_5

<Particles: tests>+≡
    subroutine particles_5 (u)

        integer, intent(in) :: u
        type(interaction_t) :: int
        type(state_flv_content_t) :: state_flv
        type(particle_set_t) :: pset
        type(flavor_t), dimension(:), allocatable :: flv
        type(quantum_numbers_t), dimension(:), allocatable :: qn
        integer :: i, j

        write (u, "(A)")  "*" Test output: Particles"
        write (u, "(A)")  "*"   Purpose: reconstruct event with duplicate entries"
        write (u, "(A)")

        write (u, "(A)")  "*" Set up a 2 -> 2 -> 3 interaction with radiation"
        write (u, "(A)")  "    + no quantum numbers"
        write (u, "(A)")

        call reset_interaction_counter ()
        call int%basic_init (0, 6, 3)
        call int%relate (1, 3)
    end subroutine particles_5

```

```

call int%relate (1, 4)
call int%relate (2, 5)
call int%relate (2, 6)
do i = 4, 6, 2
  do j = 7, 9
    call int%relate (i, j)
  end do
end do

allocate (qn (9))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
  mask = [.false., .false., .false., .false., .false., .false., &
    .true., .true., .true.])
call state_flv%set_entry (1, &
  pdg = [2011, 2012, 91, 11, 92, 12, 3, 4, 5], &
  map = [1, 2, 3, 4, 5, 6, 7, 8, 9])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 2
pset%n_in   = 2
pset%n_vir  = 4
pset%n_out  = 5
pset%n_tot  = 13

allocate (pset%prt (pset%n_tot))
call pset%prt(1)%reset_status (PRT_BEAM)
call pset%prt(2)%reset_status (PRT_BEAM)
call pset%prt(3)%reset_status (PRT_VIRTUAL)
call pset%prt(4)%reset_status (PRT_VIRTUAL)
call pset%prt(5)%reset_status (PRT_VIRTUAL)
call pset%prt(6)%reset_status (PRT_VIRTUAL)
call pset%prt(7)%reset_status (PRT_INCOMING)
call pset%prt(8)%reset_status (PRT_INCOMING)
call pset%prt( 9)%reset_status (PRT_OUTGOING)
call pset%prt(10)%reset_status (PRT_OUTGOING)
call pset%prt(11)%reset_status (PRT_OUTGOING)
call pset%prt(12)%reset_status (PRT_OUTGOING)
call pset%prt(13)%reset_status (PRT_OUTGOING)

call pset%prt(1)%set_children ([3,4])

```



```

call pset%prt(2)%set_children ([5,6])
call pset%prt(3)%set_children ([ 7])
call pset%prt(4)%set_children ([ 9])
call pset%prt(5)%set_children ([ 8])
call pset%prt(6)%set_children ([10])
call pset%prt(7)%set_children ([11,12,13])
call pset%prt(8)%set_children ([11,12,13])

call pset%prt(3)%set_parents ([1])
call pset%prt(4)%set_parents ([1])
call pset%prt(5)%set_parents ([2])
call pset%prt(6)%set_parents ([2])
call pset%prt( 7)%set_parents ([3])
call pset%prt( 8)%set_parents ([5])
call pset%prt( 9)%set_parents ([4])
call pset%prt(10)%set_parents ([6])
call pset%prt(11)%set_parents ([7,8])
call pset%prt(12)%set_parents ([7,8])
call pset%prt(13)%set_parents ([7,8])

call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (2._default))
call pset%prt(3)%set_momentum (vector4_at_rest (4._default))
call pset%prt(4)%set_momentum (vector4_at_rest (3._default))
call pset%prt(5)%set_momentum (vector4_at_rest (6._default))
call pset%prt(6)%set_momentum (vector4_at_rest (5._default))
call pset%prt(7)%set_momentum (vector4_at_rest (4._default))
call pset%prt(8)%set_momentum (vector4_at_rest (6._default))
call pset%prt( 9)%set_momentum (vector4_at_rest (3._default))
call pset%prt(10)%set_momentum (vector4_at_rest (5._default))
call pset%prt(11)%set_momentum (vector4_at_rest (7._default))
call pset%prt(12)%set_momentum (vector4_at_rest (8._default))
call pset%prt(13)%set_momentum (vector4_at_rest (9._default))

allocate (flv (13))
call flv%init ([2011, 2012, 11, 91, 12, 92, 11, 12, 91, 92, 3, 4, 5])
do i = 1, 13
    call pset%prt(i)%set_flavor (flv(i))
end do

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*"   Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "*" Cleanup"

call int%final ()
call pset%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_5"

end subroutine particles_5

```

Reconstruct an interaction with pair spectrum, e.g., beamstrahlung from a particle set.

```

<Particles: execute tests>+≡
  call test (particles_6, "particles_6", &
    "reconstruct interaction with pair spectrum", &
    u, results)

<Particles: test declarations>+≡
  public :: particles_6

<Particles: tests>+≡
  subroutine particles_6 (u)

    integer, intent(in) :: u
    type(interaction_t) :: int
    type(state_flv_content_t) :: state_flv
    type(particle_set_t) :: pset
    type(flavor_t), dimension(:), allocatable :: flv
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer :: i, j

    write (u, "(A)")  "* Test output: Particles"
    write (u, "(A)")  "* Purpose: reconstruct interaction with pair spectrum"
    write (u, "(A)")

    write (u, "(A)")  "* Set up a 2 -> 2 -> 3 interaction with radiation"
    write (u, "(A)")  "    + no quantum numbers"
    write (u, "(A)")

    call reset_interaction_counter ()
    call int%basic_init (0, 6, 3)
    do i = 1, 2
      do j = 3, 6
        call int%relate (i, j)
      end do
    end do
    do i = 5, 6
      do j = 7, 9
        call int%relate (i, j)
      end do
    end do

    allocate (qn (9))
    call int%add_state (qn)
    call int%freeze ()

    call int%basic_write (u)

    write (u, "(A)")

```

```

write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")

call state_flv%init (1, &
    mask = [.false., .false., .false., .false., .false., .false., &
    .true., .true., .true.])
call state_flv%set_entry (1, &
    pdg = [1011, 1012, 21, 22, 11, 12, 3, 4, 5], &
    map = [1, 2, 3, 4, 5, 6, 7, 8, 9])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 2
pset%n_in   = 2
pset%n_vir  = 2
pset%n_out  = 3
pset%n_tot  = 9

allocate (pset%prt (pset%n_tot))
call pset%prt(1)%reset_status (PRT_BEAM)
call pset%prt(2)%reset_status (PRT_BEAM)
call pset%prt(3)%reset_status (PRT_INCOMING)
call pset%prt(4)%reset_status (PRT_INCOMING)
call pset%prt(5)%reset_status (PRT_OUTGOING)
call pset%prt(6)%reset_status (PRT_OUTGOING)
call pset%prt(7)%reset_status (PRT_OUTGOING)
call pset%prt(8)%reset_status (PRT_OUTGOING)
call pset%prt(9)%reset_status (PRT_OUTGOING)

call pset%prt(1)%set_children ([3,4,5,6])
call pset%prt(2)%set_children ([3,4,5,6])
call pset%prt(3)%set_children ([7,8,9])
call pset%prt(4)%set_children ([7,8,9])

call pset%prt(3)%set_parents ([1,2])
call pset%prt(4)%set_parents ([1,2])
call pset%prt(5)%set_parents ([1,2])
call pset%prt(6)%set_parents ([1,2])
call pset%prt(7)%set_parents ([3,4])
call pset%prt(8)%set_parents ([3,4])
call pset%prt(9)%set_parents ([3,4])

call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (2._default))
call pset%prt(3)%set_momentum (vector4_at_rest (5._default))
call pset%prt(4)%set_momentum (vector4_at_rest (6._default))
call pset%prt(5)%set_momentum (vector4_at_rest (3._default))
call pset%prt(6)%set_momentum (vector4_at_rest (4._default))
call pset%prt(7)%set_momentum (vector4_at_rest (7._default))
call pset%prt(8)%set_momentum (vector4_at_rest (8._default))

```

```

call pset%prt(9)%set_momentum (vector4_at_rest (9._default))

allocate (flv (9))
call flv%init ([1011, 1012, 11, 12, 21, 22, 3, 4, 5])
do i = 1, 9
    call pset%prt(i)%set_flavor (flv(i))
end do

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*   Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 2, state_flv=state_flv)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_6"

end subroutine particles_6

```

Reconstruct a hard decay interaction from a shuffled particle set.

```

<Particles: execute tests>+≡
    call test (particles_7, "particles_7", &
        "reconstruct decay interaction with reordering", &
        u, results)

<Particles: test declarations>+≡
    public :: particles_7

<Particles: tests>+≡
    subroutine particles_7 (u)

        integer, intent(in) :: u
        type(interaction_t) :: int
        type(state_flv_content_t) :: state_flv
        type(particle_set_t) :: pset
        type(flavor_t), dimension(:), allocatable :: flv
        type(quantum_numbers_t), dimension(:), allocatable :: qn
        integer :: i, j

        write (u, "(A)")  "* Test output: Particles"
        write (u, "(A)")  "*   Purpose: reconstruct decay interaction with reordering"
        write (u, "(A)")

        write (u, "(A)")  "* Set up a 1 -> 3 interaction"
        write (u, "(A)")  "    + no quantum numbers"
        write (u, "(A)")
    end subroutine particles_7

```

```

call reset_interaction_counter ()
call int%basic_init (0, 1, 3)
do j = 2, 4
    call int%relate (1, j)
end do

allocate (qn (4))
call int%add_state (qn)
call int%freeze ()

call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set up a flavor-content record"
write (u, "(A)")  "* assumed interaction: 6 12 5 -11"
write (u, "(A)")

call state_flv%init (1, &
    mask = [.false., .true., .true., .true.])
call state_flv%set_entry (1, &
    pdg = [6, 5, -11, 12], &
    map = [1, 4, 2, 3])

call state_flv%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually create a matching particle set"
write (u, "(A)")

pset%n_beam = 0
pset%n_in   = 1
pset%n_vir  = 0
pset%n_out  = 3
pset%n_tot  = 4
allocate (pset%prt (pset%n_tot))
do i = 1, 1
    call pset%prt(i)%reset_status (PRT_INCOMING)
    call pset%prt(i)%set_children ([2,3,4])
end do
do i = 2, 4
    call pset%prt(i)%reset_status (PRT_OUTGOING)
    call pset%prt(i)%set_parents ([1])
end do
call pset%prt(1)%set_momentum (vector4_at_rest (1._default))
call pset%prt(2)%set_momentum (vector4_at_rest (3._default))
call pset%prt(3)%set_momentum (vector4_at_rest (2._default))
call pset%prt(4)%set_momentum (vector4_at_rest (4._default))

allocate (flv (4))
call flv%init ([6,5,12,-11])
do i = 1, 4
    call pset%prt(i)%set_flavor (flv(i))
end do

```

```

call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "*"   Fill interaction from particle set"
write (u, "(A)")

call pset%fill_interaction (int, 1, state_flg=state_flg)
call int%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "*" Cleanup"

call int%final ()
call pset%final ()

write (u, "(A)")
write (u, "(A)")  "*" Test output end: particles_7"

end subroutine particles_7

```

(Particles: execute tests)+≡

```

call test (particles_8, "particles_8", &
           "Test functions on particle sets", u, results)

```

(Particles: test declarations)+≡

```

public :: particles_8

```

(Particles: tests)+≡

```

subroutine particles_8 (u)
  integer, intent(in) :: u
  type(particle_set_t) :: particle_set
  type(particle_t), dimension(:), allocatable :: particles
  integer, allocatable, dimension(:) :: children, parents
  integer :: n_particles, i
  write (u, "(A)")  "*" Test output: particles_8"
  write (u, "(A)")  "*"   Purpose: Test functions on particle sets"
  write (u, "(A)")

  call create_test_particle_set_1 (particle_set)
  call particle_set%write (u)
  call assert_equal (u, particle_set%n_tot, 9)
  call assert_equal (u, particle_set%n_beam, 2)
  allocate (children (particle_set%prt(3)%get_n_children ()))
  children = particle_set%prt(3)%get_children()
  call assert_equal (u, particle_set%prt(children(1))%get_pdg (), 3)
  call assert_equal (u, size (particle_set%prt(1)%get_children ()), 2)
  call assert_equal (u, size (particle_set%prt(2)%get_children ()), 2)

  call particle_set%without_hadronic_remnants &
    (particles, n_particles, 3)
  call particle_set%replace (particles)
  write (u, "(A)")
  call particle_set%write (u)

```

```

call assert_equal (u, n_particles, 7)
call assert_equal (u, size(particles), 10)
call assert_equal (u, particle_set%n_tot, 10)
call assert_equal (u, particle_set%n_beam, 2)
do i = 3, 4
  if (allocated (children)) deallocate (children)
  allocate (children (particle_set%prt(i)%get_n_children ()))
  children = particle_set%prt(i)%get_children()
  call assert_equal (u, particle_set%prt(children(1))%get_pdg (), 3)
  call assert_equal (u, particle_set%prt(children(2))%get_pdg (), 4)
  call assert_equal (u, particle_set%prt(children(3))%get_pdg (), 5)
end do
do i = 5, 7
  if (allocated (parents)) deallocate (parents)
  allocate (parents (particle_set%prt(i)%get_n_parents ()))
  parents = particle_set%prt(i)%get_parents()
  call assert_equal (u, particle_set%prt(parents(1))%get_pdg (), 11)
  call assert_equal (u, particle_set%prt(parents(2))%get_pdg (), 12)
end do
call assert_equal (u, size (particle_set%prt(1)%get_children ()), &
  1, "get children of 1")
call assert_equal (u, size (particle_set%prt(2)%get_children ()), &
  1, "get children of 2")

call assert_equal (u, particle_set%find_particle &
  (particle_set%prt(1)%get_pdg (), particle_set%prt(1)%p), &
  1, "find 1st particle")
call assert_equal (u, particle_set%find_particle &
  (particle_set%prt(2)%get_pdg (), particle_set%prt(2)%p * &
    (one + tiny_07), rel_smallness=1.0E-6_default), &
  2, "find 2nd particle fuzzy")

write (u, "(A)")
write (u, "(A)")  "* Test output end: particles_8"
end subroutine particles_8

```

Order color lines into Lund string systems, without colored beam remnants first.

```

<Particles: execute tests>+≡
  call test (particles_9, "particles_9", &
    "order into Lund strings, uncolored beam remnants", &
    u, results)
<Particles: test declarations>+≡
  public :: particles_9
<Particles: tests>+≡
  subroutine particles_9 (u)
    integer, intent(in) :: u
    write (u, "(A)")  "* Test output: particles_9"
    write (u, "(A)")  "* Purpose: Order into Lund strings, "
    write (u, "(A)")  "* uncolored beam remnants"
    write (u, "(A)")
  end subroutine particles_9

```

Chapter 16

Beams

These modules implement beam configuration and beam structure, the latter in abstract terms.

beam_structures The `beam_structure_t` type is a messenger type that communicates the user settings to the **WHIZARD** core.

beams Beam configuration.

sf_aux Tools for handling structure functions and splitting

sf_mappings Mapping functions, useful for structure function implementation

sf_base The abstract structure-function interaction and structure-function chain types.

These are the implementation modules, the concrete counterparts of **sf_base**:

sf_isr ISR structure function (photon radiation inclusive and resummed in collinear and IR regions).

sf_epa Effective Photon Approximation.

sf_ewa Effective W (and Z) approximation.

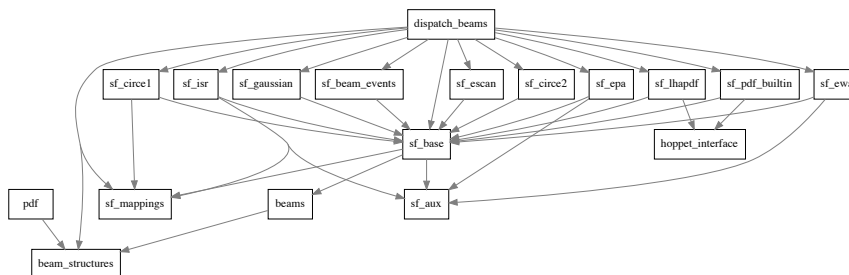


Figure 16.1: Module dependencies in `src/beams`.

sf_escan Energy spectrum that emulates a uniform energy scan.

sf_gaussian Gaussian beam spread

sf_beam_events Beam-event generator that reads its input from an external file.

sf_circe1 CIRCE1 beam spectra for electrons and photons.

sf_circe2 CIRCE2 beam spectra for electrons and photons.

hoppet_interface Support for *b*-quark matching, addon to PDF modules.

sf_pdf_builtin Direct support for selected hadron PDFs.

sf_lhapdf LHAPDF library support.

16.1 Beam structure

This module stores the beam structure definition as it is declared in the SIN-DARIN script. The structure definition is not analyzed, just recorded for later use.

We do not capture any numerical parameters, just names of particles and structure functions.

```
<beam_structures.f90>≡  
<File header>  
  
module beam_structures  
  
  <Use kinds>  
  <Use strings>  
  use io_units  
  use format_defs, only: FMT_19  
  use diagnostics  
  use lorentz  
  use polarizations  
  
  <Standard module head>  
  
  <Beam structures: public>  
  
  <Beam structures: types>  
  
  <Beam structures: interfaces>  
  
  contains  
  
  <Beam structures: procedures>  
  
end module beam_structures
```

16.1.1 Beam structure elements

An entry in a beam-structure record consists of a string that denotes a type of structure function.

```
<Beam structures: types>≡  
  type :: beam_structure_entry_t  
    logical :: is_valid = .false.  
    type(string_t) :: name  
  contains  
    <Beam structures: beam structure entry: TBP>  
  end type beam_structure_entry_t
```

Output.

```
<Beam structures: beam structure entry: TBP>≡  
  procedure :: to_string => beam_structure_entry_to_string  
  
<Beam structures: procedures>≡  
  function beam_structure_entry_to_string (object) result (string)  
    class(beam_structure_entry_t), intent(in) :: object
```

```

type(string_t) :: string
if (object%is_valid) then
    string = object%name
else
    string = "none"
end if
end function beam_structure_entry_to_string

```

A record in the beam-structure sequence denotes either a structure-function entry, a pair of such entries, or a pair spectrum.

```

⟨Beam structures: types⟩+≡
type :: beam_structure_record_t
    type(beam_structure_entry_t), dimension(:), allocatable :: entry
end type beam_structure_record_t

```

16.1.2 Beam structure type

The beam-structure object contains the beam particle(s) as simple strings. The sequence of records indicates the structure functions by name. No numerical parameters are stored.

```

⟨Beam structures: public⟩≡
public :: beam_structure_t

⟨Beam structures: types⟩+≡
type :: beam_structure_t
private
integer :: n_beam = 0
type(string_t), dimension(:), allocatable :: prt
type(beam_structure_record_t), dimension(:), allocatable :: record
type(smatrix_t), dimension(:), allocatable :: smatrix
real(default), dimension(:), allocatable :: pol_f
real(default), dimension(:), allocatable :: p
real(default), dimension(:), allocatable :: theta
real(default), dimension(:), allocatable :: phi
contains
⟨Beam structures: beam structure: TBP⟩
end type beam_structure_t

```

The finalizer deletes all contents explicitly, so we can continue with an empty beam record. (It is not needed for deallocation.) We have distinct finalizers for the independent parts of the beam structure.

```

⟨Beam structures: beam structure: TBP⟩≡
procedure :: final_sf => beam_structure_final_sf

⟨Beam structures: procedures⟩+≡
subroutine beam_structure_final_sf (object)
class(beam_structure_t), intent(inout) :: object
if (allocated (object%prt)) deallocate (object%prt)
if (allocated (object%record)) deallocate (object%record)
object%n_beam = 0
end subroutine beam_structure_final_sf

```

Output. The actual information fits in a single line, therefore we can provide a `to_string` method. The `show` method also lists the current values of relevant global variables.

```

(Beam structures: beam structure: TBP)+≡
  procedure :: write => beam_structure_write
  procedure :: to_string => beam_structure_to_string

(Beam structures: procedures)+≡
  subroutine beam_structure_write (object, unit)
    class(bean_structure_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A,A)") "Beam structure: ", char (object%to_string ())
    if (allocated (object%smatrix)) then
      do i = 1, size (object%smatrix)
        write (u, "(3x,A,I0,A)") "polarization (beam ", i, "):"
        call object%smatrix(i)%write (u, indent=2)
      end do
    end if
    if (allocated (object%pol_f)) then
      write (u, "(3x,A,F10.7,:',',F10.7)") "polarization degree =", &
        object%pol_f
    end if
    if (allocated (object%p)) then
      write (u, "(3x,A," // FMT_19 // ",:',','," // FMT_19 // &
        ")") "momentum =", object%p
    end if
    if (allocated (object%theta)) then
      write (u, "(3x,A," // FMT_19 // ",:',','," // FMT_19 // &
        ")") "angle th =", object%theta
    end if
    if (allocated (object%phi)) then
      write (u, "(3x,A," // FMT_19 // ",:',','," // FMT_19 // &
        ")") "angle ph =", object%phi
    end if
  end subroutine beam_structure_write

  function beam_structure_to_string (object, sf_only) result (string)
    class(bean_structure_t), intent(in) :: object
    logical, intent(in), optional :: sf_only
    type(string_t) :: string
    integer :: i, j
    logical :: with_beams
    with_beams = .true.; if (present (sf_only)) with_beams = .not. sf_only
    select case (object%n_beam)
    case (1)
      if (with_beams) then
        string = object%prt(1)
      else
        string = ""
      end if
    case (2)
      if (with_beams) then

```

```

        string = object%prt(1) // ", " // object%prt(2)
    else
        string = ""
    end if
    if (allocated (object%record)) then
        if (size (object%record) > 0) then
            if (with_beams) string = string // " => "
            do i = 1, size (object%record)
                if (i > 1) string = string // " => "
                do j = 1, size (object%record(i)%entry)
                    if (j > 1) string = string // ", "
                    string = string // object%record(i)%entry(j)%to_string ()
                end do
            end do
        end if
    end if
    case default
        string = "[any particles]"
    end select
end function beam_structure_to_string

```

Initializer: dimension the beam structure record. Each array element denotes the number of entries for a record within the beam-structure sequence. The number of entries is either one or two, while the number of records is unlimited.

```

<Beam structures: beam structure: TBP>+≡
    procedure :: init_sf => beam_structure_init_sf

<Beam structures: procedures>+≡
    subroutine beam_structure_init_sf (beam_structure, prt, dim_array)
        class(beam_structure_t), intent(inout) :: beam_structure
        type(string_t), dimension(:), intent(in) :: prt
        integer, dimension(:), intent(in), optional :: dim_array
        integer :: i
        call beam_structure%final_sf ()
        beam_structure%n_beam = size (prt)
        allocate (beam_structure%prt (size (prt)))
        beam_structure%prt = prt
        if (present (dim_array)) then
            allocate (beam_structure%record (size (dim_array)))
            do i = 1, size (dim_array)
                allocate (beam_structure%record(i)%entry (dim_array(i)))
            end do
        else
            allocate (beam_structure%record (0))
        end if
    end subroutine beam_structure_init_sf

```

Set an entry, specified by record number and entry number.

```

<Beam structures: beam structure: TBP>+≡
    procedure :: set_sf => beam_structure_set_sf

<Beam structures: procedures>+≡
    subroutine beam_structure_set_sf (beam_structure, i, j, name)
        class(beam_structure_t), intent(inout) :: beam_structure

```

```

integer, intent(in) :: i, j
type(string_t), intent(in) :: name
associate (entry => beam_structure%record(i)%entry(j))
    entry%name = name
    entry%is_valid = .true.
end associate
end subroutine beam_structure_set_sf

```

Expand the beam-structure object. (i) For a pair spectrum, keep the entry. (ii) For a single-particle structure function written as a single entry, replace this by a record with two entries. (ii) For a record with two nontrivial entries, separate this into two records with one trivial entry each.

To achieve this, we need a function that tells us whether an entry is a spectrum or a structure function. It returns 0 for a trivial entry, 1 for a single-particle structure function, and 2 for a two-particle spectrum.

(Beam structures: interfaces)≡

```

abstract interface
    function strfun_mode_fun (name) result (n)
        import
        type(string_t), intent(in) :: name
        integer :: n
    end function strfun_mode_fun
end interface

```

Algorithm: (1) Mark entries as invalid where necessary. (2) Count the number of entries that we will need. (3) Expand and copy entries to a new record array. (4) Replace the old array by the new one.

(Beam structures: beam structure: TBP)+≡

```

procedure :: expand => beam_structure_expand

```

(Beam structures: procedures)+≡

```

subroutine beam_structure_expand (beam_structure, strfun_mode)
    class(beam_structure_t), intent(inout) :: beam_structure
    procedure(strfun_mode_fun) :: strfun_mode
    type(beam_structure_record_t), dimension(:), allocatable :: new
    integer :: n_record, i, j
    if (.not. allocated (beam_structure%record)) return
    do i = 1, size (beam_structure%record)
        associate (entry => beam_structure%record(i)%entry)
            do j = 1, size (entry)
                select case (strfun_mode (entry(j)%name))
                    case (0); entry(j)%is_valid = .false.
                end select
            end do
        end associate
    end do
    n_record = 0
    do i = 1, size (beam_structure%record)
        associate (entry => beam_structure%record(i)%entry)
            select case (size (entry))
                case (1)
                    if (entry(1)%is_valid) then
                        select case (strfun_mode (entry(1)%name))

```

```

        case (1); n_record = n_record + 2
        case (2); n_record = n_record + 1
    end select
end if
case (2)
do j = 1, 2
    if (entry(j)%is_valid) then
        select case (strfun_mode (entry(j)%name))
            case (1); n_record = n_record + 1
            case (2)
                call beam_structure%write ()
                call msg_fatal ("Pair spectrum used as &
                    &single-particle structure function")
            end select
        end if
    end do
end select
end associate
end do
allocate (new (n_record))
n_record = 0
do i = 1, size (beam_structure%record)
    associate (entry => beam_structure%record(i)%entry)
        select case (size (entry))
            case (1)
                if (entry(1)%is_valid) then
                    select case (strfun_mode (entry(1)%name))
                        case (1)
                            n_record = n_record + 1
                            allocate (new(n_record)%entry (2))
                            new(n_record)%entry(1) = entry(1)
                            n_record = n_record + 1
                            allocate (new(n_record)%entry (2))
                            new(n_record)%entry(2) = entry(1)
                        case (2)
                            n_record = n_record + 1
                            allocate (new(n_record)%entry (1))
                            new(n_record)%entry(1) = entry(1)
                        end select
                    end if
                end if
            case (2)
                do j = 1, 2
                    if (entry(j)%is_valid) then
                        n_record = n_record + 1
                        allocate (new(n_record)%entry (2))
                        new(n_record)%entry(j) = entry(j)
                    end if
                end do
            end select
        end associate
    end do
    call move_alloc (from = new, to = beam_structure%record)
end subroutine beam_structure_expand

```

16.1.3 Polarization

To record polarization, we provide an allocatable array of `smatrix` objects, sparse matrices. The polarization structure is independent of the structure-function setup, they are combined only when an actual beam object is constructed.

```

<Beam structures: beam structure: TBP>+=
  procedure :: final_pol => beam_structure_final_pol
  procedure :: init_pol => beam_structure_init_pol

<Beam structures: procedures>+=
  subroutine beam_structure_final_pol (beam_structure)
    class(beam_structure_t), intent(inout) :: beam_structure
    if (allocated (beam_structure%smatrix)) deallocate (beam_structure%smatrix)
    if (allocated (beam_structure%pol_f)) deallocate (beam_structure%pol_f)
  end subroutine beam_structure_final_pol

  subroutine beam_structure_init_pol (beam_structure, n)
    class(beam_structure_t), intent(inout) :: beam_structure
    integer, intent(in) :: n
    if (allocated (beam_structure%smatrix)) deallocate (beam_structure%smatrix)
    allocate (beam_structure%smatrix (n))
    if (.not. allocated (beam_structure%pol_f)) &
      allocate (beam_structure%pol_f (n), source = 1._default)
  end subroutine beam_structure_init_pol

```

Check if polarized beams are used.

```

<Beam structures: beam structure: TBP>+=
  procedure :: has_polarized_beams => beam_structure_has_polarized_beams

<Beam structures: procedures>+=
  elemental function beam_structure_has_polarized_beams (beam_structure) result (pol)
    logical :: pol
    class(beam_structure_t), intent(in) :: beam_structure
    if (allocated (beam_structure%pol_f)) then
      pol = any (beam_structure%pol_f /= 0)
    else
      pol = .false.
    end if
  end function beam_structure_has_polarized_beams

```

Directly copy the spin density matrices.

```

<Beam structures: beam structure: TBP>+=
  procedure :: set_smatrix => beam_structure_set_smatrix

<Beam structures: procedures>+=
  subroutine beam_structure_set_smatrix (beam_structure, i, smatrix)
    class(beam_structure_t), intent(inout) :: beam_structure
    integer, intent(in) :: i
    type(smatrix_t), intent(in) :: smatrix
    beam_structure%smatrix(i) = smatrix
  end subroutine beam_structure_set_smatrix

```


Initialize one of the spin density matrices manually.

```

(Beam structures: beam structure: TBP)+≡
    procedure :: init_smatrix => beam_structure_init_smatrix

(Beam structures: procedures)+≡
    subroutine beam_structure_init_smatrix (beam_structure, i, n_entry)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i
        integer, intent(in) :: n_entry
        call beam_structure%smatrix(i)%init (2, n_entry)
    end subroutine beam_structure_init_smatrix

```

Set a polarization entry.

```

(Beam structures: beam structure: TBP)+≡
    procedure :: set_sentry => beam_structure_set_sentry

(Beam structures: procedures)+≡
    subroutine beam_structure_set_sentry &
        (beam_structure, i, i_entry, index, value)
        class(beam_structure_t), intent(inout) :: beam_structure
        integer, intent(in) :: i
        integer, intent(in) :: i_entry
        integer, dimension(:), intent(in) :: index
        complex(default), intent(in) :: value
        call beam_structure%smatrix(i)%set_entry (i_entry, index, value)
    end subroutine beam_structure_set_sentry

```

Set the array of polarization fractions.

```

(Beam structures: beam structure: TBP)+≡
    procedure :: set_pol_f => beam_structure_set_pol_f

(Beam structures: procedures)+≡
    subroutine beam_structure_set_pol_f (beam_structure, f)
        class(beam_structure_t), intent(inout) :: beam_structure
        real(default), dimension(:), intent(in) :: f
        if (allocated (beam_structure%pol_f)) deallocate (beam_structure%pol_f)
        allocate (beam_structure%pol_f (size (f)), source = f)
    end subroutine beam_structure_set_pol_f

```

16.1.4 Beam momenta

By default, beam momenta are deduced from the `sqrts` value or from the mass of the decaying particle, assuming a c.m. setup. Here we set them explicitly.

```

(Beam structures: beam structure: TBP)+≡
    procedure :: final_mom => beam_structure_final_mom

(Beam structures: procedures)+≡
    subroutine beam_structure_final_mom (beam_structure)
        class(beam_structure_t), intent(inout) :: beam_structure
        if (allocated (beam_structure%p)) deallocate (beam_structure%p)
        if (allocated (beam_structure%theta)) deallocate (beam_structure%theta)
        if (allocated (beam_structure%phi)) deallocate (beam_structure%phi)
    end subroutine beam_structure_final_mom

```

```

<Beam structures: beam structure: TBP>+=
  procedure :: set_momentum => beam_structure_set_momentum
  procedure :: set_theta => beam_structure_set_theta
  procedure :: set_phi => beam_structure_set_phi

<Beam structures: procedures>+=
  subroutine beam_structure_set_momentum (beam_structure, p)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: p
    if (allocated (beam_structure%p)) deallocate (beam_structure%p)
    allocate (beam_structure%p (size (p)), source = p)
  end subroutine beam_structure_set_momentum

  subroutine beam_structure_set_theta (beam_structure, theta)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: theta
    if (allocated (beam_structure%theta)) deallocate (beam_structure%theta)
    allocate (beam_structure%theta (size (theta)), source = theta)
  end subroutine beam_structure_set_theta

  subroutine beam_structure_set_phi (beam_structure, phi)
    class(beam_structure_t), intent(inout) :: beam_structure
    real(default), dimension(:), intent(in) :: phi
    if (allocated (beam_structure%phi)) deallocate (beam_structure%phi)
    allocate (beam_structure%phi (size (phi)), source = phi)
  end subroutine beam_structure_set_phi

```

16.1.5 Get contents

Look at the incoming particles. We may also have the case that beam particles are not specified, but polarization.

```

<Beam structures: beam structure: TBP>+=
  procedure :: is_set => beam_structure_is_set
  procedure :: get_n_beam => beam_structure_get_n_beam
  procedure :: get_prt => beam_structure_get_prt

<Beam structures: procedures>+=
  function beam_structure_is_set (beam_structure) result (flag)
    class(beam_structure_t), intent(in) :: beam_structure
    logical :: flag
    flag = beam_structure%n_beam > 0 .or. beam_structure%asymmetric ()
  end function beam_structure_is_set

  function beam_structure_get_n_beam (beam_structure) result (n)
    class(beam_structure_t), intent(in) :: beam_structure
    integer :: n
    n = beam_structure%n_beam
  end function beam_structure_get_n_beam

  function beam_structure_get_prt (beam_structure) result (prt)
    class(beam_structure_t), intent(in) :: beam_structure
    type(string_t), dimension(:), allocatable :: prt
    allocate (prt (size (beam_structure%prt)))

```

```

    prt = beam_structure%prt
end function beam_structure_get_prt

```

Return the number of records.

```

(Beam structures: beam structure: TBP)+≡
    procedure :: get_n_record => beam_structure_get_n_record

(Beam structures: procedures)+≡
    function beam_structure_get_n_record (beam_structure) result (n)
        class(beam_structure_t), intent(in) :: beam_structure
        integer :: n
        if (allocated (beam_structure%record)) then
            n = size (beam_structure%record)
        else
            n = 0
        end if
    end function beam_structure_get_n_record

```

Return an array consisting of the beam indices affected by the valid entries within a record. After expansion, there should be exactly one valid entry per record.

```

(Beam structures: beam structure: TBP)+≡
    procedure :: get_i_entry => beam_structure_get_i_entry

(Beam structures: procedures)+≡
    function beam_structure_get_i_entry (beam_structure, i) result (i_entry)
        class(beam_structure_t), intent(in) :: beam_structure
        integer, intent(in) :: i
        integer, dimension(:), allocatable :: i_entry
        associate (record => beam_structure%record(i))
            select case (size (record%entry))
            case (1)
                if (record%entry(1)%is_valid) then
                    allocate (i_entry (2), source = [1, 2])
                else
                    allocate (i_entry (0))
                end if
            case (2)
                if (all (record%entry%is_valid)) then
                    allocate (i_entry (2), source = [1, 2])
                else if (record%entry(1)%is_valid) then
                    allocate (i_entry (1), source = [1])
                else if (record%entry(2)%is_valid) then
                    allocate (i_entry (1), source = [2])
                else
                    allocate (i_entry (0))
                end if
            end select
        end associate
    end function beam_structure_get_i_entry

```

Return the name of the first valid entry within a record. After expansion, there should be exactly one valid entry per record.

```

(Beam structures: beam structure: TBP)+≡

```

```

    procedure :: get_name => beam_structure_get_name
<Beam structures: procedures>+≡
    function beam_structure_get_name (beam_structure, i) result (name)
        type(string_t) :: name
        class(beam_structure_t), intent(in) :: beam_structure
        integer, intent(in) :: i
        associate (record => beam_structure%record(i))
            if (record%entry(1)%is_valid) then
                name = record%entry(1)%name
            else if (size (record%entry) == 2) then
                name = record%entry(2)%name
            end if
        end associate
    end function beam_structure_get_name

<Beam structures: beam structure: TBP>+≡
    procedure :: has_pdf => beam_structure_has_pdf

<Beam structures: procedures>+≡
    function beam_structure_has_pdf (beam_structure) result (has_pdf)
        logical :: has_pdf
        class(beam_structure_t), intent(in) :: beam_structure
        integer :: i
        type(string_t) :: name
        has_pdf = .false.
        do i = 1, beam_structure%get_n_record ()
            name = beam_structure%get_name (i)
            has_pdf = has_pdf .or. name == var_str ("pdf_builtin") .or. name == var_str ("lhpdf")
        end do
    end function beam_structure_has_pdf

```

Return true if the beam structure contains a particular structure function identifier (such as lhpdf, isr, etc.)

```

<Beam structures: beam structure: TBP>+≡
    procedure :: contains => beam_structure_contains

<Beam structures: procedures>+≡
    function beam_structure_contains (beam_structure, name) result (flag)
        class(beam_structure_t), intent(in) :: beam_structure
        character(*), intent(in) :: name
        logical :: flag
        integer :: i, j
        flag = .false.
        if (allocated (beam_structure%record)) then
            do i = 1, size (beam_structure%record)
                do j = 1, size (beam_structure%record(i)%entry)
                    flag = beam_structure%record(i)%entry(j)%name == name
                    if (flag) return
                end do
            end do
        end if
    end function beam_structure_contains

```

Return polarization data.

```

(Beam structures: beam structure: TBP) +=
  procedure :: polarized => beam_structure_polarized
  procedure :: get_smatrix => beam_structure_get_smatrix
  procedure :: get_pol_f => beam_structure_get_pol_f
  procedure :: asymmetric => beam_structure_asymmetric

(Beam structures: procedures) +=
  function beam_structure_polarized (beam_structure) result (flag)
    class(beam_structure_t), intent(in) :: beam_structure
    logical :: flag
    flag = allocated (beam_structure%smatrix)
  end function beam_structure_polarized

  function beam_structure_get_smatrix (beam_structure) result (smatrix)
    class(beam_structure_t), intent(in) :: beam_structure
    type(smatrix_t), dimension(:), allocatable :: smatrix
    allocate (smatrix (size (beam_structure%smatrix)), &
      source = beam_structure%smatrix)
  end function beam_structure_get_smatrix

  function beam_structure_get_pol_f (beam_structure) result (pol_f)
    class(beam_structure_t), intent(in) :: beam_structure
    real(default), dimension(:), allocatable :: pol_f
    allocate (pol_f (size (beam_structure%pol_f)), &
      source = beam_structure%pol_f)
  end function beam_structure_get_pol_f

  function beam_structure_asymmetric (beam_structure) result (flag)
    class(beam_structure_t), intent(in) :: beam_structure
    logical :: flag
    flag = allocated (beam_structure%p) &
      .or. allocated (beam_structure%theta) &
      .or. allocated (beam_structure%phi)
  end function beam_structure_asymmetric

```

Return the beam momenta (the space part, i.e., three-momenta). This is meaningful only if momenta and, optionally, angles have been set.

```

(Beam structures: beam structure: TBP) +=
  procedure :: get_momenta => beam_structure_get_momenta

(Beam structures: procedures) +=
  function beam_structure_get_momenta (beam_structure) result (p)
    class(beam_structure_t), intent(in) :: beam_structure
    type(vector3_t), dimension(:), allocatable :: p
    real(default), dimension(:), allocatable :: theta, phi
    integer :: n, i
    if (allocated (beam_structure%p)) then
      n = size (beam_structure%p)
      if (allocated (beam_structure%theta)) then
        if (size (beam_structure%theta) == n) then
          allocate (theta (n), source = beam_structure%theta)
        else
          call msg_fatal ("Beam structure: mismatch in momentum vs. &

```

```

        &angle theta specification")
    end if
else
    allocate (theta (n), source = 0._default)
end if
if (allocated (beam_structure%phi)) then
    if (size (beam_structure%phi) == n) then
        allocate (phi (n), source = beam_structure%phi)
    else
        call msg_fatal ("Beam structure: mismatch in momentum vs. &
        &angle phi specification")
    end if
else
    allocate (phi (n), source = 0._default)
end if
allocate (p (n))
do i = 1, n
    p(i) = beam_structure%p(i) * vector3_moving ([ &
        sin (theta(i)) * cos (phi(i)), &
        sin (theta(i)) * sin (phi(i)), &
        cos (theta(i))] )
end do
if (n == 2) p(2) = - p(2)
else
    call msg_fatal ("Beam structure: angle theta/phi specified but &
    &momentum/a p undefined")
end if
end function beam_structure_get_momenta

```

Check for a complete beam structure. The `applies` flag tells if the beam structure should actually be used for a process with the given `n_in` number of incoming particles.

It is set if the beam structure matches the process as either decay or scattering. It is unset if beam structure references a scattering setup but the process is a decay. It is also unset if the beam structure itself is empty.

If the beam structure cannot be used, terminate with fatal error.

```

<Beam structures: beam structure: TBP>+≡
    procedure :: check_against_n_in => beam_structure_check_against_n_in

<Beam structures: procedures>+≡
    subroutine beam_structure_check_against_n_in (beam_structure, n_in, applies)
        class(beam_structure_t), intent(in) :: beam_structure
        integer, intent(in) :: n_in
        logical, intent(out) :: applies
        if (beam_structure%is_set ()) then
            if (n_in == beam_structure%get_n_beam ()) then
                applies = .true.
            else if (beam_structure%get_n_beam () == 0) then
                call msg_fatal &
                ("Asymmetric beams: missing beam particle specification")
                applies = .false.
            else
                call msg_fatal &

```

```

        ("Mismatch of process and beam setup (scattering/decay)")
        applies = .false.
    end if
else
    applies = .false.
end if
end subroutine beam_structure_check_against_n_in

```

16.1.6 Unit Tests

Test module, followed by the corresponding implementation module.

`<beam_structures_ut.f90>`≡

<File header>

```

module beam_structures_ut
  use unit_tests
  use beam_structures_util

```

<Standard module head>

<Beam structures: public test>

contains

<Beam structures: test driver>

```

end module beam_structures_ut

```

`<beam_structures_util.f90>`≡

<File header>

```

module beam_structures_util

```

<Use kinds>

<Use strings>

```

  use beam_structures

```

<Standard module head>

<Beam structures: test declarations>

contains

<Beam structures: tests>

<Beam structures: test auxiliary>

```

end module beam_structures_util

```

API: driver for the unit tests below.

<Beam structures: public test>≡

```

  public :: beam_structures_test

```

```

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

```

Empty structure

```

<Beam structures: execute tests>≡
  call test (beam_structures_1, "beam_structures_1", &
    "empty beam structure record", &
    u, results)

<Beam structures: test declarations>≡
  public :: beam_structures_1

<Beam structures: tests>≡
  subroutine beam_structures_1 (u)
    integer, intent(in) :: u
    type(beam_structure_t) :: beam_structure

    write (u, "(A)")  "* Test output: beam_structures_1"
    write (u, "(A)")  "* Purpose: display empty beam structure record"
    write (u, "(A)")

    call beam_structure%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: beam_structures_1"

  end subroutine beam_structures_1

```

Nontrivial configurations

```

<Beam structures: execute tests>+≡
  call test (beam_structures_2, "beam_structures_2", &
    "beam structure records", &
    u, results)

<Beam structures: test declarations>+≡
  public :: beam_structures_2

<Beam structures: tests>+≡
  subroutine beam_structures_2 (u)
    integer, intent(in) :: u
    type(beam_structure_t) :: beam_structure
    integer, dimension(0) :: empty_array
    type(string_t) :: s

    write (u, "(A)")  "* Test output: beam_structures_2"
    write (u, "(A)")  "* Purpose: setup beam structure records"
    write (u, "(A)")

```



```

s = "s"

call beam_structure%init_sf ([s], empty_array)
call beam_structure%write (u)

write (u, "(A)")

call beam_structure%init_sf ([s, s], [1])
call beam_structure%set_sf (1, 1, var_str ("a"))
call beam_structure%write (u)

write (u, "(A)")

call beam_structure%init_sf ([s, s], [2])
call beam_structure%set_sf (1, 1, var_str ("a"))
call beam_structure%set_sf (1, 2, var_str ("b"))
call beam_structure%write (u)

write (u, "(A)")

call beam_structure%init_sf ([s, s], [2, 1])
call beam_structure%set_sf (1, 1, var_str ("a"))
call beam_structure%set_sf (1, 2, var_str ("b"))
call beam_structure%set_sf (2, 1, var_str ("c"))
call beam_structure%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_structures_2"

end subroutine beam_structures_2

```

Expansion

Provide a function that tells, for the dummy structure function names used here, whether they are considered a two-particle spectrum or a single-particle structure function:

```

<Beam structures: test auxiliary>≡
function test_strfun_mode (name) result (n)
  type(string_t), intent(in) :: name
  integer :: n
  select case (char (name))
    case ("a"); n = 2
    case ("b"); n = 1
    case default; n = 0
  end select
end function test_strfun_mode

<Beam structures: execute tests>+≡
call test (beam_structures_3, "beam_structures_3", &
  "beam structure expansion", &
  u, results)

```

```

<Beam structures: test declarations>+=
    public :: beam_structures_3

<Beam structures: tests>+=
    subroutine beam_structures_3 (u)
        integer, intent(in) :: u
        type(beam_structure_t) :: beam_structure
        type(string_t) :: s

        write (u, "(A)")  "* Test output: beam_structures_3"
        write (u, "(A)")  "*   Purpose: expand beam structure records"
        write (u, "(A)")

        s = "s"

        write (u, "(A)")  "* Pair spectrum (keep as-is)"
        write (u, "(A)")

        call beam_structure%init_sf ([s, s], [1])
        call beam_structure%set_sf (1, 1, var_str ("a"))
        call beam_structure%write (u)

        write (u, "(A)")

        call beam_structure%expand (test_strfun_mode)
        call beam_structure%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Structure function pair (expand)"
        write (u, "(A)")

        call beam_structure%init_sf ([s, s], [2])
        call beam_structure%set_sf (1, 1, var_str ("b"))
        call beam_structure%set_sf (1, 2, var_str ("b"))
        call beam_structure%write (u)

        write (u, "(A)")

        call beam_structure%expand (test_strfun_mode)
        call beam_structure%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Structure function (separate and expand)"
        write (u, "(A)")

        call beam_structure%init_sf ([s, s], [1])
        call beam_structure%set_sf (1, 1, var_str ("b"))
        call beam_structure%write (u)

        write (u, "(A)")

        call beam_structure%expand (test_strfun_mode)
        call beam_structure%write (u)

        write (u, "(A)")

```

```

write (u, "(A)")  "* Combination"
write (u, "(A)")

call beam_structure%init_sf ([s, s], [1, 1])
call beam_structure%set_sf (1, 1, var_str ("a"))
call beam_structure%set_sf (2, 1, var_str ("b"))
call beam_structure%write (u)

write (u, "(A)")

call beam_structure%expand (test_strfun_mode)
call beam_structure%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_structures_3"

end subroutine beam_structures_3

```

Public methods

Check the methods that can be called to get the beam-structure contents.

```

<Beam structures: execute tests>+≡
  call test (beam_structures_4, "beam_structures_4", &
    "beam structure contents", &
    u, results)

<Beam structures: test declarations>+≡
  public :: beam_structures_4

<Beam structures: tests>+≡
  subroutine beam_structures_4 (u)
    integer, intent(in) :: u
    type(beam_structure_t) :: beam_structure
    type(string_t) :: s
    type(string_t), dimension(2) :: prt
    integer :: i

    write (u, "(A)")  "* Test output: beam_structures_4"
    write (u, "(A)")  "* Purpose: check the API"
    write (u, "(A)")

    s = "s"

    write (u, "(A)")  "* Structure-function combination"
    write (u, "(A)")

    call beam_structure%init_sf ([s, s], [1, 2, 2])
    call beam_structure%set_sf (1, 1, var_str ("a"))
    call beam_structure%set_sf (2, 1, var_str ("b"))
    call beam_structure%set_sf (3, 2, var_str ("c"))
    call beam_structure%write (u)

    write (u, *)
    write (u, "(1x,A,I0)")  "n_beam = ", beam_structure%get_n_beam ()

```

```

prt = beam_structure%get_prt ()
write (u, "(1x,A,2(1x,A))" "prt =", char (prt(1)), char (prt(2))

write (u, *)
write (u, "(1x,A,I0)") "n_record = ", beam_structure%get_n_record ()

do i = 1, 3
  write (u, "(A)")
  write (u, "(1x,A,I0,A,A)" "name(", i, ") = ", &
    char (beam_structure%get_name (i))
  write (u, "(1x,A,I0,A,2(1x,I0))" "i_entry(", i, ") =", &
    beam_structure%get_i_entry (i)
end do

write (u, "(A)")
write (u, "(A)")  "** Test output end: beam_structures_4"

end subroutine beam_structures_4

```

Polarization

The polarization properties are independent from the structure-function setup.

```

<Beam structures: execute tests>+≡
  call test (beam_structures_5, "beam_structures_5", &
    "polarization", &
    u, results)

<Beam structures: test declarations>+≡
  public :: beam_structures_5

<Beam structures: tests>+≡
  subroutine beam_structures_5 (u)
    integer, intent(in) :: u
    type(beam_structure_t) :: beam_structure
    integer, dimension(0) :: empty_array
    type(string_t) :: s

    write (u, "(A)")  "** Test output: beam_structures_5"
    write (u, "(A)")  "** Purpose: setup polarization in beam structure records"
    write (u, "(A)")

    s = "s"

    call beam_structure%init_sf ([s], empty_array)
    call beam_structure%init_pol (1)
    call beam_structure%init_smatrix (1, 1)
    call beam_structure%set_sentry (1, 1, [0,0], (1._default, 0._default))
    call beam_structure%set_pol_f ([0.5_default])
    call beam_structure%write (u)

    write (u, "(A)")
    call beam_structure%final_sf ()
    call beam_structure%final_pol ()

```

```

call beam_structure%init_sf ([s, s], [1])
call beam_structure%set_sf (1, 1, var_str ("a"))
call beam_structure%init_pol (2)
call beam_structure%init_smatrix (1, 2)
call beam_structure%set_sentry (1, 1, [-1,1], (0.5_default,-0.5_default))
call beam_structure%set_sentry (1, 2, [ 1,1], (1._default, 0._default))
call beam_structure%init_smatrix (2, 0)
call beam_structure%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_structures_5"

end subroutine beam_structures_5

```

Momenta

The momenta are independent from the structure-function setup.

```

<Beam structures: execute tests>+≡
  call test (beam_structures_6, "beam_structures_6", &
    "momenta", &
    u, results)

<Beam structures: test declarations>+≡
  public :: beam_structures_6

<Beam structures: tests>+≡
  subroutine beam_structures_6 (u)
    integer, intent(in) :: u
    type(beam_structure_t) :: beam_structure
    integer, dimension(0) :: empty_array
    type(string_t) :: s

    write (u, "(A)")  "* Test output: beam_structures_6"
    write (u, "(A)")  "* Purpose: setup momenta in beam structure records"
    write (u, "(A)")

    s = "s"

    call beam_structure%init_sf ([s], empty_array)
    call beam_structure%set_momentum ([500._default])
    call beam_structure%write (u)

    write (u, "(A)")
    call beam_structure%final_sf ()
    call beam_structure%final_mom ()

    call beam_structure%init_sf ([s, s], [1])
    call beam_structure%set_momentum ([500._default, 700._default])
    call beam_structure%set_theta ([0._default, 0.1_default])
    call beam_structure%set_phi ([0._default, 1.51_default])
    call beam_structure%write (u)

```

```

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: beam_structures_6"

    end subroutine beam_structures_6

```

16.2 Beams for collisions and decays

```

⟨beams.f90⟩≡
  ⟨File header⟩

  module beams

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use io_units
    use format_defs, only: FMT_19
    use numeric_utils
    use diagnostics
    use md5
    use lorentz
    use model_data
    use flavors
    use quantum_numbers
    use state_matrices
    use interactions
    use polarizations
    use beam_structures

    ⟨Standard module head⟩

    ⟨Beams: public⟩

    ⟨Beams: types⟩

    ⟨Beams: interfaces⟩

    contains

    ⟨Beams: procedures⟩

  end module beams

```

16.2.1 Beam data

The beam data type contains beam data for one or two beams, depending on whether we are dealing with beam collisions or particle decay. In addition, it holds the c.m. energy `sqrts`, the Lorentz transformation `L` that transforms the c.m. system into the lab system, and the pair of c.m. momenta.

```

⟨Beams: public⟩≡
  public :: beam_data_t

```

```

(Beams: types)≡
  type :: beam_data_t
    logical :: initialized = .false.
    integer :: n = 0
    type(flavor_t), dimension(:), allocatable :: flv
    real(default), dimension(:), allocatable :: mass
    type(pmatrix_t), dimension(:), allocatable :: pmatrix
    logical :: lab_is_cm = .true.
    type(vector4_t), dimension(:), allocatable :: p_cm
    type(vector4_t), dimension(:), allocatable :: p
    type(lorentz_transformation_t), allocatable :: L_cm_to_lab
    real(default) :: sqrts = 0
    character(32) :: md5sum = ""
  contains
    (Beams: beam data: TBP)
  end type beam_data_t

```

Generic initializer. This is called by the specific initializers below. Initialize either for decay or for collision.

```

(Beams: procedures)≡
  subroutine beam_data_init (beam_data, n)
    type(beam_data_t), intent(out) :: beam_data
    integer, intent(in) :: n
    beam_data%n = n
    allocate (beam_data%flv (n))
    allocate (beam_data%mass (n))
    allocate (beam_data%pmatrix (n))
    allocate (beam_data%p_cm (n))
    allocate (beam_data%p (n))
    beam_data%initialized = .true.
  end subroutine beam_data_init

```

Finalizer: needed for the polarization components of the beams.

```

(Beams: beam data: TBP)≡
  procedure :: final => beam_data_final

(Beams: procedures)+≡
  subroutine beam_data_final (beam_data)
    class(beam_data_t), intent(inout) :: beam_data
    beam_data%initialized = .false.
  end subroutine beam_data_final

```

The verbose (default) version is for debugging. The short version is for screen output in the UI.

```

(Beams: beam data: TBP)+≡
  procedure :: write => beam_data_write

(Beams: procedures)+≡
  subroutine beam_data_write (beam_data, unit, verbose, write_md5sum)
    class(beam_data_t), intent(in) :: beam_data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, write_md5sum
    integer :: prt_name_len

```

```

logical :: verb, write_md5
integer :: u
u = given_output_unit (unit); if (u < 0) return
verb = .false.; if (present (verbose)) verb = verbose
write_md5 = verb; if (present (write_md5sum)) write_md5 = write_md5sum
if (.not. beam_data%initialized) then
    write (u, "(1x,A)") "Beam data: [undefined]"
    return
end if
prt_name_len = maxval (len (beam_data%flv%get_name ()))
select case (beam_data%n)
case (1)
    write (u, "(1x,A)") "Beam data (decay):"
    if (verb) then
        call write_prt (1)
        call beam_data%pmatrix(1)%write (u)
        write (u, *) "R.f. momentum:"
        call vector4_write (beam_data%p_cm(1), u)
        write (u, *) "Lab momentum:"
        call vector4_write (beam_data%p(1), u)
    else
        call write_prt (1)
    end if
case (2)
    write (u, "(1x,A)") "Beam data (collision):"
    if (verb) then
        call write_prt (1)
        call beam_data%pmatrix(1)%write (u)
        call write_prt (2)
        call beam_data%pmatrix(2)%write (u)
        call write_sqrts
        write (u, *) "C.m. momenta:"
        call vector4_write (beam_data%p_cm(1), u)
        call vector4_write (beam_data%p_cm(2), u)
        write (u, *) "Lab momenta:"
        call vector4_write (beam_data%p(1), u)
        call vector4_write (beam_data%p(2), u)
    else
        call write_prt (1)
        call write_prt (2)
        call write_sqrts
    end if
end select
if (allocated (beam_data%L_cm_to_lab)) then
    if (verb) then
        call lorentz_transformation_write (beam_data%L_cm_to_lab, u)
    else
        write (u, "(1x,A)") "Beam structure: lab and c.m. frame differ"
    end if
end if
if (write_md5) then
    write (u, *) "MD5 sum: ", beam_data%md5sum
end if
contains

```



```

subroutine write_sqrts
  character(80) :: sqrts_str
  write (sqrts_str, "(" // FMT_19 // ")") beam_data%sqrts
  write (u, "(3x,A)") "sqrts = " // trim (adjustl (sqrts_str)) // " GeV"
end subroutine write_sqrts
subroutine write_prt (i)
  integer, intent(in) :: i
  character(80) :: name_str, mass_str
  write (name_str, "(A)") char (beam_data%flv(i)%get_name ())
  write (mass_str, "(ES13.7)") beam_data%mass(i)
  write (u, "(3x,A)", advance="no") &
    name_str(:prt_name_len) // " (mass = " &
    // trim (adjustl (mass_str)) // " GeV"
  if (beam_data%pmatrix(i)%is_polarized ()) then
    write (u, "(2x,A)") "polarized"
  else
    write (u, *)
  end if
end subroutine write_prt
end subroutine beam_data_write

```

Return initialization status:

```

(Beams: beam data: TBP)+≡
  procedure :: are_valid => beam_data_are_valid

(Beams: procedures)+≡
  function beam_data_are_valid (beam_data) result (flag)
    class(beam_data_t), intent(in) :: beam_data
    logical :: flag
    flag = beam_data%initialized
  end function beam_data_are_valid

```

Check whether beam data agree with the current values of relevant parameters.

```

(Beams: beam data: TBP)+≡
  procedure :: check_scattering => beam_data_check_scattering

(Beams: procedures)+≡
  subroutine beam_data_check_scattering (beam_data, sqrts)
    class(beam_data_t), intent(in) :: beam_data
    real(default), intent(in), optional :: sqrts
    if (beam_data_are_valid (beam_data)) then
      if (present (sqrts)) then
        if (.not. nearly_equal (sqrts, beam_data%sqrts)) then
          call msg_error ("Current setting of sqrts is inconsistent " &
            // "with beam setup (ignored).")
        end if
      end if
    else
      call msg_bug ("Beam setup: invalid beam data")
    end if
  end subroutine beam_data_check_scattering

```

Return the number of beams (1 for decays, 2 for collisions).

```

(Beams: beam data: TBP)+≡
  procedure :: get_n_in => beam_data_get_n_in

(Beams: procedures)+≡
  function beam_data_get_n_in (beam_data) result (n_in)
    class(beam_data_t), intent(in) :: beam_data
    integer :: n_in
    n_in = beam_data%n
  end function beam_data_get_n_in

```

Return the beam flavor

```

(Beams: beam data: TBP)+≡
  procedure :: get_flavor => beam_data_get_flavor

(Beams: procedures)+≡
  function beam_data_get_flavor (beam_data) result (flv)
    class(beam_data_t), intent(in) :: beam_data
    type(flavor_t), dimension(:), allocatable :: flv
    allocate (flv (beam_data%n))
    flv = beam_data%flv
  end function beam_data_get_flavor

```

Return the beam energies

```

(Beams: beam data: TBP)+≡
  procedure :: get_energy => beam_data_get_energy

(Beams: procedures)+≡
  function beam_data_get_energy (beam_data) result (e)
    class(beam_data_t), intent(in) :: beam_data
    real(default), dimension(:), allocatable :: e
    integer :: i
    allocate (e (beam_data%n))
    if (beam_data%initialized) then
      do i = 1, beam_data%n
        e(i) = energy (beam_data%p(i))
      end do
    else
      e = 0
    end if
  end function beam_data_get_energy

```

Return the c.m. energy.

```

(Beams: beam data: TBP)+≡
  procedure :: get_sqrts => beam_data_get_sqrts

(Beams: procedures)+≡
  function beam_data_get_sqrts (beam_data) result (sqrts)
    class(beam_data_t), intent(in) :: beam_data
    real(default) :: sqrts
    sqrts = beam_data%sqrts
  end function beam_data_get_sqrts

```

Return the polarization in case it is just two degrees

```

(Beams: beam data: TBP)+≡
    procedure :: get_polarization => beam_data_get_polarization

(Beams: procedures)+≡
    function beam_data_get_polarization (beam_data) result (pol)
        class(beam_data_t), intent(in) :: beam_data
        real(default), dimension(2) :: pol
        if (beam_data%n /= 2) &
            call msg_fatal ("Beam data: can only treat scattering processes.")
        pol = beam_data%pmatrix%get_simple_pol ()
    end function beam_data_get_polarization

(Beams: beam data: TBP)+≡
    procedure :: get_helicity_state_matrix => beam_data_get_helicity_state_matrix

(Beams: procedures)+≡
    function beam_data_get_helicity_state_matrix (beam_data) result (state_hel)
        type(state_matrix_t) :: state_hel
        class(beam_data_t), intent(in) :: beam_data
        type(polarization_t), dimension(:), allocatable :: pol
        integer :: i
        allocate (pol (beam_data%n))
        do i = 1, beam_data%n
            call pol(i)%init_pmatrix (beam_data%pmatrix(i))
        end do
        call combine_polarization_states (pol, state_hel)
    end function beam_data_get_helicity_state_matrix

(Beams: beam data: TBP)+≡
    procedure :: is_initialized => beam_data_is_initialized

(Beams: procedures)+≡
    function beam_data_is_initialized (beam_data) result (initialized)
        logical :: initialized
        class(beam_data_t), intent(in) :: beam_data
        initialized = any (beam_data%pmatrix%exists ())
    end function beam_data_is_initialized

```

Return a MD5 checksum for beam data. If no checksum is present (because beams have not been initialized), compute the checksum of the sqrts value.

```

(Beams: beam data: TBP)+≡
    procedure :: get_md5sum => beam_data_get_md5sum

(Beams: procedures)+≡
    function beam_data_get_md5sum (beam_data, sqrts) result (md5sum_beams)
        class(beam_data_t), intent(in) :: beam_data
        real(default), intent(in) :: sqrts
        character(32) :: md5sum_beams
        character(80) :: buffer
        if (beam_data%md5sum /= "") then
            md5sum_beams = beam_data%md5sum
        else
            write (buffer, *) sqrts

```

```

        md5sum_beams = md5sum (buffer)
    end if
end function beam_data_get_md5sum

```

16.2.2 Initializers: beam structure

Initialize the beam data object from a beam structure object, given energy and model.

```

(Beams: beam data: TBP)+≡
    procedure :: init_structure => beam_data_init_structure

(Beams: procedures)+≡
    subroutine beam_data_init_structure &
        (beam_data, structure, sqrts, model, decay_rest_frame)
    class(beam_data_t), intent(out) :: beam_data
    type(beam_structure_t), intent(in) :: structure
    integer :: n_beam
    real(default), intent(in) :: sqrts
    class(model_data_t), intent(in), target :: model
    logical, intent(in), optional :: decay_rest_frame
    type(flavor_t), dimension(:), allocatable :: flv
    n_beam = structure%get_n_beam ()
    allocate (flv (n_beam))
    call flv%init (structure%get_prt (), model)
    if (structure%asymmetric ()) then
        if (structure%polarized ()) then
            call beam_data%init_momenta (structure%get_momenta (), flv, &
                structure%get_smatrix (), structure%get_pol_f ())
        else
            call beam_data%init_momenta (structure%get_momenta (), flv)
        end if
    else
        select case (n_beam)
        case (1)
            if (structure%polarized ()) then
                call beam_data%init_decay (flv, &
                    structure%get_smatrix (), structure%get_pol_f (), &
                    rest_frame = decay_rest_frame)
            else
                call beam_data%init_decay (flv, &
                    rest_frame = decay_rest_frame)
            end if
        case (2)
            if (structure%polarized ()) then
                call beam_data%init_sqrts (sqrts, flv, &
                    structure%get_smatrix (), structure%get_pol_f ())
            else
                call beam_data%init_sqrts (sqrts, flv)
            end if
        case default
            call msg_bug ("Beam data: invalid beam structure object")
        end select
    end if
end if

```

```
end subroutine beam_data_init_structure
```

16.2.3 Initializers: collisions

This is the simplest one: just the two flavors, c.m. energy, polarization. Color is inferred from flavor. Beam momenta and c.m. momenta coincide.

(Beams: beam data: TBP)+≡

```
procedure :: init_sqrts => beam_data_init_sqrts
```

(Beams: procedures)+≡

```
subroutine beam_data_init_sqrts (beam_data, sqrts, flv, smatrix, pol_f)
  class(beam_data_t), intent(out) :: beam_data
  real(default), intent(in) :: sqrts
  type(flavor_t), dimension(:), intent(in) :: flv
  type(smatrix_t), dimension(:), intent(in), optional :: smatrix
  real(default), dimension(:), intent(in), optional :: pol_f
  real(default), dimension(size(flv)) :: E, p
  call beam_data_init (beam_data, size (flv))
  beam_data%sqrts = sqrts
  beam_data%lab_is_cm = .true.
  select case (beam_data%n)
  case (1)
    E = sqrts; p = 0
    beam_data%p_cm = vector4_moving (E, p, 3)
    beam_data%p = beam_data%p_cm
  case (2)
    beam_data%p_cm = colliding_momenta (sqrts, flv%get_mass ())
    beam_data%p = colliding_momenta (sqrts, flv%get_mass ())
  end select
  call beam_data_finish_initialization (beam_data, flv, smatrix, pol_f)
end subroutine beam_data_init_sqrts
```

This version sets beam momenta directly, assuming that they are asymmetric, i.e., lab frame and c.m. frame do not coincide. Polarization info is deferred to a common initializer.

The Lorentz transformation that we compute here is not actually used in the calculation; instead, it will be recomputed for each event in the subroutine `phs_set_incoming_momenta`. We compute it here for the nominal beam setup nevertheless, so we can print it and, in particular, include it in the MD5 sum.

(Beams: beam data: TBP)+≡

```
procedure :: init_momenta => beam_data_init_momenta
```

(Beams: procedures)+≡

```
subroutine beam_data_init_momenta (beam_data, p3, flv, smatrix, pol_f)
  class(beam_data_t), intent(out) :: beam_data
  type(vector3_t), dimension(:), intent(in) :: p3
  type(flavor_t), dimension(:), intent(in) :: flv
  type(smatrix_t), dimension(:), intent(in), optional :: smatrix
  real(default), dimension(:), intent(in), optional :: pol_f
  type(vector4_t) :: p0
  type(vector4_t), dimension(:), allocatable :: p, p_cm_rot
  real(default), dimension(size(p3)) :: e
```

```

real(default), dimension(size(flv)) :: m
type(lorentz_transformation_t) :: L_boost, L_rot
call beam_data_init (beam_data, size (flv))
m = flv%get_mass ()
e = sqrt (p3 ** 2 + m ** 2)
allocate (p (beam_data%n))
p = vector4_moving (e, p3)
p0 = sum (p)
beam_data%p = p
beam_data%lab_is_cm = .false.
beam_data%sqrts = p0 ** 1
L_boost = boost (p0, beam_data%sqrts)
allocate (p_cm_rot (beam_data%n))
p_cm_rot = inverse (L_boost) * p
allocate (beam_data%L_cm_to_lab)
select case (beam_data%n)
case (1)
    beam_data%L_cm_to_lab = L_boost
    beam_data%p_cm = vector4_at_rest (beam_data%sqrts)
case (2)
    L_rot = rotation_to_2nd (3, space_part (p_cm_rot(1)))
    beam_data%L_cm_to_lab = L_boost * L_rot
    beam_data%p_cm = &
        colliding_momenta (beam_data%sqrts, flv%get_mass ())
end select
call beam_data_finish_initialization (beam_data, flv, smatrix, pol_f)
end subroutine beam_data_init_momenta

```

Final steps: If requested, rotate the beams in the lab frame, and set the beam-data components.

(Beams: procedures)+≡

```

subroutine beam_data_finish_initialization (beam_data, flv, smatrix, pol_f)
type(beam_data_t), intent(inout) :: beam_data
type(flavor_t), dimension(:), intent(in) :: flv
type(smatrix_t), dimension(:), intent(in), optional :: smatrix
real(default), dimension(:), intent(in), optional :: pol_f
integer :: i
do i = 1, beam_data%n
    beam_data%flv(i) = flv(i)
    beam_data%mass(i) = flv(i)%get_mass ()
    if (present (smatrix)) then
        if (size (smatrix) /= beam_data%n) &
            call msg_fatal ("Beam data: &
                &polarization density array has wrong dimension")
        beam_data%pmatrx(i) = smatrix(i)
    if (present (pol_f)) then
        if (size (pol_f) /= size (smatrix)) &
            call msg_fatal ("Beam data: &
                &polarization fraction array has wrong dimension")
        call beam_data%pmatrx(i)%normalize (flv(i), pol_f(i))
    else
        call beam_data%pmatrx(i)%normalize (flv(i), 1._default)
    end if
end do

```

```

        else
            call beam_data%pmatrx(i)%init (2, 0)
            call beam_data%pmatrx(i)%normalize (flv(i), 0._default)
        end if
    end do
    call beam_data%compute_md5sum ()
end subroutine beam_data_finish_initialization

```

The MD5 sum is stored within the beam-data record, so it can be checked for integrity in subsequent runs.

```

(Beams: beam data: TBP)+≡
    procedure :: compute_md5sum => beam_data_compute_md5sum

(Beams: procedures)+≡
    subroutine beam_data_compute_md5sum (beam_data)
        class(beam_data_t), intent(inout) :: beam_data
        integer :: unit
        unit = free_unit ()
        open (unit = unit, status = "scratch", action = "readwrite")
        call beam_data%write (unit, write_md5sum = .false., &
            verbose = .true.)
        rewind (unit)
        beam_data%md5sum = md5sum (unit)
        close (unit)
    end subroutine beam_data_compute_md5sum

```

16.2.4 Initializers: decays

This is the simplest one: decay in rest frame. We need just flavor and polarization. Color is inferred from flavor. Beam momentum and c.m. momentum coincide.

```

(Beams: beam data: TBP)+≡
    procedure :: init_decay => beam_data_init_decay

(Beams: procedures)+≡
    subroutine beam_data_init_decay (beam_data, flv, smatrix, pol_f, rest_frame)
        class(beam_data_t), intent(out) :: beam_data
        type(flavor_t), dimension(1), intent(in) :: flv
        type(smatrix_t), dimension(1), intent(in), optional :: smatrix
        real(default), dimension(:), intent(in), optional :: pol_f
        logical, intent(in), optional :: rest_frame
        real(default), dimension(1) :: m
        m = flv%get_mass ()
        if (present (smatrix)) then
            call beam_data%init_sqrts (m(1), flv, smatrix, pol_f)
        else
            call beam_data%init_sqrts (m(1), flv, smatrix, pol_f)
        end if
        if (present (rest_frame)) beam_data%lab_is_cm = rest_frame
    end subroutine beam_data_init_decay

```

16.2.5 The beams type

Beam objects are interaction objects that contain the actual beam data including polarization and density matrix. For collisions, the beam object actually contains two beams.

```

(Beams: public)+≡
    public :: beam_t

(Beams: types)+≡
    type :: beam_t
    private
        type(interaction_t) :: int
    end type beam_t

```

The constructor contains code that converts beam data into the (entangled) particle-pair quantum state. First, we set the number of particles and polarization mask. (The polarization mask is handed over to all later interactions, so if helicity is diagonal or absent, this fact is used when constructing the hard-interaction events.) Then, we construct the entangled state that combines helicity, flavor and color of the two particles (where flavor and color are unique, while several helicity states are possible). Then, we transfer this state together with the associated values from the spin density matrix into the `interaction_t` object.

Calling the `add_state` method of the interaction object, we keep the entries of the helicity density matrix without adding them up. This ensures that for unpolarized states, we do not normalize but end up with an $1/N$ entry, where N is the initial-state multiplicity.

```

(Beams: public)+≡
    public :: beam_init

(Beams: procedures)+≡
    subroutine beam_init (beam, beam_data)
        type(beam_t), intent(out) :: beam
        type(beam_data_t), intent(in), target :: beam_data
        logical, dimension(beam_data%n) :: polarized, diagonal
        type(quantum_numbers_mask_t), dimension(beam_data%n) :: mask, mask_d
        type(state_matrix_t), target :: state_hel, state_fc, state_tmp
        type(state_iterator_t) :: it_hel, it_tmp
        type(quantum_numbers_t), dimension(:), allocatable :: qn
        complex(default) :: value
        real(default), parameter :: tolerance = 100 * epsilon (1._default)
        polarized = beam_data%pmatrix%is_polarized ()
        diagonal = beam_data%pmatrix%is_diagonal ()
        mask = quantum_numbers_mask (.false., .false., &
            mask_h = .not. polarized, &
            mask_hd = diagonal)
        mask_d = quantum_numbers_mask (.false., .false., .false., &
            mask_hd = polarized .and. diagonal)
        call beam%int%basic_init &
            (0, 0, beam_data%n, mask = mask, store_values = .true.)
        state_hel = beam_data%get_helicity_state_matrix ()
        allocate (qn (beam_data%n))
        call qn%init (beam_data%flv, color_from_flavor (beam_data%flv, 1))
    end subroutine beam_init

```



```

call state_fc%init ()
call state_fc%add_state (qn)
call merge_state_matrices (state_hel, state_fc, state_tmp)
call it_hel%init (state_hel)
call it_tmp%init (state_tmp)
do while (it_hel%is_valid ())
    qn = it_tmp%get_quantum_numbers ()
    value = it_hel%get_matrix_element ()
    if (any (qn%are_redundant (mask_d))) then
        ! skip off-diagonal elements for diagonal polarization
    else if (abs (value) <= tolerance) then
        ! skip zero entries
    else
        call beam%int%add_state (qn, value = value)
    end if
    call it_hel%advance ()
    call it_tmp%advance ()
end do
call beam%int%freeze ()
call beam%int%set_momenta (beam_data%p, outgoing = .true.)
call state_hel%final ()
call state_fc%final ()
call state_tmp%final ()
end subroutine beam_init

```

Finalizer:

```

(Beams: public)+≡
    public :: beam_final

(Beams: procedures)+≡
    subroutine beam_final (beam)
        type(beam_t), intent(inout) :: beam
        call beam%int%final ()
    end subroutine beam_final

```

I/O:

```

(Beams: public)+≡
    public :: beam_write

(Beams: procedures)+≡
    subroutine beam_write (beam, unit, verbose, show_momentum_sum, show_mass, col_verbose)
        type(beam_t), intent(in) :: beam
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, show_momentum_sum, show_mass
        logical, intent(in), optional :: col_verbose
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        select case (beam%int%get_n_out ())
        case (1); write (u, *) "Decaying particle:"
        case (2); write (u, *) "Colliding beams:"
        end select
        call beam%int%basic_write &
            (unit, verbose = verbose, show_momentum_sum = &
                show_momentum_sum, show_mass = show_mass, &

```

```

        col_verbose = col_verbose)
end subroutine beam_write

```

Defined assignment: deep copy

```

<Beams: public>+≡
    public :: assignment(=)

<Beams: interfaces>≡
    interface assignment(=)
        module procedure beam_assign
    end interface

<Beams: procedures>+≡
    subroutine beam_assign (beam_out, beam_in)
        type(beam_t), intent(out) :: beam_out
        type(beam_t), intent(in) :: beam_in
        beam_out%int = beam_in%int
    end subroutine beam_assign

```

16.2.6 Inherited procedures

```

<Beams: public>+≡
    public :: interaction_set_source_link

<Beams: interfaces>+≡
    interface interaction_set_source_link
        module procedure interaction_set_source_link_beam
    end interface

<Beams: procedures>+≡
    subroutine interaction_set_source_link_beam (int, i, beam1, i1)
        type(interaction_t), intent(inout) :: int
        type(beam_t), intent(in), target :: beam1
        integer, intent(in) :: i, i1
        call int%set_source_link (i, beam1%int, i1)
    end subroutine interaction_set_source_link_beam

```

16.2.7 Accessing contents

Return the interaction component – as a pointer, to avoid any copying.

```

<Beams: public>+≡
    public :: beam_get_int_ptr

<Beams: procedures>+≡
    function beam_get_int_ptr (beam) result (int)
        type(interaction_t), pointer :: int
        type(beam_t), intent(in), target :: beam
        int => beam%int
    end function beam_get_int_ptr

```

Set beam momenta directly. (Used for cascade decays.)

```
<Beams: public>+≡
    public :: beam_set_momenta

<Beams: procedures>+≡
    subroutine beam_set_momenta (beam, p)
        type(beam_t), intent(inout) :: beam
        type(vector4_t), dimension(:), intent(in) :: p
        call beam%int%set_momenta (p)
    end subroutine beam_set_momenta
```

16.2.8 Unit tests

Test module, followed by the corresponding implementation module.

```
<beams_ut.f90>≡
    <File header>

    module beams_ut
        use unit_tests
        use beams_uti

    <Standard module head>

    <Beams: public test>

    contains

    <Beams: test driver>

    end module beams_ut

<beams_uti.f90>≡
    <File header>

    module beams_uti

    <Use kinds>
        use lorentz
        use flavors
        use interactions, only: reset_interaction_counter
        use polarizations, only: smatrix_t
        use model_data
        use beam_structures

        use beams

    <Standard module head>

    <Beams: test declarations>

    contains

    <Beams: tests>
```

```
end module beams_util
```

API: driver for the unit tests below.

```
<Beams: public test>≡
```

```
public :: beams_test
```

```
<Beams: test driver>≡
```

```
subroutine beams_test (u, results)
```

```
integer, intent(in) :: u
```

```
type(test_results_t), intent(inout) :: results
```

```
<Beams: execute tests>
```

```
end subroutine beams_test
```

Test the basic beam setup.

```
<Beams: execute tests>≡
```

```
call test (beam_1, "beam_1", &
  "check basic beam setup", &
  u, results)
```

```
<Beams: test declarations>≡
```

```
public :: beam_1
```

```
<Beams: tests>≡
```

```
subroutine beam_1 (u)
```

```
integer, intent(in) :: u
```

```
type(beam_data_t), target :: beam_data
```

```
type(beam_t) :: beam
```

```
real(default) :: sqrts
```

```
type(flavor_t), dimension(2) :: flv
```

```
type(smatrix_t), dimension(2) :: smatrix
```

```
real(default), dimension(2) :: pol_f
```

```
type(model_data_t), target :: model
```

```
write (u, "(A)")  "* Test output: beam_1"
```

```
write (u, "(A)")  "* Purpose: test basic beam setup"
```

```
write (u, "(A)")
```

```
write (u, "(A)")  "* Reading model file"
```

```
write (u, "(A)")
```

```
call reset_interaction_counter ()
```

```
call model%init_sm_test ()
```

```
write (u, "(A)")  "* Unpolarized scattering, massless fermions"
```

```
write (u, "(A)")
```

```
call reset_interaction_counter ()
```

```
sqrts = 500
```

```
call flv%init ([1,-1], model)
```

```
call beam_data%init_sqrts (sqrts, flv)
```

```
call beam_data%write (u)
```

```
write (u, "(A)")
```

```
call beam_init (beam, beam_data)
```

```

call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized scattering, massless bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([22,22], model)

call beam_data%init_sqrts (sqrts, flv)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized scattering, massive bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([24,-24], model)

call beam_data%init_sqrts (sqrts, flv)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Polarized scattering, massless fermions"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([1,-1], model)

call smatrix(1)%init (2, 1)
call smatrix(1)%set_entry (1, [1,1], (1._default, 0._default))
pol_f(1) = 0.5_default

call smatrix(2)%init (2, 3)
call smatrix(2)%set_entry (1, [1,1], (1._default, 0._default))
call smatrix(2)%set_entry (2, [-1,-1], (1._default, 0._default))
call smatrix(2)%set_entry (3, [-1,1], (1._default, 0._default))
pol_f(2) = 1._default

```

```

call beam_data%init_sqrts (sqrts, flv, smatrix, pol_f)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Semi-polarized scattering, massless bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([22,22], model)

call smatrix(1)%init (2, 0)
pol_f(1) = 0._default

call smatrix(2)%init (2, 1)
call smatrix(2)%set_entry (1, [1,1], (1._default, 0._default))
pol_f(2) = 1._default

call beam_data%init_sqrts (sqrts, flv, smatrix, pol_f)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Semi-polarized scattering, massive bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([24,-24], model)

call smatrix(1)%init (2, 0)
pol_f(1) = 0._default

call smatrix(2)%init (2, 1)
call smatrix(2)%set_entry (1, [0,0], (1._default, 0._default))
pol_f(2) = 1._default

call beam_data%init_sqrts (sqrts, flv, smatrix, pol_f)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Unpolarized decay, massive boson"
write (u, "(A)")

call reset_interaction_counter ()
call flv(1)%init (23, model)

call beam_data%init_decay (flv(1:1))
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Polarized decay, massive boson"
write (u, "(A)")

call reset_interaction_counter ()
call flv(1)%init (23, model)
call smatrix(1)%init (2, 1)
call smatrix(1)%set_entry (1, [0,0], (1._default, 0._default))
pol_f(1) = 0.4_default

call beam_data%init_decay (flv(1:1), smatrix(1:1), pol_f(1:1))
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call beam_final (beam)
call beam_data%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_1"

end subroutine beam_1

```

Test advanced beam setup.

```

<Beams: execute tests>+≡
  call test (beam_2, "beam_2", &
    "beam initialization", &
    u, results)
<Beams: test declarations>+≡
  public :: beam_2
<Beams: tests>+≡
  subroutine beam_2 (u)
    integer, intent(in) :: u
    type(beam_data_t), target :: beam_data

```

```

type(beam_t) :: beam
real(default) :: sqrts
type(flavor_t), dimension(2) :: flv
integer, dimension(0) :: no_records
type(beam_structure_t) :: beam_structure
type(model_data_t), target :: model

write (u, "(A)")  "* Test output: beam_2"
write (u, "(A)")  "* Purpose: transfer beam polarization using &
    &beam structure"
write (u, "(A)")

write (u, "(A)")  "* Reading model file"
write (u, "(A)")

call model%init_sm_test ()

write (u, "(A)")  "* Unpolarized scattering, massless fermions"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([1,-1], model)
call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%final_pol ()

call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized scattering, massless bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([22,22], model)

call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%final_pol ()

call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

```



```

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized scattering, massive bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([24,-24], model)

call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%final_pol ()

call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Polarized scattering, massless fermions"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([1,-1], model)
call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%init_pol (2)

call beam_structure%init_smatrix (1, 1)
call beam_structure%set_sentry (1, 1, [1,1], (1._default, 0._default))

call beam_structure%init_smatrix (2, 3)
call beam_structure%set_sentry (2, 1, [1,1], (1._default, 0._default))
call beam_structure%set_sentry (2, 2, [-1,-1], (1._default, 0._default))
call beam_structure%set_sentry (2, 3, [-1,1], (1._default, 0._default))

call beam_structure%set_pol_f ([0.5_default, 1._default])
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

```

```

write (u, *)

call beam_init (beam, beam_data)
call beam_write (beam, u)

call beam_final (beam)
call beam_data%final ()
call beam_structure%final_pol ()
call beam_structure%final_sf ()

write (u, "(A)")
write (u, "(A)")  "* Semi-polarized scattering, massless bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([22,22], model)

call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%init_pol (2)

call beam_structure%init_smatrix (1, 0)

call beam_structure%init_smatrix (2, 1)
call beam_structure%set_sentry (2, 1, [1,1], (1._default, 0._default))

call beam_structure%set_pol_f ([0._default, 1._default])
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Semi-polarized scattering, massive bosons"
write (u, "(A)")

call reset_interaction_counter ()
sqrts = 500
call flv%init ([24,-24], model)

call beam_structure%init_sf (flv%get_name (), no_records)
call beam_structure%init_pol (2)

call beam_structure%init_smatrix (1, 0)

call beam_structure%init_smatrix (2, 1)
call beam_structure%set_sentry (2, 1, [0,0], (1._default, 0._default))

```

```

call beam_structure%write (u)

write (u, "(A)")
call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)
call beam_final (beam)
call beam_data%final ()

write (u, "(A)")
write (u, "(A)")  "* Unpolarized decay, massive boson"
write (u, "(A)")

call reset_interaction_counter ()
call flv(1)%init (23, model)

call beam_structure%init_sf ([flv(1)%get_name ()], no_records)
call beam_structure%final_pol ()
call beam_structure%write (u)

write (u, "(A)")
call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)

write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Polarized decay, massive boson"
write (u, "(A)")

call reset_interaction_counter ()
call flv(1)%init (23, model)
call beam_structure%init_sf ([flv(1)%get_name ()], no_records)

call beam_structure%init_pol (1)

call beam_structure%init_smatrix (1, 1)
call beam_structure%set_sentry (1, 1, [0,0], (1._default, 0._default))
call beam_structure%set_pol_f ([0.4_default])
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, sqrts, model)
call beam_data%write (u)
write (u, "(A)")
call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")

```

```

write (u, "(A)")  "* Cleanup"

call beam_final (beam)
call beam_data%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_2"

end subroutine beam_2

```

Test advanced beam setup, completely arbitrary momenta.

```

<Beams: execute tests>+≡
  call test (beam_3, "beam_3", &
    "generic beam momenta", &
    u, results)

<Beams: test declarations>+≡
  public :: beam_3

<Beams: tests>+≡
  subroutine beam_3 (u)
    integer, intent(in) :: u
    type(beam_data_t), target :: beam_data
    type(beam_t) :: beam
    type(flavor_t), dimension(2) :: flv
    integer, dimension(0) :: no_records
    type(model_data_t), target :: model
    type(beam_structure_t) :: beam_structure
    type(vector3_t), dimension(2) :: p3
    type(vector4_t), dimension(2) :: p

    write (u, "(A)")  "* Test output: beam_3"
    write (u, "(A)")  "* Purpose: set up beams with generic momenta"
    write (u, "(A)")

    write (u, "(A)")  "* Reading model file"
    write (u, "(A)")

    call reset_interaction_counter ()

    call model%init_sm_test ()

    write (u, "(A)")  "* 1: Scattering process"
    write (u, "(A)")

    call flv%init ([2212,2212], model)

    p3(1) = vector3_moving ([5._default, 0._default, 10._default])
    p3(2) = -vector3_moving ([1._default, 1._default, -10._default])

    call beam_structure%init_sf (flv%get_name (), no_records)
    call beam_structure%set_momentum (p3 ** 1)
    call beam_structure%set_theta (polar_angle (p3))

```

```

call beam_structure%set_phi (azimuthal_angle (p3))
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, 0._default, model)
call pacify (beam_data%l_cm_to_lab, 1e-20_default)
call beam_data%compute_md5sum ()
call beam_data%write (u, verbose = .true.)
write (u, *)

write (u, "(1x,A)") "Beam momenta reconstructed from LT:"
p = beam_data%L_cm_to_lab * beam_data%p_cm
call pacify (p, 1e-12_default)
call vector4_write (p(1), u)
call vector4_write (p(2), u)
write (u, "(A)")

call beam_init (beam, beam_data)
call beam_write (beam, u)

call beam_final (beam)
call beam_data%final ()
call beam_structure%final_sf ()
call beam_structure%final_mom ()

write (u, "(A)")
write (u, "(A)")  "* 2: Decay"
write (u, "(A)")

call flv(1)%init (23, model)
p3(1) = vector3_moving ([10._default, 5._default, 50._default])

call beam_structure%init_sf ([flv(1)%get_name ()], no_records)
call beam_structure%set_momentum ([p3(1) ** 1])
call beam_structure%set_theta ([polar_angle (p3(1))])
call beam_structure%set_phi ([azimuthal_angle (p3(1))])
call beam_structure%write (u)
write (u, *)

call beam_data%init_structure (beam_structure, 0._default, model)
call beam_data%write (u, verbose = .true.)
write (u, "(A)")

write (u, "(1x,A)") "Beam momentum reconstructed from LT:"
p(1) = beam_data%L_cm_to_lab * beam_data%p_cm(1)
call pacify (p(1), 1e-12_default)
call vector4_write (p(1), u)
write (u, "(A)")

call beam_init (beam, beam_data)
call beam_write (beam, u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call beam_final (beam)
call beam_data%final ()
call beam_structure%final_sf ()
call beam_structure%final_mom ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: beam_3"

end subroutine beam_3

```

16.3 Tools

This module contains auxiliary procedures that can be accessed by the structure function code.

```

⟨sf_aux.f90⟩≡
  ⟨File header⟩

module sf_aux

  ⟨Use kinds⟩
  use io_units
  use constants, only: twopi
  use numeric_utils

  use lorentz

  ⟨Standard module head⟩

  ⟨SF aux: public⟩

  ⟨SF aux: parameters⟩

  ⟨SF aux: types⟩

contains

  ⟨SF aux: procedures⟩

end module sf_aux

```

16.3.1 Momentum splitting

Let us consider first an incoming parton with momentum k and invariant mass squared $s = k^2$ that splits into two partons with momenta q, p and invariant masses $t = q^2$ and $u = p^2$. (This is an abuse of the Mandelstam notation. t is actually the momentum transfer, assuming that p is radiated and q initiates

the hard process.) The energy is split among the partons such that if $E = k^0$, we have $q^0 = xE$ and $p^0 = \bar{x}E$, where $\bar{x} \equiv 1 - x$.

We define the angle θ as the polar angle of p w.r.t. the momentum axis of the incoming momentum k . Ignoring azimuthal angle, we can write the four-momenta in the basis (E, p_T, p_L) as

$$k = \begin{pmatrix} E \\ 0 \\ p \end{pmatrix}, \quad p = \begin{pmatrix} \bar{x}E \\ \bar{x}\bar{p} \sin \theta \\ \bar{x}\bar{p} \cos \theta \end{pmatrix}, \quad q = \begin{pmatrix} xE \\ -\bar{x}\bar{p} \sin \theta \\ p - \bar{x}\bar{p} \cos \theta \end{pmatrix}, \quad (16.1)$$

where the first two mass-shell conditions are

$$p^2 = E^2 - s, \quad \bar{p}^2 = E^2 - \frac{u}{\bar{x}^2}. \quad (16.2)$$

The second condition implies that, for positive u , $\bar{x}^2 > u/E^2$, or equivalently

$$x < 1 - \sqrt{u}/E. \quad (16.3)$$

We are interested in the third mass-shell conditions: s and u are fixed, so we need t as a function of $\cos \theta$:

$$t = -2\bar{x} (E^2 - p\bar{p} \cos \theta) + s + u. \quad (16.4)$$

Solving for $\cos \theta$, we get

$$\cos \theta = \frac{2\bar{x}E^2 + t - s - u}{2\bar{x}p\bar{p}}. \quad (16.5)$$

We can compute $\sin \theta$ numerically as $\sin^2 \theta = 1 - \cos^2 \theta$, but it is important to reexpress this in view of numerical stability. To this end, we first determine the bounds for t . The cosine must be between -1 and 1 , so the bounds are

$$t_0 = -2\bar{x} (E^2 + p\bar{p}) + s + u, \quad (16.6)$$

$$t_1 = -2\bar{x} (E^2 - p\bar{p}) + s + u. \quad (16.7)$$

Computing $\sin^2 \theta$ from $\cos \theta$ above, we observe that the numerator is a quadratic polynomial in t which has the zeros t_0 and t_1 , while the common denominator is given by $(2\bar{x}p\bar{p})^2$. Hence, we can write

$$\sin^2 \theta = -\frac{(t - t_0)(t - t_1)}{(2\bar{x}p\bar{p})^2} \quad \text{and} \quad \cos \theta = \frac{(t - t_0) + (t - t_1)}{4\bar{x}p\bar{p}}, \quad (16.8)$$

which is free of large cancellations near $t = t_0$ or $t = t_1$.

If all is massless, i.e., $s = u = 0$, this simplifies to

$$t_0 = -4\bar{x}E^2, \quad t_1 = 0, \quad (16.9)$$

$$\sin^2 \theta = -\frac{t}{\bar{x}E^2} \left(1 + \frac{t}{4\bar{x}E^2} \right), \quad \cos \theta = 1 + \frac{t}{2\bar{x}E^2}. \quad (16.10)$$

Here is the implementation. First, we define a container for the kinematical integration limits and some further data.

Note: contents are public only for easy access in unit test.

```
<SF aux: public>≡
public :: splitting_data_t
```

```

<SF aux: types>≡
  type :: splitting_data_t
  !
    private
      logical :: collinear = .false.
      real(default) :: x0 = 0
      real(default) :: x1
      real(default) :: t0
      real(default) :: t1
      real(default) :: phi0 = 0
      real(default) :: phi1 = twopi
      real(default) :: E, p, s, u, m2
      real(default) :: x, xb, pb
      real(default) :: t = 0
      real(default) :: phi = 0
    contains
      <SF aux: splitting data: TBP>
  end type splitting_data_t

```

I/O for debugging:

```

<SF aux: splitting data: TBP>≡
  procedure :: write => splitting_data_write

<SF aux: procedures>≡
  subroutine splitting_data_write (d, unit)
    class(splitting_data_t), intent(in) :: d
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(A)") "Splitting data:"
    write (u, "(2x,A,L1)") "collinear = ", d%collinear
1   format (2x,A,1x,ES15.8)
    write (u, 1) "x0  =", d%x0
    write (u, 1) "x   =", d%x
    write (u, 1) "xb  =", d%xb
    write (u, 1) "x1  =", d%x1
    write (u, 1) "t0  =", d%t0
    write (u, 1) "t   =", d%t
    write (u, 1) "t1  =", d%t1
    write (u, 1) "phi0 =", d%phi0
    write (u, 1) "phi  =", d%phi
    write (u, 1) "phi1 =", d%phi1
    write (u, 1) "E   =", d%E
    write (u, 1) "p   =", d%p
    write (u, 1) "pb  =", d%pb
    write (u, 1) "s   =", d%s
    write (u, 1) "u   =", d%u
    write (u, 1) "m2  =", d%m2
  end subroutine splitting_data_write

```

16.3.2 Constant data

This is the initializer for the data. The input consists of the incoming momentum, its invariant mass squared, and the invariant mass squared of the radiated

particle. m_2 is the *physical* mass squared of the outgoing particle. The t bounds depend on the chosen x value and cannot be determined yet.

```

<SF aux: splitting data: TBP>+≡
  procedure :: init => splitting_data_init

<SF aux: procedures>+≡
  subroutine splitting_data_init (d, k, mk2, mr2, mo2, collinear)
    class(splitting_data_t), intent(out) :: d
    type(vector4_t), intent(in) :: k
    real(default), intent(in) :: mk2, mr2, mo2
    logical, intent(in), optional :: collinear
    if (present (collinear)) d%collinear = collinear
    d%E = energy (k)
    d%x1 = 1 - sqrt (max (mr2, 0._default)) / d%E
    d%p = sqrt (d%E**2 - mk2)
    d%s = mk2
    d%u = mr2
    d%m2 = mo2
  end subroutine splitting_data_init

```

Retrieve the x bounds, if needed for x sampling. Generating an x value is done by the caller, since this is the part that depends on the nature of the structure function.

```

<SF aux: splitting data: TBP>+≡
  procedure :: get_x_bounds => splitting_get_x_bounds

<SF aux: procedures>+≡
  function splitting_get_x_bounds (d) result (x)
    class(splitting_data_t), intent(in) :: d
    real(default), dimension(2) :: x
    x = [ d%x0, d%x1 ]
  end function splitting_get_x_bounds

```

Now set the momentum fraction and compute t_0 and t_1 .

[The calculation of t_1 is subject to numerical problems. The exact formula is ($s = m_i^2$, $u = m_r^2$)

$$t_1 = -2\bar{x}E^2 + m_i^2 + m_r^2 + 2\bar{x}\sqrt{E^2 - m_i^2}\sqrt{E^2 - m_r^2/\bar{x}^2}. \quad (16.11)$$

The structure-function paradigm is useful only if $E \gg m_i, m_r$. In a Taylor expansion for large E , the leading term cancels. The expansion of the square roots (to subleading order) yields

$$t_1 = xm_i^2 - \frac{x}{\bar{x}}m_r^2. \quad (16.12)$$

There are two cases of interest: $m_i = m_o$ and $m_r = 0$,

$$t_1 = xm_o^2 \quad (16.13)$$

and $m_i = m_r$ and $m_o = 0$,

$$t_1 = -\frac{x^2}{\bar{x}}m_i^2. \quad (16.14)$$

In both cases, $t_1 \leq m_o^2$]

That said, it turns out that taking the t_1 evaluation at face value leads to less problems than the approximation. We express the angles in terms of $t - t_0$ and $t - t_1$. Numerical noise in t_1 can then be tolerated.

```

<SF aux: splitting data: TBP>+≡
  procedure :: set_t_bounds => splitting_set_t_bounds

<SF aux: procedures>+≡
  elemental subroutine splitting_set_t_bounds (d, x, xb)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in), optional :: x, xb
    real(default) :: tp, tm
    if (present (x)) d%x = x
    if (present (xb)) d%xb = xb
    if (vanishes (d%u)) then
      d%pb = d%E
    else
      if (.not. vanishes (d%xb)) then
        d%pb = sqrt (max (d%E**2 - d%u / d%xb**2, 0._default))
      else
        d%pb = 0
      end if
    end if
    tp = -2 * d%xb * d%E**2 + d%s + d%u
    tm = -2 * d%xb * d%p * d%pb
    d%t0 = tp + tm
    d%t1 = tp - tm
    d%t = d%t1
  end subroutine splitting_set_t_bounds

```

16.3.3 Sampling recoil

Compute a value for the momentum transfer t , using a random number r . We assume a logarithmic distribution for $t - m^2$, corresponding to the propagator $1/(t - m^2)$ with the physical mass m for the outgoing particle. Optionally, we can narrow the kinematical bounds.

If all three masses in the splitting vanish, the upper limit for t is zero. In that case, the t value is set to zero and the splitting will be collinear.

```

<SF aux: splitting data: TBP>+≡
  procedure :: sample_t => splitting_sample_t

<SF aux: procedures>+≡
  subroutine splitting_sample_t (d, r, t0, t1)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in) :: r
    real(default), intent(in), optional :: t0, t1
    real(default) :: tt0, tt1, tt0m, tt1m
    if (d%collinear) then
      d%t = d%t1
    else
      tt0 = d%t0; if (present (t0)) tt0 = max (t0, tt0)
      tt1 = d%t1; if (present (t1)) tt1 = min (t1, tt1)
    end if
  end subroutine splitting_sample_t

```

```

tt0m = tt0 - d%m2
tt1m = tt1 - d%m2
if (tt0m < 0 .and. tt1m < 0 .and. abs(tt0m) > &
    epsilon(tt0m) .and. abs(tt1m) > epsilon(tt0m)) then
    d%t = d%m2 + tt0m * exp (r * log (tt1m / tt0m))
else
    d%t = tt1
end if
end if
end subroutine splitting_sample_t

```

The inverse operation: Given t , we recover the value of r that would have produced this value.

```

<SF aux: splitting data: TBP>+≡
  procedure :: inverse_t => splitting_inverse_t

<SF aux: procedures>+≡
  subroutine splitting_inverse_t (d, r, t0, t1)
    class(splitting_data_t), intent(in) :: d
    real(default), intent(out) :: r
    real(default), intent(in), optional :: t0, t1
    real(default) :: tt0, tt1, tt0m, tt1m
    if (d%collinear) then
        r = 0
    else
        tt0 = d%t0; if (present (t0)) tt0 = max (t0, tt0)
        tt1 = d%t1; if (present (t1)) tt1 = min (t1, tt1)
        tt0m = tt0 - d%m2
        tt1m = tt1 - d%m2
        if (tt0m < 0 .and. tt1m < 0) then
            r = log ((d%t - d%m2) / tt0m) / log (tt1m / tt0m)
        else
            r = 0
        end if
    end if
  end subroutine splitting_inverse_t

```

This is trivial, but provided for convenience:

```

<SF aux: splitting data: TBP>+≡
  procedure :: sample_phi => splitting_sample_phi

<SF aux: procedures>+≡
  subroutine splitting_sample_phi (d, r)
    class(splitting_data_t), intent(inout) :: d
    real(default), intent(in) :: r
    if (d%collinear) then
        d%phi = 0
    else
        d%phi = (1-r) * d%phi0 + r * d%phi1
    end if
  end subroutine splitting_sample_phi

```

Inverse:

```

<SF aux: splitting data: TBP>+≡
  procedure :: inverse_phi => splitting_inverse_phi

<SF aux: procedures>+≡
  subroutine splitting_inverse_phi (d, r)
    class(splitting_data_t), intent(in) :: d
    real(default), intent(out) :: r
    if (d%collinear) then
      r = 0
    else
      r = (d%phi - d%phi0) / (d%phi1 - d%phi0)
    end if
  end subroutine splitting_inverse_phi

```

16.3.4 Splitting

In this function, we actually perform the splitting. The incoming momentum k is split into (if no recoil) $q_1 = (1 - x)k$ and $q_2 = xk$.

Apart from the splitting data, we need the incoming momentum k , the momentum transfer t , and the azimuthal angle ϕ . The momentum fraction x is already known here.

Alternatively, we can split without recoil. The azimuthal angle is irrelevant, and the momentum transfer is always equal to the upper limit t_1 , so the polar angle is zero. Obviously, if there are nonzero masses it is not possible to keep both energy-momentum conservation and at the same time all particles on shell. We choose for dropping the on-shell condition here.

```

<SF aux: splitting data: TBP>+≡
  procedure :: split_momentum => splitting_split_momentum

<SF aux: procedures>+≡
  function splitting_split_momentum (d, k) result (q)
    class(splitting_data_t), intent(in) :: d
    type(vector4_t), dimension(2) :: q
    type(vector4_t), intent(in) :: k
    real(default) :: st2, ct2, st, ct, cp, sp
    type(lorentz_transformation_t) :: rot
    real(default) :: tt0, tt1, den
    type(vector3_t) :: kk, q1, q2
    if (d%collinear) then
      if (vanishes(d%s) .and. vanishes(d%u)) then
        q(1) = d%xb * k
        q(2) = d%x * k
      else
        kk = space_part (k)
        q1 = d%xb * (d%pb / d%p) * kk
        q2 = kk - q1
        q(1) = vector4_moving (d%xb * d%E, q1)
        q(2) = vector4_moving (d%x * d%E, q2)
      end if
    else
      den = 2 * d%xb * d%p * d%pb
    end if
  end function splitting_split_momentum

```

```

tt0 = max (d%t - d%t0, 0._default)
tt1 = min (d%t - d%t1, 0._default)
if (den**2 <= epsilon(den)) then
  st2 = 0
else
  st2 = - (tt0 * tt1) / den ** 2
end if
if (st2 > 1) then
  st2 = 1
end if
ct2 = 1 - st2
st = sqrt (max (st2, 0._default))
ct = sqrt (max (ct2, 0._default))
if ((d%t - d%t0 + d%t - d%t1) < 0) then
  ct = - ct
end if
sp = sin (d%phi)
cp = cos (d%phi)
rot = rotation_to_2nd (3, space_part (k))
q1 = vector3_moving (d%xb * d%pb * [st * cp, st * sp, ct])
q2 = vector3_moving (d%p, 3) - q1
q(1) = rot * vector4_moving (d%xb * d%E, q1)
q(2) = rot * vector4_moving (d%x * d%E, q2)
end if
end function splitting_split_momentum

```

Momenta generated by splitting will in general be off-shell. They are on-shell only if they are collinear and massless. This subroutine puts them on shell by brute force, violating either momentum or energy conservation. The direction of three-momentum is always retained.

If the energy is below mass shell, we return a zero momentum.

```

<SF aux: parameters>≡
  integer, parameter, public :: KEEP_ENERGY = 0, KEEP_MOMENTUM = 1

<SF aux: public>+≡
  public :: on_shell

<SF aux: procedures>+≡
  elemental subroutine on_shell (p, m2, keep)
    type(vector4_t), intent(inout) :: p
    real(default), intent(in) :: m2
    integer, intent(in) :: keep
    real(default) :: E, E2, pn
    select case (keep)
    case (KEEP_ENERGY)
      E = energy (p)
      E2 = E ** 2
      if (E2 >= m2) then
        pn = sqrt (E2 - m2)
        p = vector4_moving (E, pn * direction (space_part (p)))
      else
        p = vector4_null
      end if
    case (KEEP_MOMENTUM)

```

```

      E = sqrt (space_part (p) ** 2 + m2)
      p = vector4_moving (E, space_part (p))
    end select
  end subroutine on_shell

```

16.3.5 Recovering the splitting

This is the inverse problem. We have on-shell momenta and want to deduce the splitting parameters x , t , and ϕ .

Update 2018-08-22: As a true inverse to `splitting_split_momentum`, we now use not just a single momentum `q2` as before, but the momentum pair `q1`, `q2` for recovering x and \bar{x} separately. If x happens to be close to 1, we would completely lose the tiny \bar{x} value, otherwise, and thus get a meaningless result.

```

<SF aux: splitting data: TBP>+≡
  procedure :: recover => splitting_recover

<SF aux: procedures>+≡
  subroutine splitting_recover (d, k, q, keep)
    class(splitting_data_t), intent(inout) :: d
    type(vector4_t), intent(in) :: k
    type(vector4_t), dimension(2), intent(in) :: q
    integer, intent(in) :: keep
    type(lorentz_transformation_t) :: rot
    type(vector4_t) :: k0
    type(vector4_t), dimension(2) :: q0
    real(default) :: p1, p2, p3, pt2, pp2, pl
    real(default) :: aux, den, norm
    real(default) :: st2, ct2, ct
    rot = inverse (rotation_to_2nd (3, space_part (k)))
    q0 = rot * q
    p1 = vector4_get_component (q0(2), 1)
    p2 = vector4_get_component (q0(2), 2)
    p3 = vector4_get_component (q0(2), 3)
    pt2 = p1 ** 2 + p2 ** 2
    pp2 = p1 ** 2 + p2 ** 2 + p3 ** 2
    pl = abs (p3)
    k0 = vector4_moving (d%E, d%p, 3)
    select case (keep)
    case (KEEP_ENERGY)
      d%x = energy (q0(2)) / d%E
      d%xb = energy (q0(1)) / d%E
      call d%set_t_bounds ()
      if (.not. d%collinear) then
        aux = (d%xb * d%pb) ** 2 * pp2 - d%p ** 2 * pt2
        den = d%p ** 2 - (d%xb * d%pb) ** 2
        if (aux >= 0 .and. den > 0) then
          norm = (d%p * pl + sqrt (aux)) / den
        else
          norm = 1
        end if
      end if
    case (KEEP_MOMENTUM)

```

```

    d%xb = sqrt (space_part (q0(1)) ** 2 + d%u) / d%E
    d%x = 1 - d%xb
    call d%set_t_bounds ()
    norm = 1
end select
if (d%collinear) then
    d%t = d%t1
    d%phi = 0
else
    if ((d%xb * d%pb * norm)**2 < epsilon(d%xb)) then
        st2 = 1
    else
        st2 = pt2 / (d%xb * d%pb * norm) ** 2
    end if
    if (st2 > 1) then
        st2 = 1
    end if
    ct2 = 1 - st2
    ct = sqrt (max (ct2, 0._default))
    if (.not. vanishes (1 + ct)) then
        d%t = d%t1 - 2 * d%xb * d%p * d%pb * st2 / (1 + ct)
    else
        d%t = d%t0
    end if
    if (.not. vanishes (p1) .or. .not. vanishes (p2)) then
        d%phi = atan2 (-p2, -p1)
    else
        d%phi = 0
    end if
end if
end subroutine splitting_recover

```

16.3.6 Extract data

```

<SF aux: splitting data: TBP>+≡
  procedure :: get_x => splitting_get_x
  procedure :: get_xb => splitting_get_xb

<SF aux: procedures>+≡
  function splitting_get_x (sd) result (x)
    class(splitting_data_t), intent(in) :: sd
    real(default) :: x
    x = sd%x
  end function splitting_get_x

  function splitting_get_xb (sd) result (xb)
    class(splitting_data_t), intent(in) :: sd
    real(default) :: xb
    xb = sd%xb
  end function splitting_get_xb

```

16.3.7 Unit tests

Test module, followed by the corresponding implementation module.

```
<sf_aux_ut.f90>≡  
  <File header>  
  
  module sf_aux_ut  
    use unit_tests  
    use sf_aux_uti  
  
    <Standard module head>  
  
    <SF aux: public test>  
  
    contains  
  
    <SF aux: test driver>  
  
  end module sf_aux_ut  
<sf_aux_uti.f90>≡  
  <File header>  
  
  module sf_aux_uti  
  
    <Use kinds>  
    use lorentz  
  
    use sf_aux  
  
    <Standard module head>  
  
    <SF aux: test declarations>  
  
    contains  
  
    <SF aux: tests>  
  
  end module sf_aux_uti
```

API: driver for the unit tests below.

```
<SF aux: public test>≡  
  public :: sf_aux_test  
<SF aux: test driver>≡  
  subroutine sf_aux_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <SF aux: execute tests>  
  end subroutine sf_aux_test
```

Momentum splitting: massless radiation

Compute momentum splitting for generic kinematics. It turns out that for $x = 0.5$, where $t - m^2$ is the geometric mean between its upper and lower bounds (this

can be directly seen from the logarithmic distribution in the function `sample_t` for $r \equiv x = 1 - x = 0.5$), we arrive at an exact number $t = -0.15$ for the given input values.

```

<SF aux: execute tests>≡
  call test (sf_aux_1, "sf_aux_1", &
    "massless radiation", &
    u, results)

<SF aux: test declarations>≡
  public :: sf_aux_1

<SF aux: tests>≡
  subroutine sf_aux_1 (u)
    integer, intent(in) :: u
    type(splitting_data_t) :: sd
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q, q0
    real(default) :: E, mk, mp, mq
    real(default) :: x, r1, r2, r1o, r2o
    real(default) :: k2, q0_2, q1_2, q2_2

    write (u, "(A)")  "* Test output: sf_aux_1"
    write (u, "(A)")  "* Purpose: compute momentum splitting"
    write (u, "(A)")  "          (massless radiated particle)"
    write (u, "(A)")

    E = 1
    mk = 0.3_default
    mp = 0
    mq = mk

    k = vector4_moving (E, sqrt (E**2 - mk**2), 3)
    k2 = k ** 2; call pacify (k2, 1e-10_default)

    x = 0.6_default
    r1 = 0.5_default
    r2 = 0.125_default

    write (u, "(A)")  "* (1) Non-collinear setup"
    write (u, "(A)")

    call sd%init (k, mk**2, mp**2, mq**2)
    call sd%set_t_bounds (x, 1 - x)
    call sd%sample_t (r1)
    call sd%sample_phi (r2)

    call sd%write (u)

    q = sd%split_momentum (k)
    q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
    q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

    write (u, "(A)")
    write (u, "(A)")  "Incoming momentum k ="
    call vector4_write (k, u)

```

```

write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "Extract: x, 1-x"
write (u, "(2(1x,F11.8))") sd%get_x (), sd%get_xb ()

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q0_2 = q0(2) ** 2; call pacify (q0_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q0_2
write (u, "(A)")

```

```

write (u, "(A)")  "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))")  x, sd%x
write (u, "(A)")  "Compare: t"
write (u, "(2(1x,F11.8))")  q2_2, sd%t

call sd%inverse_t (r1o)

write (u, "(A)")  "Compare: r1"
write (u, "(2(1x,F11.8))")  r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)")  "Compare: r2"
write (u, "(2(1x,F11.8))")  r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)")  "Compare: mo^2"
q0_2 = q0(2) ** 2; call pacify (q0_2, 1e-10_default)
write (u, "(2(1x,F11.8))")  sd%m2, q0_2
write (u, "(A)")

write (u, "(A)")  "* Recover parameters from outgoing momentum"
write (u, "(A)")

```

```

call sd%init (k, mk**2, mp**2, mq**2)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o)

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* (2) Collinear setup"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, 1 - x)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

```

```

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q0_2 = q0(2) ** 2; call pacify (q0_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q0_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

```

```

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q0_2 = q0(2) ** 2; call pacify (q0_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q0_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_aux_1"

end subroutine sf_aux_1

```

Momentum splitting: massless parton

Compute momentum splitting for generic kinematics. It turns out that for $x = 0.5$, where $t - m^2$ is the geometric mean between its upper and lower bounds, we arrive at an exact number $t = -0.36$ for the given input values.

```

<SF aux: execute tests>+≡
  call test (sf_aux_2, "sf_aux_2", &
    "massless parton", &
    u, results)

<SF aux: test declarations>+≡
  public :: sf_aux_2

<SF aux: tests>+≡
  subroutine sf_aux_2 (u)

```

```

integer, intent(in) :: u
type(splitting_data_t) :: sd
type(vector4_t) :: k
type(vector4_t), dimension(2) :: q, q0
real(default) :: E, mk, mp, mq
real(default) :: x, r1, r2, r1o, r2o
real(default) :: k2, q02_2, q1_2, q2_2

write (u, "(A)")  "* Test output: sf_aux_2"
write (u, "(A)")  "*   Purpose: compute momentum splitting"
write (u, "(A)")  "               (massless outgoing particle)"
write (u, "(A)")

E = 1
mk = 0.3_default
mp = mk
mq = 0

k = vector4_moving (E, sqrt (E**2 - mk**2), 3)
k2 = k ** 2;  call pacify (k2, 1e-10_default)

x = 0.6_default
r1 = 0.5_default
r2 = 0.125_default

write (u, "(A)")  "* (1) Non-collinear setup"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%sample_t (r1)
call sd%sample_phi (r2)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2;  call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2;  call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)")  "Compare: s"

```

```

write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o)

```



```

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o)

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

```

```

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* (2) Collinear setup"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, 1 - x)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

```

```

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

```

```

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_aux_2"

end subroutine sf_aux_2

```

Momentum splitting: all massless

Compute momentum splitting for massless kinematics. In the non-collinear case, we need a lower cutoff for $|t|$, otherwise a logarithmic distribution is not possible.

```

<SF aux: execute tests>+≡
  call test (sf_aux_3, "sf_aux_3", &
    "massless parton", &
    u, results)

<SF aux: test declarations>+≡
  public :: sf_aux_3

<SF aux: tests>+≡
  subroutine sf_aux_3 (u)
    integer, intent(in) :: u
    type(splitting_data_t) :: sd
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q, q0
    real(default) :: E, mk, mp, mq, qmin, qmax
    real(default) :: x, r1, r2, rio, r2o
    real(default) :: k2, q02_2, q1_2, q2_2

    write (u, "(A)") "* Test output: sf_aux_3"
    write (u, "(A)") "* Purpose: compute momentum splitting"
    write (u, "(A)") " (all massless, q cuts)"
    write (u, "(A)")

```

```

E = 1
mk = 0
mp = 0
mq = 0
qmin = 1e-2_default
qmax = 1e0_default

k = vector4_moving (E, sqrt (E**2 - mk**2), 3)
k2 = k ** 2; call pacify (k2, 1e-10_default)

x = 0.6_default
r1 = 0.5_default
r2 = 0.125_default

write (u, "(A)")  "* (1) Non-collinear setup"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%sample_t (r1, t1 = - qmin ** 2, t0 = - qmax **2)
call sd%sample_phi (r2)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)")  "Compare: s"
write (u, "(2(1x,F11.8))")  sd%s, k2

write (u, "(A)")  "Compare: t"
write (u, "(2(1x,F11.8))")  sd%t, q2_2

write (u, "(A)")  "Compare: u"
write (u, "(2(1x,F11.8))")  sd%u, q1_2

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))")  sd%x, energy (q(2)) / energy (k)

```

```

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

call sd%inverse_t (r1o, t1 = - qmin ** 2, t0 = - qmax ** 2)

write (u, "(A)") "Compare: r1"
write (u, "(2(1x,F11.8))") r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)") "Compare: r2"
write (u, "(2(1x,F11.8))") r2, r2o

write (u, "(A)")
call sd%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "** Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)")  "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))")  sd%m2, q02_2
write (u, "(A)")

write (u, "(A)")  "** Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))")  x, sd%x
write (u, "(A)")  "Compare: t"
write (u, "(2(1x,F11.8))")  q2_2, sd%t

call sd%inverse_t (r1o, t1 = - qmin ** 2, t0 = - qmax **2)

write (u, "(A)")  "Compare: r1"
write (u, "(2(1x,F11.8))")  r1, r1o

call sd%inverse_phi (r2o)

write (u, "(A)")  "Compare: r2"
write (u, "(2(1x,F11.8))")  r2, r2o

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)")  "** (2) Collinear setup"
write (u, "(A)")

```

```

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, 1 - x)

call sd%write (u)

q = sd%split_momentum (k)
q1_2 = q(1) ** 2; call pacify (q1_2, 1e-10_default)
q2_2 = q(2) ** 2; call pacify (q2_2, 1e-10_default)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: s"
write (u, "(2(1x,F11.8))") sd%s, k2

write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") sd%t, q2_2

write (u, "(A)") "Compare: u"
write (u, "(2(1x,F11.8))") sd%u, q1_2

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") sd%x, energy (q(2)) / energy (k)

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") sd%xb, energy (q(1)) / energy (k)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep energy)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_ENERGY)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)

```



```

write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)
call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Project on-shell (keep momentum)"

q0 = q
call on_shell (q0, [mp**2, mq**2], KEEP_MOMENTUM)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q0), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q0(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q0(2), u)
write (u, "(A)")

write (u, "(A)") "Compare: mo^2"
q02_2 = q0(2) ** 2; call pacify (q02_2, 1e-10_default)
write (u, "(2(1x,F11.8))") sd%m2, q02_2
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momentum"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2)

```

```

call sd%set_t_bounds (x, 1 - x)
call sd%recover (k, q0, KEEP_MOMENTUM)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x
write (u, "(A)") "Compare: t"
write (u, "(2(1x,F11.8))") q2_2, sd%t

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_aux_3"

end subroutine sf_aux_3

```

Endpoint stability

Compute momentum splitting for collinear kinematics close to both endpoints. In particular, check both directions $x \rightarrow$ momenta and momenta $\rightarrow x$.

For purely massless collinear splitting, the KEEP_XXX flag is irrelevant. We choose KEEP_ENERGY here.

```

<SF aux: execute tests>+≡
  call test (sf_aux_4, "sf_aux_4", &
    "endpoint numerics", &
    u, results)

<SF aux: test declarations>+≡
  public :: sf_aux_4

<SF aux: tests>+≡
  subroutine sf_aux_4 (u)
    integer, intent(in) :: u
    type(splitting_data_t) :: sd
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E, mk, mp, mq, qmin, qmax
    real(default) :: x, xb

    write (u, "(A)") "* Test output: sf_aux_4"
    write (u, "(A)") "* Purpose: compute massless collinear splitting near endpoint"

    E = 1
    mk = 0
    mp = 0
    mq = 0
    qmin = 1e-2_default
    qmax = 1e0_default

    k = vector4_moving (E, sqrt (E**2 - mk**2), 3)

    x = 0.1_default
    xb = 1 - x

```

```

write (u, "(A)")
write (u, "(A)")  "* (1) Collinear setup, moderate kinematics"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)

call sd%write (u)

q = sd%split_momentum (k)

write (u, "(A)")
write (u, "(A)")  "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)")  "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)")  "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)")  "* Recover parameters from outgoing momenta"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)
call sd%recover (k, q, KEEP_ENERGY)

write (u, "(A)")  "Compare: x"
write (u, "(2(1x,F11.8))")  x, sd%x

write (u, "(A)")  "Compare: 1-x"
write (u, "(2(1x,F11.8))")  xb, sd%xb

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)")  "* (2) Close to x=0"
write (u, "(A)")

x = 1e-9_default
xb = 1 - x

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)

call sd%write (u)

```

```

q = sd%split_momentum (k)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="
call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momenta"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)
call sd%recover (k, q, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") xb, sd%xb

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* (3) Close to x=1"
write (u, "(A)")

xb = 1e-9_default
x = 1 - xb

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)

call sd%write (u)

q = sd%split_momentum (k)

write (u, "(A)")
write (u, "(A)") "Incoming momentum k ="
call vector4_write (k, u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum sum p + q ="
call vector4_write (sum (q), u)
write (u, "(A)")
write (u, "(A)") "Radiated momentum p ="

```

```

call vector4_write (q(1), u)
write (u, "(A)")
write (u, "(A)") "Outgoing momentum q ="
call vector4_write (q(2), u)
write (u, "(A)")

write (u, "(A)") "* Recover parameters from outgoing momenta"
write (u, "(A)")

call sd%init (k, mk**2, mp**2, mq**2, collinear = .true.)
call sd%set_t_bounds (x, xb)
call sd%recover (k, q, KEEP_ENERGY)

write (u, "(A)") "Compare: x"
write (u, "(2(1x,F11.8))") x, sd%x

write (u, "(A)") "Compare: 1-x"
write (u, "(2(1x,F11.8))") xb, sd%xb

write (u, "(A)")
call sd%write (u)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_aux_4"

end subroutine sf_aux_4

```

16.4 Mappings for structure functions

In this module, we provide a wrapper for useful mappings of the unit (hyper-)square that we can apply to a set of structure functions.

In some cases it is useful, or even mandatory, to map the MC input parameters nontrivially onto a set of structure functions for the two beams. In all cases considered here, instead of x_1, x_2, \dots as parameters for the beams, we generate one parameter that is equal, or related to, the product $x_1 x_2 \dots$ (so it directly corresponds to \sqrt{s}). The other parameters describe the distribution of energy (loss) between beams and radiations.

`<sf_mappings.f90>`≡

<File header>

```
module sf_mappings
```

<Use kinds>

```

use kinds, only: double
use io_units
use constants, only: pi, zero, one
use numeric_utils
use diagnostics

```

<Standard module head>

```

    <SF mappings: public>

    <SF mappings: parameters>

    <SF mappings: types>

    <SF mappings: interfaces>

contains

    <SF mappings: procedures>

end module sf_mappings

```

16.4.1 Base type

First, we define an abstract base type for the mapping. In all cases we need to store the indices of the parameters on which the mapping applies. Additional parameters can be stored in the extensions of this type.

```

<SF mappings: public>≡
    public :: sf_mapping_t

<SF mappings: types>≡
    type, abstract :: sf_mapping_t
        integer, dimension(:), allocatable :: i
    contains
        <SF mappings: sf mapping: TBP>
    end type sf_mapping_t

```

The output routine is deferred:

```

<SF mappings: sf mapping: TBP>≡
    procedure (sf_mapping_write), deferred :: write

<SF mappings: interfaces>≡
    abstract interface
        subroutine sf_mapping_write (object, unit)
            import
            class(sf_mapping_t), intent(in) :: object
            integer, intent(in), optional :: unit
        end subroutine sf_mapping_write
    end interface

```

Initializer for the base type. The array of parameter indices is allocated but initialized to zero.

```

<SF mappings: sf mapping: TBP>+≡
    procedure :: base_init => sf_mapping_base_init

<SF mappings: procedures>≡
    subroutine sf_mapping_base_init (mapping, n_par)
        class(sf_mapping_t), intent(out) :: mapping
        integer, intent(in) :: n_par
        allocate (mapping%i (n_par))
        mapping%i = 0
    end subroutine

```

```
end subroutine sf_mapping_base_init
```

Set an index value.

```
<SF mappings: sf mapping: TBP>+≡
  procedure :: set_index => sf_mapping_set_index

<SF mappings: procedures>+≡
  subroutine sf_mapping_set_index (mapping, j, i)
    class(sf_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
    mapping%i(j) = i
  end subroutine sf_mapping_set_index
```

Retrieve an index value.

```
<SF mappings: sf mapping: TBP>+≡
  procedure :: get_index => sf_mapping_get_index

<SF mappings: procedures>+≡
  function sf_mapping_get_index (mapping, j) result (i)
    class(sf_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j
    integer :: i
    i = mapping%i(j)
  end function sf_mapping_get_index
```

Return the dimensionality, i.e., the number of parameters.

```
<SF mappings: sf mapping: TBP>+≡
  procedure :: get_n_dim => sf_mapping_get_n_dim

<SF mappings: procedures>+≡
  function sf_mapping_get_n_dim (mapping) result (n)
    class(sf_mapping_t), intent(in) :: mapping
    integer :: n
    n = size (mapping%i)
  end function sf_mapping_get_n_dim
```

Computation: the values **p** are the input parameters, the values **r** are the output parameters. The values **rb** are defined as $\bar{r} = 1 - r$, but provided explicitly. They allow us to avoid numerical problems near $r = 1$.

The extra parameter **x_free** indicates that the total energy has already been renormalized by this factor. We have to take such a factor into account in a resonance or on-shell mapping.

The Jacobian is **f**. We modify only the two parameters indicated by the indices **i**.

```
<SF mappings: sf mapping: TBP>+≡
  procedure (sf_mapping_compute), deferred :: compute

<SF mappings: interfaces>+≡
  abstract interface
    subroutine sf_mapping_compute (mapping, r, rb, f, p, pb, x_free)
      import
      class(sf_mapping_t), intent(inout) :: mapping
      real(default), dimension(:), intent(out) :: r, rb
```

```

        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
    end subroutine sf_mapping_compute
end interface

```

The inverse mapping. Use *r* and/or *rb* to reconstruct *p* and also compute *f*.

```

<SF mappings: sf mapping: TBP>+≡
    procedure (sf_mapping_inverse), deferred :: inverse

<SF mappings: interfaces>+≡
    abstract interface
        subroutine sf_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
            import
            class(sf_mapping_t), intent(inout) :: mapping
            real(default), dimension(:), intent(in) :: r, rb
            real(default), intent(out) :: f
            real(default), dimension(:), intent(out) :: p, pb
            real(default), intent(inout), optional :: x_free
        end subroutine sf_mapping_inverse
    end interface

```

16.4.2 Methods for self-tests

This is a shorthand for: inject parameters, compute the mapping, display results, compute the inverse, display again. We provide an output format for the parameters and, optionally, a different output format for the Jacobians.

```

<SF mappings: sf mapping: TBP>+≡
    procedure :: check => sf_mapping_check

<SF mappings: procedures>+≡
    subroutine sf_mapping_check (mapping, u, p_in, pb_in, fmt_p, fmt_f)
        class(sf_mapping_t), intent(inout) :: mapping
        integer, intent(in) :: u
        real(default), dimension(:), intent(in) :: p_in, pb_in
        character(*), intent(in) :: fmt_p
        character(*), intent(in), optional :: fmt_f
        real(default), dimension(size(p_in)) :: p, pb, r, rb
        real(default) :: f, tolerance
        tolerance = 1.5E-17
        p = p_in
        pb = pb_in
        call mapping%compute (r, rb, f, p, pb)
        call pacify (p, tolerance)
        call pacify (pb, tolerance)
        call pacify (r, tolerance)
        call pacify (rb, tolerance)
        write (u, "(3x,A,9(1x," // fmt_p // "))" ) "p =", p
        write (u, "(3x,A,9(1x," // fmt_p // "))" ) "pb=", pb
        write (u, "(3x,A,9(1x," // fmt_p // "))" ) "r =", r
        write (u, "(3x,A,9(1x," // fmt_p // "))" ) "rb=", rb
        if (present (fmt_f)) then

```



```

        write (u, "(3x,A,9(1x," // fmt_f // "))") "f =", f
    else
        write (u, "(3x,A,9(1x," // fmt_p // "))") "f =", f
    end if
    write (u, *)
    call mapping%inverse (r, rb, f, p, pb)
    call pacify (p, tolerance)
    call pacify (pb, tolerance)
    call pacify (r, tolerance)
    call pacify (rb, tolerance)
    write (u, "(3x,A,9(1x," // fmt_p // "))") "p =", p
    write (u, "(3x,A,9(1x," // fmt_p // "))") "pb=", pb
    write (u, "(3x,A,9(1x," // fmt_p // "))") "r =", r
    write (u, "(3x,A,9(1x," // fmt_p // "))") "rb=", rb
    if (present (fmt_f)) then
        write (u, "(3x,A,9(1x," // fmt_f // "))") "f =", f
    else
        write (u, "(3x,A,9(1x," // fmt_p // "))") "f =", f
    end if
    write (u, *)
    write (u, "(3x,A,9(1x," // fmt_p // "))") "*r=", product (r)
end subroutine sf_mapping_check

```

This is a consistency check for the self-tests: the integral over the unit square should be unity. We estimate this by a simple binning and adding up the values; this should be sufficient for a self-test.

The argument is the requested number of sampling points. We take the square root for binning in both dimensions, so the precise number might be different.

```

<SF mappings: sf mapping: TBP>+≡
    procedure :: integral => sf_mapping_integral

<SF mappings: procedures>+≡
    function sf_mapping_integral (mapping, n_calls) result (integral)
        class(sf_mapping_t), intent(inout) :: mapping
        integer, intent(in) :: n_calls
        real(default) :: integral
        integer :: n_dim, n_bin, k
        real(default), dimension(:), allocatable :: p, pb, r, rb
        integer, dimension(:), allocatable :: ii
        real(default) :: dx, f, s

        n_dim = mapping%get_n_dim ()
        allocate (p (n_dim))
        allocate (pb(n_dim))
        allocate (r (n_dim))
        allocate (rb(n_dim))
        allocate (ii(n_dim))
        n_bin = nint (real (n_calls, default) ** (1._default / n_dim))
        dx = 1._default / n_bin
        s = 0
        ii = 1

    SAMPLE: do

```

```

do k = 1, n_dim
  p(k) = ii(k) * dx - dx/2
  pb(k) = (n_bin - ii(k)) * dx + dx/2
end do
call mapping%compute (r, rb, f, p, pb)
s = s + f
INCR: do k = 1, n_dim
  ii(k) = ii(k) + 1
  if (ii(k) <= n_bin) then
    exit INCR
  else if (k < n_dim) then
    ii(k) = 1
  else
    exit SAMPLE
  end if
end do INCR
end do SAMPLE

integral = s / real (n_bin, default) ** n_dim

end function sf_mapping_integral

```

16.4.3 Implementation: standard mapping

This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio.

```

<SF mappings: public>+≡
  public :: sf_s_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_s_mapping_t
    logical :: power_set = .false.
    real(default) :: power = 1
  contains
    <SF mappings: sf standard mapping: TBP>
  end type sf_s_mapping_t

```

Output.

```

<SF mappings: sf standard mapping: TBP>≡
  procedure :: write => sf_s_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_s_mapping_write (object, unit)
    class(sf_s_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,',',',',I0,')')'", advance="no") object%i
    end if
    write (u, "(A,F7.5,A)" ": standard (", object%power, ")")
  end subroutine sf_s_mapping_write

```

Initialize: index pair and power parameter.

```

<SF mappings: sf standard mapping: TBP>+≡
  procedure :: init => sf_s_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_s_mapping_init (mapping, power)
    class(sf_s_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: power
    call mapping%base_init (2)
    if (present (power)) then
      mapping%power_set = .true.
      mapping%power = power
    end if
  end subroutine sf_s_mapping_init

```

Apply mapping.

```

<SF mappings: sf standard mapping: TBP>+≡
  procedure :: compute => sf_s_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_s_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_s_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: r2
    integer :: j
    if (mapping%power_set) then
      call map_unit_square (r2, f, p(mapping%i), mapping%power)
    else
      call map_unit_square (r2, f, p(mapping%i))
    end if
    r = p
    rb = pb
    do j = 1, 2
      r (mapping%i(j)) = r2(j)
      rb(mapping%i(j)) = 1 - r2(j)
    end do
  end subroutine sf_s_mapping_compute

```

Apply inverse.

```

<SF mappings: sf standard mapping: TBP>+≡
  procedure :: inverse => sf_s_mapping_inverse

<SF mappings: procedures>+≡
  subroutine sf_s_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_s_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: p2

```

```

integer :: j
if (mapping%power_set) then
  call map_unit_square_inverse (r(mapping%i), f, p2, mapping%power)
else
  call map_unit_square_inverse (r(mapping%i), f, p2)
end if
p = r
pb= rb
do j = 1, 2
  p (mapping%i(j)) = p2(j)
  pb(mapping%i(j)) = 1 - p2(j)
end do
end subroutine sf_s_mapping_inverse

```

16.4.4 Implementation: resonance pair mapping

This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio, then it maps p_1 to itself according to a Breit-Wigner shape, i.e., a flat prior distribution in p_1 results in a Breit-Wigner distribution. Mass and width of the BW are rescaled by the energy, thus dimensionless fractions.

```

<SF mappings: public>+≡
  public :: sf_res_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_res_mapping_t
    real(default) :: m = 0
    real(default) :: w = 0
  contains
    <SF mappings: sf resonance mapping: TBP>
  end type sf_res_mapping_t

```

Output.

```

<SF mappings: sf resonance mapping: TBP>≡
  procedure :: write => sf_res_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_res_mapping_write (object, unit)
    class(sf_res_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,',',',I0,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,',',',F7.5,A)") ": resonance (", object%m, object%w, ")"
  end subroutine sf_res_mapping_write

```

Initialize: index pair and dimensionless mass and width parameters.

```

<SF mappings: sf resonance mapping: TBP>+≡
  procedure :: init => sf_res_mapping_init

```

```

<SF mappings: procedures>+≡
subroutine sf_res_mapping_init (mapping, m, w)
  class(sf_res_mapping_t), intent(out) :: mapping
  real(default), intent(in) :: m, w
  call mapping%base_init (2)
  mapping%m = m
  mapping%w = w
end subroutine sf_res_mapping_init

```

Apply mapping.

```

<SF mappings: sf resonance mapping: TBP>+≡
  procedure :: compute => sf_res_mapping_compute

<SF mappings: procedures>+≡
subroutine sf_res_mapping_compute (mapping, r, rb, f, p, pb, x_free)
  class(sf_res_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(out) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(in) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(2) :: r2, p2
  real(default) :: fbw, f2, p1m
  integer :: j
  p2 = p(mapping%i)
  call map_breit_wigner &
    (p1m, fbw, p2(1), mapping%m, mapping%w, x_free)
  call map_unit_square (r2, f2, [p1m, p2(2)])
  f = fbw * f2
  r = p
  rb= pb
  do j = 1, 2
    r (mapping%i(j)) = r2(j)
    rb(mapping%i(j)) = 1 - r2(j)
  end do
end subroutine sf_res_mapping_compute

```

Apply inverse.

```

<SF mappings: sf resonance mapping: TBP>+≡
  procedure :: inverse => sf_res_mapping_inverse

<SF mappings: procedures>+≡
subroutine sf_res_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
  class(sf_res_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(in) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(2) :: p2
  real(default) :: fbw, f2, p1m
  call map_unit_square_inverse (r(mapping%i), f2, p2)
  call map_breit_wigner_inverse &
    (p2(1), fbw, p1m, mapping%m, mapping%w, x_free)
  p = r
  pb= rb

```

```

p (mapping%i(1)) = p1m
pb(mapping%i(1)) = 1 - p1m
p (mapping%i(2)) = p2(2)
pb(mapping%i(2)) = 1 - p2(2)
f = fbw * f2
end subroutine sf_res_mapping_inverse

```

16.4.5 Implementation: resonance single mapping

While simpler, this is needed for structure-function setups only in exceptional cases.

This maps the unit interval (r_1) to itself according to a Breit-Wigner shape, i.e., a flat prior distribution in r_1 results in a Breit-Wigner distribution. Mass and width of the BW are rescaled by the energy, thus dimensionless fractions.

```

<SF mappings: public>+≡
public :: sf_res_mapping_single_t

<SF mappings: types>+≡
type, extends (sf_mapping_t) :: sf_res_mapping_single_t
    real(default) :: m = 0
    real(default) :: w = 0
contains
    <SF mappings: sf resonance single mapping: TBP>
end type sf_res_mapping_single_t

```

Output.

```

<SF mappings: sf resonance single mapping: TBP>≡
procedure :: write => sf_res_mapping_single_write

<SF mappings: procedures>+≡
subroutine sf_res_mapping_single_write (object, unit)
    class(sf_res_mapping_single_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
        write (u, "('(',I0,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,', ',F7.5,A)" ": resonance (" , object%m, object%w, ")")
end subroutine sf_res_mapping_single_write

```

Initialize: single index (!) and dimensionless mass and width parameters.

```

<SF mappings: sf resonance single mapping: TBP>+≡
procedure :: init => sf_res_mapping_single_init

<SF mappings: procedures>+≡
subroutine sf_res_mapping_single_init (mapping, m, w)
    class(sf_res_mapping_single_t), intent(out) :: mapping
    real(default), intent(in) :: m, w
    call mapping%base_init (1)
    mapping%m = m

```

```

        mapping%w = w
    end subroutine sf_res_mapping_single_init

```

Apply mapping.

```

<SF mappings: sf resonance single mapping: TBP>+≡
    procedure :: compute => sf_res_mapping_single_compute

<SF mappings: procedures>+≡
    subroutine sf_res_mapping_single_compute (mapping, r, rb, f, p, pb, x_free)
        class(sf_res_mapping_single_t), intent(inout) :: mapping
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: p, pb
        real(default), intent(inout), optional :: x_free
        real(default), dimension(1) :: r2, p2
        real(default) :: fbw
        integer :: j
        p2 = p(mapping%i)
        call map_breit_wigner &
            (r2(1), fbw, p2(1), mapping%m, mapping%w, x_free)
        f = fbw
        r = p
        rb= pb
        r (mapping%i(1)) = r2(1)
        rb(mapping%i(1)) = 1 - r2(1)
    end subroutine sf_res_mapping_single_compute

```

Apply inverse.

```

<SF mappings: sf resonance single mapping: TBP>+≡
    procedure :: inverse => sf_res_mapping_single_inverse

<SF mappings: procedures>+≡
    subroutine sf_res_mapping_single_inverse (mapping, r, rb, f, p, pb, x_free)
        class(sf_res_mapping_single_t), intent(inout) :: mapping
        real(default), dimension(:), intent(in) :: r, rb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(out) :: p, pb
        real(default), intent(inout), optional :: x_free
        real(default), dimension(1) :: p2
        real(default) :: fbw
        call map_breit_wigner_inverse &
            (r(mapping%i(1)), fbw, p2(1), mapping%m, mapping%w, x_free)
        p = r
        pb= rb
        p (mapping%i(1)) = p2(1)
        pb(mapping%i(1)) = 1 - p2(1)
        f = fbw
    end subroutine sf_res_mapping_single_inverse

```

16.4.6 Implementation: on-shell mapping

This is a degenerate version of the unit-square mapping where the product $r_1 r_2$ is constant. This product is given by the rescaled squared mass. We introduce

an artificial first parameter p_1 to keep the counting, but nothing depends on it. The second parameter is the same p_2 as for the standard unit-square mapping for $\alpha = 1$, it parameterizes the ratio of r_1 and r_2 .

```

<SF mappings: public>+≡
  public :: sf_os_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_os_mapping_t
    real(default) :: m = 0
    real(default) :: lm2 = 0
  contains
    <SF mappings: sf on-shell mapping: TBP>
  end type sf_os_mapping_t

```

Output.

```

<SF mappings: sf on-shell mapping: TBP>≡
  procedure :: write => sf_os_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_os_mapping_write (object, unit)
    class(sf_os_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',IO,',',',IO,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,A)" " ": on-shell (" , object%m, ")")
  end subroutine sf_os_mapping_write

```

Initialize: index pair and dimensionless mass parameter.

```

<SF mappings: sf on-shell mapping: TBP>+≡
  procedure :: init => sf_os_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_os_mapping_init (mapping, m)
    class(sf_os_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: m
    call mapping%base_init (2)
    mapping%m = m
    mapping%lm2 = abs (2 * log (mapping%m))
  end subroutine sf_os_mapping_init

```

Apply mapping. The `x_free` parameter rescales the total energy, which must be accounted for in the enclosed mapping.

```

<SF mappings: sf on-shell mapping: TBP>+≡
  procedure :: compute => sf_os_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_os_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f

```



```

real(default), dimension(:), intent(in) :: p, pb
real(default), intent(inout), optional :: x_free
real(default), dimension(2) :: r2, p2
integer :: j
p2 = p(mapping%i)
call map_on_shell (r2, f, p2, mapping%lm2, x_free)
r = p
rb= pb
do j = 1, 2
  r (mapping%i(j)) = r2(j)
  rb(mapping%i(j)) = 1 - r2(j)
end do
end subroutine sf_os_mapping_compute

```

Apply inverse. The irrelevant parameter p_1 is always set zero.

<SF mappings: sf on-shell mapping: TBP>+≡

```

procedure :: inverse => sf_os_mapping_inverse

```

<SF mappings: procedures>+≡

```

subroutine sf_os_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
  class(sf_os_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(in) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(2) :: p2, r2
  r2 = r(mapping%i)
  call map_on_shell_inverse (r2, f, p2, mapping%lm2, x_free)
  p = r
  pb= rb
  p (mapping%i(1)) = p2(1)
  pb(mapping%i(1)) = 1 - p2(1)
  p (mapping%i(2)) = p2(2)
  pb(mapping%i(2)) = 1 - p2(2)
end subroutine sf_os_mapping_inverse

```

16.4.7 Implementation: on-shell single mapping

This is a degenerate version of the unit-interval mapping where the result r is constant. The value is given by the rescaled squared mass. The input parameter p_1 is actually ignored, nothing depends on it.

<SF mappings: public>+≡

```

public :: sf_os_mapping_single_t

```

<SF mappings: types>+≡

```

type, extends (sf_mapping_t) :: sf_os_mapping_single_t
  real(default) :: m = 0
  real(default) :: lm2 = 0
contains
  <SF mappings: sf on-shell mapping single: TBP>
end type sf_os_mapping_single_t

```

Output.

```

<SF mappings: sf on-shell mapping single: TBP>≡
  procedure :: write => sf_os_mapping_single_write

<SF mappings: procedures>+≡
  subroutine sf_os_mapping_single_write (object, unit)
    class(sf_os_mapping_single_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',IO,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,A)" ": on-shell (" , object%m, ")")
  end subroutine sf_os_mapping_single_write

```

Initialize: index pair and dimensionless mass parameter.

```

<SF mappings: sf on-shell mapping single: TBP>+≡
  procedure :: init => sf_os_mapping_single_init

<SF mappings: procedures>+≡
  subroutine sf_os_mapping_single_init (mapping, m)
    class(sf_os_mapping_single_t), intent(out) :: mapping
    real(default), intent(in) :: m
    call mapping%base_init (1)
    mapping%m = m
    mapping%lm2 = abs (2 * log (mapping%m))
  end subroutine sf_os_mapping_single_init

```

Apply mapping. The `x_free` parameter rescales the total energy, which must be accounted for in the enclosed mapping.

```

<SF mappings: sf on-shell mapping single: TBP>+≡
  procedure :: compute => sf_os_mapping_single_compute

<SF mappings: procedures>+≡
  subroutine sf_os_mapping_single_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_single_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(1) :: r2, p2
    integer :: j
    p2 = p(mapping%i)
    call map_on_shell_single (r2, f, p2, mapping%lm2, x_free)
    r = p
    rb = pb
    r (mapping%i(1)) = r2(1)
    rb(mapping%i(1)) = 1 - r2(1)
  end subroutine sf_os_mapping_single_compute

```

Apply inverse. The irrelevant parameter p_1 is always set zero.

```

<SF mappings: sf on-shell mapping single: TBP>+≡
  procedure :: inverse => sf_os_mapping_single_inverse

<SF mappings: procedures>+≡
  subroutine sf_os_mapping_single_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_os_mapping_single_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(1) :: p2, r2
    r2 = r(mapping%i)
    call map_on_shell_single_inverse (r2, f, p2, mapping%lm2, x_free)
    p = r
    pb= rb
    p (mapping%i(1)) = p2(1)
    pb(mapping%i(1)) = 1 - p2(1)
  end subroutine sf_os_mapping_single_inverse

```

16.4.8 Implementation: endpoint mapping

This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio. Furthermore, we enhance the region at $r_1 = 1$ and $r_2 = 1$, which translates into $p_1 = 1$ and $p_2 = 0, 1$. The enhancement is such that any power-like singularity is caught. This is useful for beamstrahlung spectra.

In addition, we allow for a delta-function singularity in r_1 and/or r_2 . The singularity is smeared to an interval of width ϵ . If nonzero, we distinguish the kinematical momentum fractions r_i from effective values x_i , which should go into the structure-function evaluation. A bin of width ϵ in r is mapped to $x = 1$ exactly, while the interval $(0, 1 - \epsilon)$ is mapped to $(0, 1)$ in x . The Jacobian reflects this distinction, and the logical `in_peak` allows for an unambiguous distinction.

The delta-peak fraction is used only for the integration self-test.

```

<SF mappings: public>+≡
  public :: sf_ep_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ep_mapping_t
    real(default) :: a = 1
  contains
    <SF mappings: sf endpoint mapping: TBP>
  end type sf_ep_mapping_t

```

Output.

```

<SF mappings: sf endpoint mapping: TBP>≡
  procedure :: write => sf_ep_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_ep_mapping_write (object, unit)
    class(sf_ep_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u

```

```

u = given_output_unit (unit)
write (u, "(1x,A)", advance="no") "map"
if (any (object%i /= 0)) then
    write (u, "('(',I0,',',',I0,')')", advance="no") object%i
end if
write (u, "(A,ES12.5,A)") ": endpoint (a =", object%a, ")"
end subroutine sf_ep_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf endpoint mapping: TBP>+≡
  procedure :: init => sf_ep_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_ep_mapping_init (mapping, a)
    class(sf_ep_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: a
    call mapping%base_init (2)
    if (present (a)) mapping%a = a
  end subroutine sf_ep_mapping_init

```

Apply mapping.

```

<SF mappings: sf endpoint mapping: TBP>+≡
  procedure :: compute => sf_ep_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_ep_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_ep_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, r2
    real(default) :: f1, f2
    integer :: j
    call map_endpoint_1 (px(1), f1, p(mapping%i(1)), mapping%a)
    call map_endpoint_01 (px(2), f2, p(mapping%i(2)), mapping%a)
    call map_unit_square (r2, f, px)
    f = f * f1 * f2
    r = p
    rb = pb
    do j = 1, 2
        r (mapping%i(j)) = r2(j)
        rb(mapping%i(j)) = 1 - r2(j)
    end do
  end subroutine sf_ep_mapping_compute

```

Apply inverse.

```

<SF mappings: sf endpoint mapping: TBP>+≡
  procedure :: inverse => sf_ep_mapping_inverse

<SF mappings: procedures>+≡
  subroutine sf_ep_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ep_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb

```

```

real(default), intent(out) :: f
real(default), dimension(:), intent(out) :: p, pb
real(default), intent(inout), optional :: x_free
real(default), dimension(2) :: r2, px, p2
real(default) :: f1, f2
integer :: j
do j = 1, 2
    r2(j) = r(mapping%i(j))
end do
call map_unit_square_inverse (r2, f, px)
call map_endpoint_inverse_1 (px(1), f1, p2(1), mapping%a)
call map_endpoint_inverse_01 (px(2), f2, p2(2), mapping%a)
f = f * f1 * f2
p = r
pb= rb
do j = 1, 2
    p (mapping%i(j)) = p2(j)
    pb(mapping%i(j)) = 1 - p2(j)
end do
end subroutine sf_ep_mapping_inverse

```

16.4.9 Implementation: endpoint mapping with resonance

Like the endpoint mapping for p_2 , but replace the endpoint mapping by a Breit-Wigner mapping for p_1 . This covers resonance production in the presence of beamstrahlung.

If the flag `resonance` is unset, we skip the resonance mapping, so the parameter p_1 remains equal to $r_1 r_2$, as in the standard s-channel mapping.

```

<SF mappings: public>+≡
    public :: sf_epr_mapping_t

<SF mappings: types>+≡
    type, extends (sf_mapping_t) :: sf_epr_mapping_t
        real(default) :: a = 1
        real(default) :: m = 0
        real(default) :: w = 0
        logical :: resonance = .true.
    contains
        <SF mappings: sf endpoint/res mapping: TBP>
    end type sf_epr_mapping_t

```

Output.

```

<SF mappings: sf endpoint/res mapping: TBP>≡
    procedure :: write => sf_epr_mapping_write

<SF mappings: procedures>+≡
    subroutine sf_epr_mapping_write (object, unit)
        class(sf_epr_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "map"
    end subroutine sf_epr_mapping_write

```

```

if (any (object%i /= 0)) then
  write (u, "('(',I0,',',I0,')')", advance="no") object%i
end if
if (object%resonance) then
  write (u, "(A,F7.5,A,F7.5,', ',F7.5,A)") ": ep/res (a = ", object%a, &
    " | ", object%m, object%w, ")")
else
  write (u, "(A,F7.5,A)") ": ep/nores (a = ", object%a, ")")
end if
end subroutine sf_epr_mapping_write

```

Initialize: if mass and width are not given, we initialize a non-resonant version of the mapping.

```

<SF mappings: sf endpoint/res mapping: TBP>+≡
  procedure :: init => sf_epr_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_epr_mapping_init (mapping, a, m, w)
    class(sf_epr_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a
    real(default), intent(in), optional :: m, w
    call mapping%base_init (2)
    mapping%a = a
    if (present (m) .and. present (w)) then
      mapping%m = m
      mapping%w = w
    else
      mapping%resonance = .false.
    end if
  end subroutine sf_epr_mapping_init

```

Apply mapping.

```

<SF mappings: sf endpoint/res mapping: TBP>+≡
  procedure :: compute => sf_epr_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_epr_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_epr_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, r2
    real(default) :: f1, f2
    integer :: j
    if (mapping%resonance) then
      call map_breit_wigner &
        (px(1), f1, p(mapping%i(1)), mapping%m, mapping%w, x_free)
    else
      px(1) = p(mapping%i(1))
      f1 = 1
    end if
    call map_endpoint_01 (px(2), f2, p(mapping%i(2)), mapping%a)
    call map_unit_square (r2, f, px)
  end subroutine sf_epr_mapping_compute

```

```

f = f * f1 * f2
r = p
rb= pb
do j = 1, 2
  r (mapping%i(j)) = r2(j)
  rb(mapping%i(j)) = 1 - r2(j)
end do
end subroutine sf_epr_mapping_compute

```

Apply inverse.

```

⟨SF mappings: sf endpoint/res mapping: TBP⟩+≡
  procedure :: inverse => sf_epr_mapping_inverse

⟨SF mappings: procedures⟩+≡
  subroutine sf_epr_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_epr_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, p2
    real(default) :: f1, f2
    integer :: j
    call map_unit_square_inverse (r(mapping%i), f, px)
    if (mapping%resonance) then
      call map_breit_wigner_inverse &
        (px(1), f1, p2(1), mapping%m, mapping%w, x_free)
    else
      p2(1) = px(1)
      f1 = 1
    end if
    call map_endpoint_inverse_01 (px(2), f2, p2(2), mapping%a)
    f = f * f1 * f2
    p = r
    pb= rb
    do j = 1, 2
      p (mapping%i(j)) = p2(j)
      pb(mapping%i(j)) = 1 - p2(j)
    end do
  end subroutine sf_epr_mapping_inverse

```

16.4.10 Implementation: endpoint mapping for on-shell particle

Analogous to the resonance mapping, but the p_1 input is ignored altogether. This covers on-shell particle production in the presence of beamstrahlung.

```

⟨SF mappings: public⟩+≡
  public :: sf_epo_mapping_t

⟨SF mappings: types⟩+≡
  type, extends (sf_mapping_t) :: sf_epo_mapping_t
    real(default) :: a = 1

```

```

        real(default) :: m = 0
        real(default) :: lm2 = 0
contains
  <SF mappings: sf endpoint/os mapping: TBP>
end type sf_epo_mapping_t

```

Output.

```

<SF mappings: sf endpoint/os mapping: TBP>≡
  procedure :: write => sf_epo_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_epo_mapping_write (object, unit)
    class(sf_epo_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',IO,',',IO,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,A,F7.5,A)") ": ep/on-shell (a = ", object%a, &
      " | ", object%m, ") "
  end subroutine sf_epo_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf endpoint/os mapping: TBP>+≡
  procedure :: init => sf_epo_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_epo_mapping_init (mapping, a, m)
    class(sf_epo_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a, m
    call mapping%base_init (2)
    mapping%a = a
    mapping%m = m
    mapping%lm2 = abs (2 * log (mapping%m))
  end subroutine sf_epo_mapping_init

```

Apply mapping.

```

<SF mappings: sf endpoint/os mapping: TBP>+≡
  procedure :: compute => sf_epo_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_epo_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_epo_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, r2
    real(default) :: f2
    integer :: j
    px(1) = 0
    call map_endpoint_01 (px(2), f2, p(mapping%i(2)), mapping%a)

```



```

call map_on_shell (r2, f, px, mapping%lm2)
f = f * f2
r = p
rb= pb
do j = 1, 2
  r (mapping%i(j)) = r2(j)
  rb(mapping%i(j)) = 1 - r2(j)
end do
end subroutine sf_epo_mapping_compute

```

Apply inverse.

```

⟨SF mappings: sf endpoint/os mapping: TBP⟩+≡
  procedure :: inverse => sf_epo_mapping_inverse

⟨SF mappings: procedures⟩+≡
  subroutine sf_epo_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_epo_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, p2
    real(default) :: f2
    integer :: j
    call map_on_shell_inverse (r(mapping%i), f, px, mapping%lm2)
    p2(1) = 0
    call map_endpoint_inverse_01 (px(2), f2, p2(2), mapping%a)
    f = f * f2
    p = r
    pb= rb
    do j = 1, 2
      p (mapping%i(j)) = p2(j)
      pb(mapping%i(j)) = 1 - p2(j)
    end do
  end subroutine sf_epo_mapping_inverse

```

16.4.11 Implementation: ISR endpoint mapping

Similar to the endpoint mapping above: This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio. Furthermore, we enhance the region at $r_1 = 1$ and $r_2 = 1$, which translates into $p_1 = 1$ and $p_2 = 0, 1$.

The enhancement is such that ISR singularity $(1 - x)^{-1+\epsilon}$ is flattened. This would be easy in one dimension, but becomes nontrivial in two dimensions.

```

⟨SF mappings: public⟩+≡
  public :: sf_ip_mapping_t

⟨SF mappings: types⟩+≡
  type, extends (sf_mapping_t) :: sf_ip_mapping_t
    real(default) :: eps = 0
  contains
    ⟨SF mappings: sf power mapping: TBP⟩

```

```
end type sf_ip_mapping_t
```

Output.

```
<SF mappings: sf power mapping: TBP>≡
  procedure :: write => sf_ip_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_ip_mapping_write (object, unit)
    class(sf_ip_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',IO,',',IO,')')", advance="no") object%i
    end if
    write (u, "(A,ES12.5,A)") ": isr (eps =", object%eps, ")"
  end subroutine sf_ip_mapping_write
```

Initialize: no extra parameters.

```
<SF mappings: sf power mapping: TBP>+≡
  procedure :: init => sf_ip_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_ip_mapping_init (mapping, eps)
    class(sf_ip_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: eps
    call mapping%base_init (2)
    if (present (eps)) mapping%eps = eps
    if (mapping%eps <= 0) &
      call msg_fatal ("ISR mapping: regulator epsilon must not be zero")
  end subroutine sf_ip_mapping_init
```

Apply mapping.

```
<SF mappings: sf power mapping: TBP>+≡
  procedure :: compute => sf_ip_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_ip_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_ip_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, pxb, r2, r2b
    real(default) :: f1, f2, xb, y, yb
    integer :: j
    call map_power_1 (xb, f1, pb(mapping%i(1)), 2 * mapping%eps)
    call map_power_01 (y, yb, f2, pb(mapping%i(2)), mapping%eps)
    px(1) = 1 - xb
    pxb(1) = xb
    px(2) = y
    pxb(2) = yb
    call map_unit_square_prec (r2, r2b, f, px, pxb)
```

```

f = f * f1 * f2
r = p
rb= pb
do j = 1, 2
  r (mapping%i(j)) = r2 (j)
  rb(mapping%i(j)) = r2b(j)
end do
end subroutine sf_ip_mapping_compute

```

Apply inverse.

(SF mappings: sf power mapping: TBP)+≡

```

procedure :: inverse => sf_ip_mapping_inverse

```

(SF mappings: procedures)+≡

```

subroutine sf_ip_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
  class(sf_ip_mapping_t), intent(inout) :: mapping
  real(default), dimension(:), intent(in) :: r, rb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: p, pb
  real(default), intent(inout), optional :: x_free
  real(default), dimension(2) :: r2, r2b, px, pxb, p2, p2b
  real(default) :: f1, f2, xb, y, yb
  integer :: j
  do j = 1, 2
    r2 (j) = r (mapping%i(j))
    r2b(j) = rb(mapping%i(j))
  end do
  call map_unit_square_inverse_prec (r2, r2b, f, px, pxb)
  xb = pxb(1)
  if (px(1) > 0) then
    y = px(2)
    yb = pxb(2)
  else
    y = 0.5_default
    yb = 0.5_default
  end if
  call map_power_inverse_1 (xb, f1, p2b(1), 2 * mapping%eps)
  call map_power_inverse_01 (y, yb, f2, p2b(2), mapping%eps)
  p2 = 1 - p2b
  f = f * f1 * f2
  p = r
  pb= rb
  do j = 1, 2
    p (mapping%i(j)) = p2(j)
    pb(mapping%i(j)) = p2b(j)
  end do
end subroutine sf_ip_mapping_inverse

```

16.4.12 Implementation: ISR endpoint mapping, resonant

Similar to the endpoint mapping above: This maps the unit square (r_1, r_2) such that p_1 is the product $r_1 r_2$, while p_2 is related to the ratio. Furthermore, we

enhance the region at $r_1 = 1$ and $r_2 = 1$, which translates into $p_1 = 1$ and $p_2 = 0, 1$.

The enhancement is such that ISR singularity $(1 - x)^{-1+\epsilon}$ is flattened. This would be easy in one dimension, but becomes nontrivial in two dimensions.

The resonance can be turned off by the flag **resonance**.

```

<SF mappings: public>+≡
  public :: sf_ipr_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ipr_mapping_t
    real(default) :: eps = 0
    real(default) :: m = 0
    real(default) :: w = 0
    logical :: resonance = .true.
  contains
    <SF mappings: sf power/res mapping: TBP>
  end type sf_ipr_mapping_t

```

Output.

```

<SF mappings: sf power/res mapping: TBP>≡
  procedure :: write => sf_ipr_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_ipr_mapping_write (object, unit)
    class(sf_ipr_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,',',I0,')')", advance="no") object%i
    end if
    if (object%resonance) then
      write (u, "(A,F7.5,A,F7.5,', ',F7.5,A)") ": isr/res (eps = ", &
        object%eps, " | ", object%m, object%w, ") "
    else
      write (u, "(A,F7.5,A)") ": isr/res (eps = ", object%eps, ") "
    end if
  end subroutine sf_ipr_mapping_write

```

Initialize:

```

<SF mappings: sf power/res mapping: TBP>+≡
  procedure :: init => sf_ipr_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_ipr_mapping_init (mapping, eps, m, w)
    class(sf_ipr_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: eps, m, w
    call mapping%base_init (2)
    if (present (eps)) mapping%eps = eps
    if (mapping%eps <= 0) &
      call msg_fatal ("ISR mapping: regulator epsilon must not be zero")
    if (present (m) .and. present (w)) then
      mapping%m = m

```

```

        mapping%w = w
    else
        mapping%resonance = .false.
    end if
end subroutine sf_ipr_mapping_init

```

Apply mapping.

```

<SF mappings: sf power/res mapping: TBP>+≡
  procedure :: compute => sf_ipr_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_ipr_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_ipr_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, pxb, r2, r2b
    real(default) :: f1, f2, y, yb
    integer :: j
    if (mapping%resonance) then
        call map_breit_wigner &
            (px(1), f1, p(mapping%i(1)), mapping%m, mapping%w, x_free)
    else
        px(1) = p(mapping%i(1))
        f1 = 1
    end if
    call map_power_01 (y, yb, f2, pb(mapping%i(2)), mapping%eps)
    pxb(1) = 1 - px(1)
    px(2) = y
    pxb(2) = yb
    call map_unit_square_prec (r2, r2b, f, px, pxb)
    f = f * f1 * f2
    r = p
    rb = pb
    do j = 1, 2
        r (mapping%i(j)) = r2 (j)
        rb(mapping%i(j)) = r2b(j)
    end do
  end subroutine sf_ipr_mapping_compute

```

Apply inverse.

```

<SF mappings: sf power/res mapping: TBP>+≡
  procedure :: inverse => sf_ipr_mapping_inverse

<SF mappings: procedures>+≡
  subroutine sf_ipr_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ipr_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: r2, r2b, px, pxb, p2, p2b
    real(default) :: f1, f2, y, yb

```

```

integer :: j
do j = 1, 2
  r2 (j) = r (mapping%i(j))
  r2b(j) = rb(mapping%i(j))
end do
call map_unit_square_inverse_prec (r2, r2b, f, px, pxb)
if (px(1) > 0) then
  y = px(2)
  yb = pxb(2)
else
  y = 0.5_default
  yb = 0.5_default
end if
if (mapping%resonance) then
  call map_breit_wigner_inverse &
    (px(1), f1, p2(1), mapping%m, mapping%w, x_free)
else
  p2(1) = px(1)
  f1 = 1
end if
call map_power_inverse_01 (y, yb, f2, p2b(2), mapping%eps)
p2b(1) = 1 - p2(1)
p2 (2) = 1 - p2b(2)
f = f * f1 * f2
p = r
pb= rb
do j = 1, 2
  p (mapping%i(j)) = p2(j)
  pb(mapping%i(j)) = p2b(j)
end do
end subroutine sf_ipr_mapping_inverse

```

16.4.13 Implementation: ISR on-shell mapping

Similar to the endpoint mapping above: This maps the unit square (r_1, r_2) such that p_1 is ignored while the product $r_1 r_2$ is constant. p_2 is related to the ratio. Furthermore, we enhance the region at $r_1 = 1$ and $r_2 = 1$, which translates into $p_1 = 1$ and $p_2 = 0, 1$.

The enhancement is such that ISR singularity $(1 - x)^{-1+\epsilon}$ is flattened. This would be easy in one dimension, but becomes nontrivial in two dimensions.

```

<SF mappings: public>+≡
  public :: sf_ipo_mapping_t

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ipo_mapping_t
    real(default) :: eps = 0
    real(default) :: m = 0
  contains
    <SF mappings: sf power/os mapping: TBP>
  end type sf_ipo_mapping_t

```

Output.

```

<SF mappings: sf power/os mapping: TBP>≡
  procedure :: write => sf_ipo_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_ipo_mapping_write (object, unit)
    class(sf_ipo_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',IO,',',IO,')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,A,F7.5,A)" " : isr/os (eps = ", object%eps, &
      " | ", object%m, ")")
  end subroutine sf_ipo_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf power/os mapping: TBP>+≡
  procedure :: init => sf_ipo_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_ipo_mapping_init (mapping, eps, m)
    class(sf_ipo_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: eps, m
    call mapping%base_init (2)
    if (present (eps)) mapping%eps = eps
    if (mapping%eps <= 0) &
      call msg_fatal ("ISR mapping: regulator epsilon must not be zero")
    mapping%m = m
  end subroutine sf_ipo_mapping_init

```

Apply mapping.

```

<SF mappings: sf power/os mapping: TBP>+≡
  procedure :: compute => sf_ipo_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_ipo_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_ipo_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: px, pxb, r2, r2b
    real(default) :: f1, f2, y, yb
    integer :: j
    call map_power_01 (y, yb, f2, pb(mapping%i(2)), mapping%eps)
    px(1) = mapping%m ** 2
    if (present (x_free)) px(1) = px(1) / x_free
    pxb(1) = 1 - px(1)
    px(2) = y
    pxb(2) = yb
    call map_unit_square_prec (r2, r2b, f1, px, pxb)
  end subroutine sf_ipo_mapping_compute

```

```

f = f1 * f2
r = p
rb= pb
do j = 1, 2
  r (mapping%i(j)) = r2 (j)
  rb(mapping%i(j)) = r2b(j)
end do
end subroutine sf_ipo_mapping_compute

```

Apply inverse.

```

⟨SF mappings: sf power/os mapping: TBP⟩+≡
  procedure :: inverse => sf_ipo_mapping_inverse

⟨SF mappings: procedures⟩+≡
  subroutine sf_ipo_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ipo_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(2) :: r2, r2b, px, pxb, p2, p2b
    real(default) :: f1, f2, y, yb
    integer :: j
    do j = 1, 2
      r2 (j) = r (mapping%i(j))
      r2b(j) = rb(mapping%i(j))
    end do
    call map_unit_square_inverse_prec (r2, r2b, f1, px, pxb)
    y  = px(2)
    yb = pxb(2)
    call map_power_inverse_01 (y, yb, f2, p2b(2), mapping%eps)
    p2(1) = 0
    p2b(1) = 1
    p2(2) = 1 - p2b(2)
    f = f1 * f2
    p = r
    pb= rb
    do j = 1, 2
      p (mapping%i(j)) = p2(j)
      pb(mapping%i(j)) = p2b(j)
    end do
  end subroutine sf_ipo_mapping_inverse

```

16.4.14 Implementation: Endpoint + ISR power mapping

This is a combination of endpoint (i.e., beamstrahlung) and ISR power mapping. The first two parameters apply to the beamstrahlung spectrum, the last two to the ISR function for the first and second beam, respectively.

```

⟨SF mappings: public⟩+≡
  public :: sf_ei_mapping_t

```



```

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_ei_mapping_t
    type(sf_ep_mapping_t) :: ep
    type(sf_ip_mapping_t) :: ip
  contains
    <SF mappings: sf ep-ip mapping: TBP>
  end type sf_ei_mapping_t

```

Output.

```

<SF mappings: sf ep-ip mapping: TBP>≡
  procedure :: write => sf_ei_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_ei_mapping_write (object, unit)
    class(sf_ei_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,3(' ',I0),')')", advance="no") object%i
    end if
    write (u, "(A,ES12.5,A,ES12.5,A)") ": ep/isr (a =", object%ep%a, &
      ", eps =", object%ip%eps, ")"
  end subroutine sf_ei_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf ep-ip mapping: TBP>+≡
  procedure :: init => sf_ei_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_ei_mapping_init (mapping, a, eps)
    class(sf_ei_mapping_t), intent(out) :: mapping
    real(default), intent(in), optional :: a, eps
    call mapping%base_init (4)
    call mapping%ep%init (a)
    call mapping%ip%init (eps)
  end subroutine sf_ei_mapping_init

```

Set an index value. We should communicate the appropriate indices to the enclosed sub-mappings, therefore override the method.

```

<SF mappings: sf ep-ip mapping: TBP>+≡
  procedure :: set_index => sf_ei_mapping_set_index

<SF mappings: procedures>+≡
  subroutine sf_ei_mapping_set_index (mapping, j, i)
    class(sf_ei_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
    mapping%i(j) = i
    select case (j)
    case (1:2); call mapping%ep%set_index (j, i)
    case (3:4); call mapping%ip%set_index (j-2, i)
    end select

```

```
end subroutine sf_ei_mapping_set_index
```

Apply mapping. Now, the beamstrahlung and ISR mappings are independent of each other. The parameter subsets that are actually used should not overlap. The Jacobians are multiplied.

```
<SF mappings: sf ep-ip mapping: TBP>+≡
  procedure :: compute => sf_ei_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_ei_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_ei_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: q, qb
    real(default) :: f1, f2
    call mapping%ep%compute (q, qb, f1, p, pb, x_free)
    call mapping%ip%compute (r, rb, f2, q, qb, x_free)
    f = f1 * f2
  end subroutine sf_ei_mapping_compute
```

Apply inverse.

```
<SF mappings: sf ep-ip mapping: TBP>+≡
  procedure :: inverse => sf_ei_mapping_inverse

<SF mappings: procedures>+≡
  subroutine sf_ei_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_ei_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: q, qb
    real(default) :: f1, f2
    call mapping%ip%inverse (r, rb, f2, q, qb, x_free)
    call mapping%ep%inverse (q, qb, f1, p, pb, x_free)
    f = f1 * f2
  end subroutine sf_ei_mapping_inverse
```

16.4.15 Implementation: Endpoint + ISR + resonance

This is a combination of endpoint (i.e., beamstrahlung) and ISR power mapping, adapted for an s-channel resonance. The first two internal parameters apply to the beamstrahlung spectrum, the last two to the ISR function for the first and second beam, respectively. The first and third parameters are the result of an overall resonance mapping, so on the outside, the first parameter is the total momentum fraction, the third one describes the distribution between beamstrahlung and ISR.

```
<SF mappings: public>+≡
  public :: sf_eir_mapping_t
```

```

<SF mappings: types>+≡
  type, extends (sf_mapping_t) :: sf_eir_mapping_t
    type(sf_res_mapping_t) :: res
    type(sf_epr_mapping_t) :: ep
    type(sf_ipr_mapping_t) :: ip
  contains
    <SF mappings: sf ep-ip-res mapping: TBP>
  end type sf_eir_mapping_t

```

Output.

```

<SF mappings: sf ep-ip-res mapping: TBP>≡
  procedure :: write => sf_eir_mapping_write

<SF mappings: procedures>+≡
  subroutine sf_eir_mapping_write (object, unit)
    class(sf_eir_mapping_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "map"
    if (any (object%i /= 0)) then
      write (u, "('(',I0,3(' ',I0),')')", advance="no") object%i
    end if
    write (u, "(A,F7.5,A,F7.5,A,F7.5,', ',F7.5,A)") &
      ": ep/isr/res (a =", object%ep%a, &
      ", eps =", object%ip%eps, " | ", object%res%m, object%res%w, ") "
  end subroutine sf_eir_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf ep-ip-res mapping: TBP>+≡
  procedure :: init => sf_eir_mapping_init

<SF mappings: procedures>+≡
  subroutine sf_eir_mapping_init (mapping, a, eps, m, w)
    class(sf_eir_mapping_t), intent(out) :: mapping
    real(default), intent(in) :: a, eps, m, w
    call mapping%base_init (4)
    call mapping%res%init (m, w)
    call mapping%ep%init (a)
    call mapping%ip%init (eps)
  end subroutine sf_eir_mapping_init

```

Set an index value. We should communicate the appropriate indices to the enclosed sub-mappings, therefore override the method.

```

<SF mappings: sf ep-ip-res mapping: TBP>+≡
  procedure :: set_index => sf_eir_mapping_set_index

<SF mappings: procedures>+≡
  subroutine sf_eir_mapping_set_index (mapping, j, i)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
    mapping%i(j) = i
    select case (j)

```

```

case (1); call mapping%res%set_index (1, i)
case (3); call mapping%res%set_index (2, i)
end select
select case (j)
case (1:2); call mapping%ep%set_index (j, i)
case (3:4); call mapping%ip%set_index (j-2, i)
end select
end subroutine sf_eir_mapping_set_index

```

Apply mapping. Now, the beamstrahlung and ISR mappings are independent of each other. The parameter subsets that are actually used should not overlap. The Jacobians are multiplied.

```

<SF mappings: sf ep-ip-res mapping: TBP>+≡
  procedure :: compute => sf_eir_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_eir_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: px, pxb, q, qb
    real(default) :: f0, f1, f2
    call mapping%res%compute (px, pxb, f0, p, pb, x_free)
    call mapping%ep%compute (q, qb, f1, px, pxb, x_free)
    call mapping%ip%compute (r, rb, f2, q, qb, x_free)
    f = f0 * f1 * f2
  end subroutine sf_eir_mapping_compute

```

Apply inverse.

```

<SF mappings: sf ep-ip-res mapping: TBP>+≡
  procedure :: inverse => sf_eir_mapping_inverse

<SF mappings: procedures>+≡
  subroutine sf_eir_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_eir_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: px, pxb, q, qb
    real(default) :: f0, f1, f2
    call mapping%ip%inverse (r, rb, f2, q, qb, x_free)
    call mapping%ep%inverse (q, qb, f1, px, pxb, x_free)
    call mapping%res%inverse (px, pxb, f0, p, pb, x_free)
    f = f0 * f1 * f2
  end subroutine sf_eir_mapping_inverse

```

16.4.16 Implementation: Endpoint + ISR power mapping, on-shell

This is a combination of endpoint (i.e., beamstrahlung) and ISR power mapping. The first two parameters apply to the beamstrahlung spectrum, the last two to the ISR function for the first and second beam, respectively. On top of that, we map the first and third parameter such that the product is constant. From the outside, the first parameter is irrelevant while the third parameter describes the distribution of energy (loss) among beamstrahlung and ISR.

```

<SF mappings: public>+≡
    public :: sf_eio_mapping_t

<SF mappings: types>+≡
    type, extends (sf_mapping_t) :: sf_eio_mapping_t
        type(sf_os_mapping_t) :: os
        type(sf_epr_mapping_t) :: ep
        type(sf_ipr_mapping_t) :: ip
    contains
        <SF mappings: sf ep-ip-os mapping: TBP>
    end type sf_eio_mapping_t

```

Output.

```

<SF mappings: sf ep-ip-os mapping: TBP>≡
    procedure :: write => sf_eio_mapping_write

<SF mappings: procedures>+≡
    subroutine sf_eio_mapping_write (object, unit)
        class(sf_eio_mapping_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)", advance="no") "map"
        if (any (object%i /= 0)) then
            write (u, "('(',I0,3(' ',I0),')')", advance="no") object%i
        end if
        write (u, "(A,F7.5,A,F7.5,A,F7.5,A)") ": ep/isr/os (a =", object%ep%a, &
            ", eps =", object%ip%eps, " | ", object%os%m, ")"
    end subroutine sf_eio_mapping_write

```

Initialize: no extra parameters.

```

<SF mappings: sf ep-ip-os mapping: TBP>+≡
    procedure :: init => sf_eio_mapping_init

<SF mappings: procedures>+≡
    subroutine sf_eio_mapping_init (mapping, a, eps, m)
        class(sf_eio_mapping_t), intent(out) :: mapping
        real(default), intent(in), optional :: a, eps, m
        call mapping%base_init (4)
        call mapping%os%init (m)
        call mapping%ep%init (a)
        call mapping%ip%init (eps)
    end subroutine sf_eio_mapping_init

```

Set an index value. We should communicate the appropriate indices to the enclosed sub-mappings, therefore override the method.

```

<SF mappings: sf ep-ip-os mapping: TBP>+≡
  procedure :: set_index => sf_eio_mapping_set_index

<SF mappings: procedures>+≡
  subroutine sf_eio_mapping_set_index (mapping, j, i)
    class(sf_eio_mapping_t), intent(inout) :: mapping
    integer, intent(in) :: j, i
    mapping%i(j) = i
    select case (j)
    case (1); call mapping%os%set_index (1, i)
    case (3); call mapping%os%set_index (2, i)
    end select
    select case (j)
    case (1:2); call mapping%ep%set_index (j, i)
    case (3:4); call mapping%ip%set_index (j-2, i)
    end select
  end subroutine sf_eio_mapping_set_index

```

Apply mapping. Now, the beamstrahlung and ISR mappings are independent of each other. The parameter subsets that are actually used should not overlap. The Jacobians are multiplied.

```

<SF mappings: sf ep-ip-os mapping: TBP>+≡
  procedure :: compute => sf_eio_mapping_compute

<SF mappings: procedures>+≡
  subroutine sf_eio_mapping_compute (mapping, r, rb, f, p, pb, x_free)
    class(sf_eio_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: px, pxb, q, qb
    real(default) :: f0, f1, f2
    call mapping%os%compute (px, pxb, f0, p, pb, x_free)
    call mapping%ep%compute (q, qb, f1, px, pxb, x_free)
    call mapping%ip%compute (r, rb, f2, q, qb, x_free)
    f = f0 * f1 * f2
  end subroutine sf_eio_mapping_compute

```

Apply inverse.

```

<SF mappings: sf ep-ip-os mapping: TBP>+≡
  procedure :: inverse => sf_eio_mapping_inverse

<SF mappings: procedures>+≡
  subroutine sf_eio_mapping_inverse (mapping, r, rb, f, p, pb, x_free)
    class(sf_eio_mapping_t), intent(inout) :: mapping
    real(default), dimension(:), intent(in) :: r, rb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: p, pb
    real(default), intent(inout), optional :: x_free
    real(default), dimension(size(p)) :: px, pxb, q, qb
    real(default) :: f0, f1, f2

```

```

call mapping%ip%inverse (r, rb, f2, q, qb, x_free)
call mapping%ep%inverse (q, qb, f1, px, pxb, x_free)
call mapping%os%inverse (px, pxb, f0, p, pb, x_free)
f = f0 * f1 * f2
end subroutine sf_eio_mapping_inverse

```

16.4.17 Basic formulas

Standard mapping of the unit square

This mapping of the unit square is appropriate in particular for structure functions which are concentrated at the lower end. Instead of a rectangular grid, one set of grid lines corresponds to constant parton c.m. energy. The other set is chosen such that the jacobian is only mildly singular ($\ln x$ which is zero at $x = 1$), corresponding to an initial concentration of sampling points at the maximum energy. If **power** is greater than one (the default), points are also concentrated at the lower end.

The formula is (**power**= α):

$$r_1 = (p_1^{p_2})^\alpha \quad (16.15)$$

$$r_2 = (p_1^{1-p_2})^\alpha \quad (16.16)$$

$$f = \alpha^2 p_1^{\alpha-1} |\log p_1| \quad (16.17)$$

and for the default case $\alpha = 1$:

$$r_1 = p_1^{p_2} \quad (16.18)$$

$$r_2 = p_1^{1-p_2} \quad (16.19)$$

$$f = |\log p_1| \quad (16.20)$$

(SF mappings: procedures) +≡

```

subroutine map_unit_square (r, factor, p, power)
  real(default), dimension(2), intent(out) :: r
  real(default), intent(out) :: factor
  real(default), dimension(2), intent(in) :: p
  real(default), intent(in), optional :: power
  real(default) :: xx, yy
  factor = 1
  xx = p(1)
  yy = p(2)
  if (present(power)) then
    if (p(1) > 0 .and. power > 1) then
      xx = p(1)**power
      factor = factor * power * xx / p(1)
    end if
  end if
  if (.not. vanishes (xx)) then
    r(1) = xx ** yy
    r(2) = xx / r(1)
    factor = factor * abs (log (xx))
  else
    r = 0
  end if
end subroutine map_unit_square

```

```

        end if
    end subroutine map_unit_square

```

This is the inverse mapping.

```

⟨SF mappings: procedures⟩+≡
subroutine map_unit_square_inverse (r, factor, p, power)
    real(kind=default), dimension(2), intent(in) :: r
    real(kind=default), intent(out) :: factor
    real(kind=default), dimension(2), intent(out) :: p
    real(kind=default), intent(in), optional :: power
    real(kind=default) :: lg, xx, yy
    factor = 1
    xx = r(1) * r(2)
    if (.not. vanishes (xx)) then
        lg = log (xx)
        if (.not. vanishes (lg)) then
            yy = log (r(1)) / lg
        else
            yy = 0
        end if
        p(2) = yy
        factor = factor * abs (lg)
        if (present(power)) then
            p(1) = xx**(1._default/power)
            factor = factor * power * xx / p(1)
        else
            p(1) = xx
        end if
    else
        p = 0
    end if
end subroutine map_unit_square_inverse

```

Precise mapping of the unit square

A more precise version (with unit power parameter). This version should be numerically stable near $x = 1$ and $y = 0, 1$. The formulas are again

$$r_1 = p_1^{p_2}, \quad r_2 = p_1^{\bar{p}_2}, \quad f = -\log p_1 \quad (16.21)$$

but we compute both r_i and \bar{r}_i simultaneously and make direct use of both p_i and \bar{p}_i as appropriate.

```

⟨SF mappings: procedures⟩+≡
subroutine map_unit_square_prec (r, rb, factor, p, pb)
    real(default), dimension(2), intent(out) :: r
    real(default), dimension(2), intent(out) :: rb
    real(default), intent(out) :: factor
    real(default), dimension(2), intent(in) :: p
    real(default), dimension(2), intent(in) :: pb
    if (p(1) > 0.5_default) then
        call compute_prec_xy_1 (r(1), rb(1), p(1), pb(1), p (2))
        call compute_prec_xy_1 (r(2), rb(2), p(1), pb(1), pb(2))
    end if
end subroutine map_unit_square_prec

```



```

        factor = - log_prec (p(1), pb(1))
    else if (.not. vanishes (p(1))) then
        call compute_prec_xy_0 (r(1), rb(1), p(1), pb(1), p (2))
        call compute_prec_xy_0 (r(2), rb(2), p(1), pb(1), pb(2))
        factor = - log_prec (p(1), pb(1))
    else
        r  = 0
        rb = 1
        factor = 0
    end if
end subroutine map_unit_square_prec

```

This is the inverse mapping.

(SF mappings: procedures)+≡

```

subroutine map_unit_square_inverse_prec (r, rb, factor, p, pb)
    real(default), dimension(2), intent(in) :: r
    real(default), dimension(2), intent(in) :: rb
    real(default), intent(out) :: factor
    real(default), dimension(2), intent(out) :: p
    real(default), dimension(2), intent(out) :: pb
    call inverse_prec_x (r, rb, p(1), pb(1))
    if (all (r > 0)) then
        if (rb(1) < rb(2)) then
            call inverse_prec_y (r, rb, p(2), pb(2))
        else
            call inverse_prec_y ([r(2),r(1)], [rb(2),rb(1)], pb(2), p(2))
        end if
        factor = - log_prec (p(1), pb(1))
    else
        p(1) = 0
        pb(1) = 1
        p(2) = 0.5_default
        pb(2) = 0.5_default
        factor = 0
    end if
end subroutine map_unit_square_inverse_prec

```

This is an auxiliary function: evaluate the expression $\bar{z} = 1 - x^y$ in a numerically stable way. Instabilities occur for $y = 0$ and $x = 1$. The idea is to replace the bracket by the first terms of its Taylor expansion around $x = 1$ (read $\bar{x} \equiv 1 - x$)

$$1 - x^y = y\bar{x} \left(1 + \frac{1}{2}(1-y)\bar{x} + \frac{1}{6}(2-y)(1-y)\bar{x}^2 \right) \quad (16.22)$$

whenever this is the better approximation. Actually, the relative numerical error of the exact formula is about $\eta/(y\bar{x})$ where η is given by `epsilon(KIND)` in Fortran. The relative error of the approximation is better than the last included term divided by $(y\bar{x})$.

The first subroutine computes z and \bar{z} near $x = 1$ where $\log x$ should be expanded, the second one near $x = 0$ where $\log x$ can be kept.

(SF mappings: procedures)+≡

```

subroutine compute_prec_xy_1 (z, zb, x, xb, y)
    real(default), intent(out) :: z, zb

```

```

real(default), intent(in) :: x, xb, y
real(default) :: a1, a2, a3
a1 = y * xb
a2 = a1 * (1 - y) * xb / 2
a3 = a2 * (2 - y) * xb / 3
if (abs (a3) < epsilon (a3)) then
    zb = a1 + a2 + a3
    z = 1 - zb
else
    z = x ** y
    zb = 1 - z
end if
end subroutine compute_prec_xy_1

subroutine compute_prec_xy_0 (z, zb, x, xb, y)
real(default), intent(out) :: z, zb
real(default), intent(in) :: x, xb, y
real(default) :: a1, a2, a3, lx
lx = -log (x)
a1 = y * lx
a2 = a1 * y * lx / 2
a3 = a2 * y * lx / 3
if (abs (a3) < epsilon (a3)) then
    zb = a1 + a2 + a3
    z = 1 - zb
else
    z = x ** y
    zb = 1 - z
end if
end subroutine compute_prec_xy_0

```

For the inverse calculation, we evaluate $x = r_1 r_2$ in a stable way. Since it is just a polynomial, the expansion near $x = 1$ is analytically exact, and we don't need to choose based on precision.

(SF mappings: procedures)+≡

```

subroutine inverse_prec_x (r, rb, x, xb)
real(default), dimension(2), intent(in) :: r, rb
real(default), intent(out) :: x, xb
real(default) :: a0, a1
a0 = rb(1) + rb(2)
a1 = rb(1) * rb(2)
if (a0 > 0.5_default) then
    xb = a0 - a1
    x = 1 - xb
else
    x = r(1) * r(2)
    xb = 1 - x
end if
end subroutine inverse_prec_x

```

The inverse calculation for the relative momentum fraction

$$y = \frac{1}{1 + \frac{\log r_2}{\log r_1}} \quad (16.23)$$

is slightly more complicated. We should take the precise form of the logarithm, so we are safe near $r_i = 1$. A series expansion is required if $r_1 \ll r_2$, since then y becomes small. (We assume $r_1 < r_2$ here; for the opposite case, the arguments can be exchanged.)

```

(SF mappings: procedures)+≡
subroutine inverse_prec_y (r, rb, y, yb)
  real(default), dimension(2), intent(in) :: r, rb
  real(default), intent(out) :: y, yb
  real(default) :: log1, log2, a1, a2, a3
  log1 = log_prec (r(1), rb(1))
  log2 = log_prec (r(2), rb(2))
  if (abs (log2**3) < epsilon (one)) then
    if (abs(log1) < epsilon (one)) then
      y = zero
    else
      y = one / (one + log2 / log1)
    end if
    if (abs(log2) < epsilon (one)) then
      yb = zero
    else
      yb = one / (one + log1 / log2)
    end if
    return
  end if
  a1 = - rb(1) / log2
  a2 = - rb(1) ** 2 * (one / log2**2 + one / (2 * log2))
  a3 = - rb(1) ** 3 * (one / log2**3 + one / log2**2 + one/(3 * log2))
  if (abs (a3) < epsilon (a3)) then
    y = a1 + a2 + a3
    yb = one - y
  else
    y = one / (one + log2 / log1)
    yb = one / (one + log1 / log2)
  end if
end subroutine inverse_prec_y

```

Mapping for on-shell s-channel

The limiting case, if the product $r_1 r_2$ is fixed for on-shell production. The parameter p_1 is ignored. In the inverse mapping, it is returned zero.

The parameter `x_free`, if present, rescales the total energy. If it is less than one, the rescaled mass parameter m^2 should be increased accordingly.

Public for access in unit test.

```

(SF mappings: public)+≡
public :: map_on_shell
public :: map_on_shell_inverse

(SF mappings: procedures)+≡
subroutine map_on_shell (r, factor, p, lm2, x_free)
  real(default), dimension(2), intent(out) :: r
  real(default), intent(out) :: factor
  real(default), dimension(2), intent(in) :: p

```

```

real(default), intent(in) :: lm2
real(default), intent(in), optional :: x_free
real(default) :: lx
lx = lm2; if (present (x_free)) lx = lx + log (x_free)
r(1) = exp (- p(2) * lx)
r(2) = exp (- (1 - p(2)) * lx)
factor = lx
end subroutine map_on_shell

subroutine map_on_shell_inverse (r, factor, p, lm2, x_free)
real(default), dimension(2), intent(in) :: r
real(default), intent(out) :: factor
real(default), dimension(2), intent(out) :: p
real(default), intent(in) :: lm2
real(default), intent(in), optional :: x_free
real(default) :: lx
lx = lm2; if (present (x_free)) lx = lx + log (x_free)
p(1) = 0
p(2) = abs (log (r(1))) / lx
factor = lx
end subroutine map_on_shell_inverse

```

Mapping for on-shell s-channel, single parameter

This is a pseudo-mapping which applies if there is actually just one parameter p . The output parameter r is fixed for on-shell production. The lone parameter p_1 is ignored. In the inverse mapping, it is returned zero.

The parameter x_free , if present, rescales the total energy. If it is less than one, the rescaled mass parameter m^2 should be increased accordingly.

Public for access in unit test.

```

<SF mappings: public>+≡
public :: map_on_shell_single
public :: map_on_shell_single_inverse

<SF mappings: procedures>+≡
subroutine map_on_shell_single (r, factor, p, lm2, x_free)
real(default), dimension(1), intent(out) :: r
real(default), intent(out) :: factor
real(default), dimension(1), intent(in) :: p
real(default), intent(in) :: lm2
real(default), intent(in), optional :: x_free
real(default) :: lx
lx = lm2; if (present (x_free)) lx = lx + log (x_free)
r(1) = exp (- lx)
factor = 1
end subroutine map_on_shell_single

subroutine map_on_shell_single_inverse (r, factor, p, lm2, x_free)
real(default), dimension(1), intent(in) :: r
real(default), intent(out) :: factor
real(default), dimension(1), intent(out) :: p
real(default), intent(in) :: lm2
real(default), intent(in), optional :: x_free

```

```

real(default) :: lx
lx = lm2; if (present (x_free)) lx = lx + log (x_free)
p(1) = 0
factor = 1
end subroutine map_on_shell_single_inverse

```

Mapping for a Breit-Wigner resonance

This is the standard Breit-Wigner mapping. We apply it to a single variable, independently of or in addition to a unit-square mapping. We assume here that the limits for the variable are 0 and 1, and that the mass m and width w are rescaled appropriately, so they are dimensionless and usually between 0 and 1.

If `x_free` is set, it rescales the total energy and thus mass and width, since these are defined with respect to the total energy.

(SF mappings: procedures)+≡

```

subroutine map_breit_wigner (r, factor, p, m, w, x_free)
  real(default), intent(out) :: r
  real(default), intent(out) :: factor
  real(default), intent(in) :: p
  real(default), intent(in) :: m
  real(default), intent(in) :: w
  real(default), intent(in), optional :: x_free
  real(default) :: m2, mw, a1, a2, a3, z, tmp
  m2 = m ** 2
  mw = m * w
  if (present (x_free)) then
    m2 = m2 / x_free
    mw = mw / x_free
  end if
  a1 = atan (- m2 / mw)
  a2 = atan ((1 - m2) / mw)
  a3 = (a2 - a1) * mw
  z = (1-p) * a1 + p * a2
  if (-pi/2 < z .and. z < pi/2) then
    tmp = tan (z)
    r = max (m2 + mw * tmp, 0._default)
    factor = a3 * (1 + tmp ** 2)
  else
    r = 0
    factor = 0
  end if
end subroutine map_breit_wigner

subroutine map_breit_wigner_inverse (r, factor, p, m, w, x_free)
  real(default), intent(in) :: r
  real(default), intent(out) :: factor
  real(default), intent(out) :: p
  real(default), intent(in) :: m
  real(default), intent(in) :: w
  real(default) :: m2, mw, a1, a2, a3, tmp
  real(default), intent(in), optional :: x_free
  m2 = m ** 2

```

```

mw = m * w
if (present (x_free)) then
  m2 = m2 / x_free
  mw = mw / x_free
end if
a1 = atan (- m2 / mw)
a2 = atan ((1 - m2) / mw)
a3 = (a2 - a1) * mw
tmp = (r - m2) / mw
p = (atan (tmp) - a1) / (a2 - a1)
factor = a3 * (1 + tmp ** 2)
end subroutine map_breit_wigner_inverse

```

Mapping with endpoint enhancement

This is a mapping which is close to the unit mapping, except that at the endpoint(s), the output values are exponentially enhanced.

$$y = \tanh(a \tan(\frac{\pi}{2}x)) \quad (16.24)$$

We have two variants: one covers endpoints at 0 and 1 symmetrically, while the other one (which essentially maps one-half of the range), covers only the endpoint at 1.

```

<SF mappings: procedures>+≡
subroutine map_endpoint_1 (x3, factor, x1, a)
  real(default), intent(out) :: x3, factor
  real(default), intent(in) :: x1
  real(default), intent(in) :: a
  real(default) :: x2
  if (abs (x1) < 1) then
    x2 = tan (x1 * pi / 2)
    x3 = tanh (a * x2)
    factor = a * pi/2 * (1 + x2 ** 2) * (1 - x3 ** 2)
  else
    x3 = x1
    factor = 0
  end if
end subroutine map_endpoint_1

subroutine map_endpoint_inverse_1 (x3, factor, x1, a)
  real(default), intent(in) :: x3
  real(default), intent(out) :: x1, factor
  real(default), intent(in) :: a
  real(default) :: x2
  if (abs (x3) < 1) then
    x2 = atanh (x3) / a
    x1 = 2 / pi * atan (x2)
    factor = a * pi/2 * (1 + x2 ** 2) * (1 - x3 ** 2)
  else
    x1 = x3
    factor = 0
  end if

```

```

end subroutine map_endpoint_inverse_1

subroutine map_endpoint_01 (x4, factor, x0, a)
  real(default), intent(out) :: x4, factor
  real(default), intent(in) :: x0
  real(default), intent(in) :: a
  real(default) :: x1, x3
  x1 = 2 * x0 - 1
  call map_endpoint_1 (x3, factor, x1, a)
  x4 = (x3 + 1) / 2
end subroutine map_endpoint_01

subroutine map_endpoint_inverse_01 (x4, factor, x0, a)
  real(default), intent(in) :: x4
  real(default), intent(out) :: x0, factor
  real(default), intent(in) :: a
  real(default) :: x1, x3
  x3 = 2 * x4 - 1
  call map_endpoint_inverse_1 (x3, factor, x1, a)
  x0 = (x1 + 1) / 2
end subroutine map_endpoint_inverse_01

```

Mapping with endpoint enhancement (ISR)

This is another endpoint mapping. It is designed to flatten the ISR singularity which is of power type at $x = 1$, i.e., if

$$\sigma = \int_0^1 dx f(x) G(x) = \int_0^1 dx \epsilon (1-x)^{-1+\epsilon} G(x), \quad (16.25)$$

we replace this by

$$r = x^\epsilon \implies \sigma = \int_0^1 dr G(1 - (1-r)^{1/\epsilon}). \quad (16.26)$$

We expect that ϵ is small.

The actual mapping is $r \rightarrow x$ (so x emerges closer to 1). The Jacobian that we return is thus $1/f(x)$. We compute the mapping in terms of $\bar{x} \equiv 1 - x$, so we can achieve the required precision. Because some compilers show quite wild numeric fluctuations, we internally convert numeric types to explicit `double` precision.

```

<SF mappings: public>+≡
  public :: map_power_1
  public :: map_power_inverse_1

<SF mappings: procedures>+≡
  subroutine map_power_1 (xb, factor, rb, eps)
    real(default), intent(out) :: xb, factor
    real(default), intent(in) :: rb
    real(double) :: rb_db, factor_db, eps_db, xb_db
    real(default), intent(in) :: eps
    rb_db = real (rb, kind=double)
    eps_db = real (eps, kind=double)

```

```

xb_db = rb_db ** (1 / eps_db)
if (rb_db > 0) then
    factor_db = xb_db / rb_db / eps_db
    factor = real (factor_db, kind=default)
else
    factor = 0
end if
xb = real (xb_db, kind=default)
end subroutine map_power_1

subroutine map_power_inverse_1 (xb, factor, rb, eps)
    real(default), intent(in) :: xb
    real(default), intent(out) :: rb, factor
    real(double) :: xb_db, factor_db, eps_db, rb_db
    real(default), intent(in) :: eps
    xb_db = real (xb, kind=double)
    eps_db = real (eps, kind=double)
    rb_db = xb_db ** eps_db
    if (xb_db > 0) then
        factor_db = xb_db / rb_db / eps_db
        factor = real (factor_db, kind=default)
    else
        factor = 0
    end if
    rb = real (rb_db, kind=default)
end subroutine map_power_inverse_1

```

Here we apply a power mapping to both endpoints. We divide the interval in two equal halves and apply the power mapping for the nearest endpoint, either 0 or 1.

(SF mappings: procedures) + \equiv

```

subroutine map_power_01 (y, yb, factor, r, eps)
    real(default), intent(out) :: y, yb, factor
    real(default), intent(in) :: r
    real(default), intent(in) :: eps
    real(default) :: u, ub, zp, zm
    u = 2 * r - 1
    if (u > 0) then
        ub = 2 * (1 - r)
        call map_power_1 (zm, factor, ub, eps)
        zp = 2 - zm
    else if (u < 0) then
        ub = 2 * r
        call map_power_1 (zp, factor, ub, eps)
        zm = 2 - zp
    else
        factor = 1 / eps
        zp = 1
        zm = 1
    end if
    y = zp / 2
    yb = zm / 2
end subroutine map_power_01

```



```

subroutine map_power_inverse_01 (y, yb, factor, r, eps)
  real(default), intent(in) :: y, yb
  real(default), intent(out) :: r, factor
  real(default), intent(in) :: eps
  real(default) :: ub, zp, zm
  zp = 2 * y
  zm = 2 * yb
  if (zm < zp) then
    call map_power_inverse_1 (zm, factor, ub, eps)
    r = 1 - ub / 2
  else if (zp < zm) then
    call map_power_inverse_1 (zp, factor, ub, eps)
    r = ub / 2
  else
    factor = 1 / eps
    ub = 1
    r = ub / 2
  end if
end subroutine map_power_inverse_01

```

Structure-function channels

A structure-function chain parameterization (channel) may contain a mapping that applies to multiple structure functions. This is described by an extension of the `sf_mapping_t` type. In addition, it may contain mappings that apply to (other) individual structure functions. The details of these mappings are implementation-specific.

The `sf_channel_t` type combines this information. It contains an array of map codes, one for each structure-function entry. The code values are:

none MC input parameters r directly become energy fractions x

single default mapping for a single structure-function entry

multi/s map $r \rightarrow x$ such that one MC input parameter is \hat{s}/s

multi/resonance as before, adapted to s-channel resonance

multi/on-shell as before, adapted to an on-shell particle in the s channel

multi/endpoint like multi/s, but enhance the region near $r_i = 1$

multi/endpoint/res endpoint mapping with resonance

multi/endpoint/os endpoint mapping for on-shell

multi/power/os like multi/endpoint, regulating a power singularity

$\langle SF \text{ mappings: parameters} \rangle \equiv$

```

integer, parameter :: SFMAP_NONE = 0
integer, parameter :: SFMAP_SINGLE = 1
integer, parameter :: SFMAP_MULTI_S = 2
integer, parameter :: SFMAP_MULTI_RES = 3

```

```

integer, parameter :: SFMAP_MULTI_ONS = 4
integer, parameter :: SFMAP_MULTI_EP = 5
integer, parameter :: SFMAP_MULTI_EPR = 6
integer, parameter :: SFMAP_MULTI_EPO = 7
integer, parameter :: SFMAP_MULTI_IP = 8
integer, parameter :: SFMAP_MULTI_IPR = 9
integer, parameter :: SFMAP_MULTI_IPO = 10
integer, parameter :: SFMAP_MULTI_EI = 11
integer, parameter :: SFMAP_MULTI_SRS = 13
integer, parameter :: SFMAP_MULTI_SON = 14

```

Then, it contains an allocatable entry for the multi mapping. This entry holds the MC-parameter indices on which the mapping applies (there may be more than one MC parameter per structure-function entry) and any parameters associated with the mapping.

There can be only one multi-mapping per channel.

```

<SF mappings: public>+≡
  public :: sf_channel_t

<SF mappings: types>+≡
  type :: sf_channel_t
    integer, dimension(:), allocatable :: map_code
    class(sf_mapping_t), allocatable :: multi_mapping
    contains
    <SF mappings: sf channel: TBP>
  end type sf_channel_t

```

The output format prints a single character for each structure-function entry and, if applicable, an account of the mapping parameters.

```

<SF mappings: sf channel: TBP>≡
  procedure :: write => sf_channel_write

<SF mappings: procedures>+≡
  subroutine sf_channel_write (object, unit)
    class(sf_channel_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    if (allocated (object%map_code)) then
      do i = 1, size (object%map_code)
        select case (object%map_code (i))
          case (SFMAP_NONE)
            write (u, "(1x,A)", advance="no") "-"
          case (SFMAP_SINGLE)
            write (u, "(1x,A)", advance="no") "+"
          case (SFMAP_MULTI_S)
            write (u, "(1x,A)", advance="no") "s"
          case (SFMAP_MULTI_RES, SFMAP_MULTI_SRS)
            write (u, "(1x,A)", advance="no") "r"
          case (SFMAP_MULTI_ONS, SFMAP_MULTI_SON)
            write (u, "(1x,A)", advance="no") "o"
          case (SFMAP_MULTI_EP)
            write (u, "(1x,A)", advance="no") "e"

```

```

        case (SFMAP_MULTI_EPR)
            write (u, "(1x,A)", advance="no") "p"
        case (SFMAP_MULTI_EPO)
            write (u, "(1x,A)", advance="no") "q"
        case (SFMAP_MULTI_IP)
            write (u, "(1x,A)", advance="no") "i"
        case (SFMAP_MULTI_IPR)
            write (u, "(1x,A)", advance="no") "i"
        case (SFMAP_MULTI_IPO)
            write (u, "(1x,A)", advance="no") "i"
        case (SFMAP_MULTI_EI)
            write (u, "(1x,A)", advance="no") "i"
        case default
            write (u, "(1x,A)", advance="no") "?"
        end select
    end do
else
    write (u, "(1x,A)", advance="no") "-"
end if
if (allocated (object%multi_mapping)) then
    write (u, "(1x,')'", advance="no")
    call object%multi_mapping%write (u)
else
    write (u, *)
end if
end subroutine sf_channel_write

```

Initializer for a single `sf_channel` object.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: init => sf_channel_init

<SF mappings: procedures>+≡
    subroutine sf_channel_init (channel, n_strfun)
        class(sf_channel_t), intent(out) :: channel
        integer, intent(in) :: n_strfun
        allocate (channel%map_code (n_strfun))
        channel%map_code = SFMAP_NONE
    end subroutine sf_channel_init

```

Assignment. This merely copies intrinsic assignment.

```

<SF mappings: sf channel: TBP>+≡
    generic :: assignment (=) => sf_channel_assign
    procedure :: sf_channel_assign

<SF mappings: procedures>+≡
    subroutine sf_channel_assign (copy, original)
        class(sf_channel_t), intent(out) :: copy
        type(sf_channel_t), intent(in) :: original
        allocate (copy%map_code (size (original%map_code)))
        copy%map_code = original%map_code
        if (allocated (original%multi_mapping)) then
            allocate (copy%multi_mapping, source = original%multi_mapping)
        end if
    end subroutine sf_channel_assign

```

This initializer allocates an array of channels with common number of structure-function entries, therefore it is not a type-bound procedure.

```

<SF mappings: public>+≡
    public :: allocate_sf_channels

<SF mappings: procedures>+≡
    subroutine allocate_sf_channels (channel, n_channel, n_strfun)
        type(sf_channel_t), dimension(:), intent(out), allocatable :: channel
        integer, intent(in) :: n_channel
        integer, intent(in) :: n_strfun
        integer :: c
        allocate (channel (n_channel))
        do c = 1, n_channel
            call channel(c)%init (n_strfun)
        end do
    end subroutine allocate_sf_channels

```

This marks a given subset of indices as single-mapping.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: activate_mapping => sf_channel_activate_mapping

<SF mappings: procedures>+≡
    subroutine sf_channel_activate_mapping (channel, i_sf)
        class(sf_channel_t), intent(inout) :: channel
        integer, dimension(:), intent(in) :: i_sf
        channel%map_code(i_sf) = SFMAP_SINGLE
    end subroutine sf_channel_activate_mapping

```

This sets an s-channel multichannel mapping. The parameter indices are not yet set.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: set_s_mapping => sf_channel_set_s_mapping

<SF mappings: procedures>+≡
    subroutine sf_channel_set_s_mapping (channel, i_sf, power)
        class(sf_channel_t), intent(inout) :: channel
        integer, dimension(:), intent(in) :: i_sf
        real(default), intent(in), optional :: power
        channel%map_code(i_sf) = SFMAP_MULTI_S
        allocate (sf_s_mapping_t :: channel%multi_mapping)
        select type (mapping => channel%multi_mapping)
            type is (sf_s_mapping_t)
                call mapping%init (power)
            end select
    end subroutine sf_channel_set_s_mapping

```

This sets an s-channel resonance multichannel mapping.

```

<SF mappings: sf channel: TBP>+≡
    procedure :: set_res_mapping => sf_channel_set_res_mapping

```

```

<SF mappings: procedures>+≡
subroutine sf_channel_set_res_mapping (channel, i_sf, m, w, single)
  class(sf_channel_t), intent(inout) :: channel
  integer, dimension(:), intent(in) :: i_sf
  real(default), intent(in) :: m, w
  logical, intent(in) :: single
  if (single) then
    channel%map_code(i_sf) = SFMAP_MULTI_SRS
    allocate (sf_res_mapping_single_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_res_mapping_single_t)
      call mapping%init (m, w)
    end select
  else
    channel%map_code(i_sf) = SFMAP_MULTI_RES
    allocate (sf_res_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_res_mapping_t)
      call mapping%init (m, w)
    end select
  end if
end subroutine sf_channel_set_res_mapping

```

This sets an s-channel on-shell multichannel mapping. The length of the `i_sf` array must be 2. (The first parameter actually becomes an irrelevant dummy.)

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_os_mapping => sf_channel_set_os_mapping

<SF mappings: procedures>+≡
subroutine sf_channel_set_os_mapping (channel, i_sf, m, single)
  class(sf_channel_t), intent(inout) :: channel
  integer, dimension(:), intent(in) :: i_sf
  real(default), intent(in) :: m
  logical, intent(in) :: single
  if (single) then
    channel%map_code(i_sf) = SFMAP_MULTI_SON
    allocate (sf_os_mapping_single_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_os_mapping_single_t)
      call mapping%init (m)
    end select
  else
    channel%map_code(i_sf) = SFMAP_MULTI_ONS
    allocate (sf_os_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_os_mapping_t)
      call mapping%init (m)
    end select
  end if
end subroutine sf_channel_set_os_mapping

```

This sets an s-channel endpoint mapping. The parameter a is the slope parameter (default 1); increasing it moves the endpoint region (at $x = 1$ to lower values

in the input parameter. region even more.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_ep_mapping => sf_channel_set_ep_mapping

<SF mappings: procedures>+≡
  subroutine sf_channel_set_ep_mapping (channel, i_sf, a)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    real(default), intent(in), optional :: a
    channel%map_code(i_sf) = SFMAP_MULTI_EP
    allocate (sf_ep_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_ep_mapping_t)
      call mapping%init (a = a)
    end select
  end subroutine sf_channel_set_ep_mapping

```

This sets a resonant endpoint mapping.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_epr_mapping => sf_channel_set_epr_mapping

<SF mappings: procedures>+≡
  subroutine sf_channel_set_epr_mapping (channel, i_sf, a, m, w)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    real(default), intent(in) :: a, m, w
    channel%map_code(i_sf) = SFMAP_MULTI_EPR
    allocate (sf_epr_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_epr_mapping_t)
      call mapping%init (a, m, w)
    end select
  end subroutine sf_channel_set_epr_mapping

```

This sets an on-shell endpoint mapping.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_epo_mapping => sf_channel_set_epo_mapping

<SF mappings: procedures>+≡
  subroutine sf_channel_set_epo_mapping (channel, i_sf, a, m)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    real(default), intent(in) :: a, m
    channel%map_code(i_sf) = SFMAP_MULTI_EPO
    allocate (sf_epo_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_epo_mapping_t)
      call mapping%init (a, m)
    end select
  end subroutine sf_channel_set_epo_mapping

```

This sets an s-channel power mapping, regulating a singularity of type $(1 - x)^{-1+\epsilon}$. The parameter ϵ depends on the structure function.

```

<SF mappings: sf channel: TBP>+≡

```

```

    procedure :: set_ip_mapping => sf_channel_set_ip_mapping
  <SF mappings: procedures>+≡
    subroutine sf_channel_set_ip_mapping (channel, i_sf, eps)
      class(sf_channel_t), intent(inout) :: channel
      integer, dimension(:), intent(in) :: i_sf
      real(default), intent(in), optional :: eps
      channel%map_code(i_sf) = SFMAP_MULTI_IP
      allocate (sf_ip_mapping_t :: channel%multi_mapping)
      select type (mapping => channel%multi_mapping)
        type is (sf_ip_mapping_t)
          call mapping%init (eps)
        end select
      end subroutine sf_channel_set_ip_mapping

```

This sets an s-channel resonant power mapping, regulating a singularity of type $(1-x)^{-1+\epsilon}$ in the presence of an s-channel resonance. The parameter ϵ depends on the structure function.

```

  <SF mappings: sf channel: TBP>+≡
    procedure :: set_ipr_mapping => sf_channel_set_ipr_mapping
  <SF mappings: procedures>+≡
    subroutine sf_channel_set_ipr_mapping (channel, i_sf, eps, m, w)
      class(sf_channel_t), intent(inout) :: channel
      integer, dimension(:), intent(in) :: i_sf
      real(default), intent(in), optional :: eps, m, w
      channel%map_code(i_sf) = SFMAP_MULTI_IPR
      allocate (sf_ipr_mapping_t :: channel%multi_mapping)
      select type (mapping => channel%multi_mapping)
        type is (sf_ipr_mapping_t)
          call mapping%init (eps, m, w)
        end select
      end subroutine sf_channel_set_ipr_mapping

```

This sets an on-shell power mapping, regulating a singularity of type $(1-x)^{-1+\epsilon}$ for the production of a single on-shell particle.. The parameter ϵ depends on the structure function.

```

  <SF mappings: sf channel: TBP>+≡
    procedure :: set_ipo_mapping => sf_channel_set_ipo_mapping
  <SF mappings: procedures>+≡
    subroutine sf_channel_set_ipo_mapping (channel, i_sf, eps, m)
      class(sf_channel_t), intent(inout) :: channel
      integer, dimension(:), intent(in) :: i_sf
      real(default), intent(in), optional :: eps, m
      channel%map_code(i_sf) = SFMAP_MULTI_IPO
      allocate (sf_ipo_mapping_t :: channel%multi_mapping)
      select type (mapping => channel%multi_mapping)
        type is (sf_ipo_mapping_t)
          call mapping%init (eps, m)
        end select
      end subroutine sf_channel_set_ipo_mapping

```

This sets a combined endpoint/ISR mapping.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_ei_mapping => sf_channel_set_ei_mapping

<SF mappings: procedures>+≡
  subroutine sf_channel_set_ei_mapping (channel, i_sf, a, eps)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    real(default), intent(in), optional :: a, eps
    channel%map_code(i_sf) = SFMAP_MULTI_EI
    allocate (sf_ei_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_ei_mapping_t)
      call mapping%init (a, eps)
    end select
  end subroutine sf_channel_set_ei_mapping

```

This sets a combined endpoint/ISR mapping with resonance.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_eir_mapping => sf_channel_set_eir_mapping

<SF mappings: procedures>+≡
  subroutine sf_channel_set_eir_mapping (channel, i_sf, a, eps, m, w)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    real(default), intent(in), optional :: a, eps, m, w
    channel%map_code(i_sf) = SFMAP_MULTI_EI
    allocate (sf_eir_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_eir_mapping_t)
      call mapping%init (a, eps, m, w)
    end select
  end subroutine sf_channel_set_eir_mapping

```

This sets a combined endpoint/ISR mapping, on-shell.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: set_eio_mapping => sf_channel_set_eio_mapping

<SF mappings: procedures>+≡
  subroutine sf_channel_set_eio_mapping (channel, i_sf, a, eps, m)
    class(sf_channel_t), intent(inout) :: channel
    integer, dimension(:), intent(in) :: i_sf
    real(default), intent(in), optional :: a, eps, m
    channel%map_code(i_sf) = SFMAP_MULTI_EI
    allocate (sf_eio_mapping_t :: channel%multi_mapping)
    select type (mapping => channel%multi_mapping)
    type is (sf_eio_mapping_t)
      call mapping%init (a, eps, m)
    end select
  end subroutine sf_channel_set_eio_mapping

```

Return true if the mapping code at position i_sf is SFMAP_SINGLE.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: is_single_mapping => sf_channel_is_single_mapping

```



```

<SF mappings: procedures>+≡
function sf_channel_is_single_mapping (channel, i_sf) result (flag)
  class(sf_channel_t), intent(in) :: channel
  integer, intent(in) :: i_sf
  logical :: flag
  flag = channel%map_code(i_sf) == SFMAP_SINGLE
end function sf_channel_is_single_mapping

```

Return true if the mapping code at position `i_sf` is any of the `SFMAP_MULTI` mappings.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: is_multi_mapping => sf_channel_is_multi_mapping

<SF mappings: procedures>+≡
function sf_channel_is_multi_mapping (channel, i_sf) result (flag)
  class(sf_channel_t), intent(in) :: channel
  integer, intent(in) :: i_sf
  logical :: flag
  select case (channel%map_code(i_sf))
  case (SFMAP_NONE, SFMAP_SINGLE)
    flag = .false.
  case default
    flag = .true.
  end select
end function sf_channel_is_multi_mapping

```

Return the number of parameters that the multi-mapping requires. The mapping object must be allocated.

```

<SF mappings: sf channel: TBP>+≡
  procedure :: get_multi_mapping_n_par => sf_channel_get_multi_mapping_n_par

<SF mappings: procedures>+≡
function sf_channel_get_multi_mapping_n_par (channel) result (n_par)
  class(sf_channel_t), intent(in) :: channel
  integer :: n_par
  if (allocated (channel%multi_mapping)) then
    n_par = channel%multi_mapping%get_n_dim ()
  else
    n_par = 0
  end if
end function sf_channel_get_multi_mapping_n_par

```

Return true if there is any nontrivial mapping in any of the channels.

```

<SF mappings: public>+≡
  public :: any_sf_channel_has_mapping

<SF mappings: procedures>+≡
function any_sf_channel_has_mapping (channel) result (flag)
  type(sf_channel_t), dimension(:), intent(in) :: channel
  logical :: flag
  integer :: c
  flag = .false.
  do c = 1, size (channel)

```

```

        flag = flag .or. any (channel(c)%map_code /= SFMAP_NONE)
    end do
end function any_sf_channel_has_mapping

```

Set a parameter index for an active multi mapping. We assume that the index array is allocated properly.

```

⟨SF mappings: sf channel: TBP⟩+≡
    procedure :: set_par_index => sf_channel_set_par_index

⟨SF mappings: procedures⟩+≡
    subroutine sf_channel_set_par_index (channel, j, i_par)
        class(sf_channel_t), intent(inout) :: channel
        integer, intent(in) :: j
        integer, intent(in) :: i_par
        associate (mapping => channel%multi_mapping)
            if (j >= 1 .and. j <= mapping%get_n_dim ()) then
                if (mapping%get_index (j) == 0) then
                    call channel%multi_mapping%set_index (j, i_par)
                else
                    call msg_bug ("Structure-function setup: mapping index set twice")
                end if
            else
                call msg_bug ("Structure-function setup: mapping index out of range")
            end if
        end associate
    end subroutine sf_channel_set_par_index

```

16.4.18 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sf_mappings_ut.f90⟩≡
    ⟨File header⟩

    module sf_mappings_ut
        use unit_tests
        use sf_mappings_uti

    ⟨Standard module head⟩

    ⟨SF mappings: public test⟩

    contains

    ⟨SF mappings: test driver⟩

    end module sf_mappings_ut

⟨sf_mappings_uti.f90⟩≡
    ⟨File header⟩

    module sf_mappings_uti

```

```

    <Use kinds>
    use format_defs, only: FMT_11, FMT_12, FMT_13, FMT_14, FMT_15, FMT_16

    use sf_mappings

    <Standard module head>

    <SF mappings: test declarations>

contains

    <SF mappings: tests>

end module sf_mappings_util
API: driver for the unit tests below.
<SF mappings: public test>≡
    public :: sf_mappings_test
<SF mappings: test driver>≡
    subroutine sf_mappings_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <SF mappings: execute tests>
end subroutine sf_mappings_test

```

Check standard mapping

Probe the standard mapping of the unit square for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>≡
    call test (sf_mappings_1, "sf_mappings_1", &
        "standard pair mapping", &
        u, results)
<SF mappings: test declarations>≡
    public :: sf_mappings_1
<SF mappings: tests>≡
    subroutine sf_mappings_1 (u)
        integer, intent(in) :: u
        class(sf_mapping_t), allocatable :: mapping
        real(default), dimension(2) :: p

        write (u, "(A)")  "* Test output: sf_mappings_1"
        write (u, "(A)")  "*   Purpose: probe standard mapping"
        write (u, "(A)")

        allocate (sf_s_mapping_t :: mapping)
        select type (mapping)
        type is (sf_s_mapping_t)
            call mapping%init ()
            call mapping%set_index (1, 1)

```

```

        call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)") "Probe at (0,0):"
    p = [0._default, 0._default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)") "Probe at (0.5,0.5):"
    p = [0.5_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)") "Probe at (0.1,0.5):"
    p = [0.1_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)") "Probe at (0.1,0.1):"
    p = [0.1_default, 0.1_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)") "Compute integral:"
    write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

    deallocate (mapping)
    allocate (sf_s_mapping_t :: mapping)
    select type (mapping)
    type is (sf_s_mapping_t)
        call mapping%init (power=2._default)
        call mapping%set_index (1, 1)
        call mapping%set_index (2, 2)
    end select

    write (u, *)
    call mapping%write (u)

    write (u, *)
    write (u, "(A)") "Probe at (0,0):"
    p = [0._default, 0._default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)") "Probe at (0.5,0.5):"
    p = [0.5_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)") "Probe at (0.1,0.5):"
    p = [0.1_default, 0.5_default]

```

```

call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1,0.1):"
p = [0.1_default, 0.1_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_1"

end subroutine sf_mappings_1

```

Channel entries

Construct channel entries and print them.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_2, "sf_mappings_2", &
    "structure-function mapping channels", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_2

<SF mappings: tests>+≡
  subroutine sf_mappings_2 (u)
    integer, intent(in) :: u
    type(sf_channel_t), dimension(:), allocatable :: channel
    integer :: c

    write (u, "(A)") "* Test output: sf_mappings_2"
    write (u, "(A)") "* Purpose: construct and display &
      &mapping-channel objects"
    write (u, "(A)")

    call allocate_sf_channels (channel, n_channel = 8, n_strfun = 2)
    call channel(2)%activate_mapping ([1])
    call channel(3)%set_s_mapping ([1,2])
    call channel(4)%set_s_mapping ([1,2], power=2._default)
    call channel(5)%set_res_mapping ([1,2], m = 0.5_default, w = 0.1_default, single = .false.)
    call channel(6)%set_os_mapping ([1,2], m = 0.5_default, single = .false.)
    call channel(7)%set_res_mapping ([1], m = 0.5_default, w = 0.1_default, single = .true.)
    call channel(8)%set_os_mapping ([1], m = 0.5_default, single = .true.)

    call channel(3)%set_par_index (1, 1)
    call channel(3)%set_par_index (2, 4)

    call channel(4)%set_par_index (1, 1)
    call channel(4)%set_par_index (2, 4)

    call channel(5)%set_par_index (1, 1)

```

```

call channel(5)%set_par_index (2, 3)

call channel(6)%set_par_index (1, 1)
call channel(6)%set_par_index (2, 2)

call channel(7)%set_par_index (1, 1)

call channel(8)%set_par_index (1, 1)

do c = 1, size (channel)
  write (u, "(I0,':')", advance="no")  c
  call channel(c)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_2"

end subroutine sf_mappings_2

```

Check resonance mapping

Probe the resonance mapping of the unit square for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

The resonance mass is at $1/2$ the energy, the width is $1/10$.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_3, "sf_mappings_3", &
    "resonant pair mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_3

<SF mappings: tests>+≡
  subroutine sf_mappings_3 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p

    write (u, "(A)")  "* Test output: sf_mappings_3"
    write (u, "(A)")  "* Purpose: probe resonance pair mapping"
    write (u, "(A)")

    allocate (sf_res_mapping_t :: mapping)
    select type (mapping)
    type is (sf_res_mapping_t)
      call mapping%init (0.5_default, 0.1_default)
      call mapping%set_index (1, 1)
      call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

```

```

write (u, *)
write (u, "(A)") "Probe at (0,0):"
p = [0._default, 0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1,0.5):"
p = [0.1_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1,0.1):"
p = [0.1_default, 0.1_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_3"

end subroutine sf_mappings_3

```

Check on-shell mapping

Probe the on-shell mapping of the unit square for different parameter values. Also calculates integrals. In this case, the Jacobian is constant and given by $|\log m^2|$, so this is also the value of the integral. The factor results from the variable change in the δ function $\delta(m^2 - x_1 x_2)$ which multiplies the cross section for the case at hand.

For the test, the (rescaled) resonance mass is set at $1/2$ the energy.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_4, "sf_mappings_4", &
    "on-shell pair mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_4

<SF mappings: tests>+≡
  subroutine sf_mappings_4 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p

```

```

write (u, "(A)")  "* Test output: sf_mappings_4"
write (u, "(A)")  "* Purpose: probe on-shell pair mapping"
write (u, "(A)")

allocate (sf_os_mapping_t :: mapping)
select type (mapping)
type is (sf_os_mapping_t)
  call mapping%init (0.5_default)
  call mapping%set_index (1, 1)
  call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)")  "Probe at (0,0):"
p = [0._default, 0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Probe at (0,0.1):"
p = [0._default, 0.1_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Probe at (0,1.0):"
p = [0._default, 1.0_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)")  "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_4"

end subroutine sf_mappings_4

```

Check endpoint mapping

Probe the endpoint mapping of the unit square for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>+=
  call test (sf_mappings_5, "sf_mappings_5", &

```



```

        "endpoint pair mapping", &
        u, results)
<SF mappings: test declarations>+≡
    public :: sf_mappings_5
<SF mappings: tests>+≡
    subroutine sf_mappings_5 (u)
        integer, intent(in) :: u
        class(sf_mapping_t), allocatable :: mapping
        real(default), dimension(2) :: p

        write (u, "(A)")  "* Test output: sf_mappings_5"
        write (u, "(A)")  "*   Purpose: probe endpoint pair mapping"
        write (u, "(A)")

        allocate (sf_ep_mapping_t :: mapping)
        select type (mapping)
        type is (sf_ep_mapping_t)
            call mapping%init ()
            call mapping%set_index (1, 1)
            call mapping%set_index (2, 2)
        end select

        call mapping%write (u)

        write (u, *)
        write (u, "(A)")  "Probe at (0,0):"
        p = [0._default, 0._default]
        call mapping%check (u, p, 1-p, "F7.5")

        write (u, *)
        write (u, "(A)")  "Probe at (0.5,0.5):"
        p = [0.5_default, 0.5_default]
        call mapping%check (u, p, 1-p, "F7.5")

        write (u, *)
        write (u, "(A)")  "Probe at (0.1,0.5):"
        p = [0.1_default, 0.5_default]
        call mapping%check (u, p, 1-p, "F7.5")

        write (u, *)
        write (u, "(A)")  "Probe at (0.7,0.2):"
        p = [0.7_default, 0.2_default]
        call mapping%check (u, p, 1-p, "F7.5")

        write (u, *)
        write (u, "(A)")  "Compute integral:"
        write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

        deallocate (mapping)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: sf_mappings_5"

```

```
end subroutine sf_mappings_5
```

Check endpoint resonant mapping

Probe the endpoint mapping with resonance. Also calculates integrals.

```
<SF mappings: execute tests>+≡
  call test (sf_mappings_6, "sf_mappings_6", &
    "endpoint resonant mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_6

<SF mappings: tests>+≡
  subroutine sf_mappings_6 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(2) :: p

    write (u, "(A)")  "* Test output: sf_mappings_6"
    write (u, "(A)")  "* Purpose: probe endpoint resonant mapping"
    write (u, "(A)")

    allocate (sf_epr_mapping_t :: mapping)
    select type (mapping)
    type is (sf_epr_mapping_t)
      call mapping%init (a = 1._default, m = 0.5_default, w = 0.1_default)
      call mapping%set_index (1, 1)
      call mapping%set_index (2, 2)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)")  "Probe at (0,0):"
    p = [0._default, 0._default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0.5,0.5):"
    p = [0.5_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0.1,0.5):"
    p = [0.1_default, 0.5_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0.7,0.2):"
    p = [0.7_default, 0.2_default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
```

```

write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Same mapping without resonance:"
write (u, "(A)")

allocate (sf_epr_mapping_t :: mapping)
select type (mapping)
type is (sf_epr_mapping_t)
  call mapping%init (a = 1._default)
  call mapping%set_index (1, 1)
  call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0,0):"
p = [0._default, 0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1,0.5):"
p = [0.1_default, 0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_6"

end subroutine sf_mappings_6

```

Check endpoint on-shell mapping

Probe the endpoint mapping with an on-shell particle. Also calculates integrals.

```

<SF mappings: execute tests>+≡
    call test (sf_mappings_7, "sf_mappings_7", &
        "endpoint on-shell mapping", &
        u, results)

<SF mappings: test declarations>+≡
    public :: sf_mappings_7

<SF mappings: tests>+≡
    subroutine sf_mappings_7 (u)
        integer, intent(in) :: u
        class(sf_mapping_t), allocatable :: mapping
        real(default), dimension(2) :: p

        write (u, "(A)")  "* Test output: sf_mappings_7"
        write (u, "(A)")  "* Purpose: probe endpoint on-shell mapping"
        write (u, "(A)")

        allocate (sf_epo_mapping_t :: mapping)
        select type (mapping)
        type is (sf_epo_mapping_t)
            call mapping%init (a = 1._default, m = 0.5_default)
            call mapping%set_index (1, 1)
            call mapping%set_index (2, 2)
        end select

        call mapping%write (u)

        write (u, *)
        write (u, "(A)")  "Probe at (0,0):"
        p = [0._default, 0._default]
        call mapping%check (u, p, 1-p, "F7.5")

        write (u, *)
        write (u, "(A)")  "Probe at (0.5,0.5):"
        p = [0.5_default, 0.5_default]
        call mapping%check (u, p, 1-p, "F7.5")

        write (u, *)
        write (u, "(A)")  "Probe at (0.1,0.5):"
        p = [0.1_default, 0.5_default]
        call mapping%check (u, p, 1-p, "F7.5")

        write (u, *)
        write (u, "(A)")  "Probe at (0.7,0.2):"
        p = [0.7_default, 0.2_default]
        call mapping%check (u, p, 1-p, "F7.5")

        write (u, *)
        write (u, "(A)")  "Compute integral:"
        write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

        deallocate (mapping)

        write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: sf_mappings_7"

    end subroutine sf_mappings_7

```

Check power mapping

Probe the power mapping of the unit square for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>+≡
    call test (sf_mappings_8, "sf_mappings_8", &
        "power pair mapping", &
        u, results)

<SF mappings: test declarations>+≡
    public :: sf_mappings_8

<SF mappings: tests>+≡
    subroutine sf_mappings_8 (u)
        integer, intent(in) :: u
        class(sf_mapping_t), allocatable :: mapping
        real(default), dimension(2) :: p, pb

        write (u, "(A)")  "* Test output: sf_mappings_8"
        write (u, "(A)")  "* Purpose: probe power pair mapping"
        write (u, "(A)")

        allocate (sf_ip_mapping_t :: mapping)
        select type (mapping)
        type is (sf_ip_mapping_t)
            call mapping%init (eps = 0.1_default)
            call mapping%set_index (1, 1)
            call mapping%set_index (2, 2)
        end select

        call mapping%write (u)

        write (u, *)
        write (u, "(A)")  "Probe at (0,0.5):"
        p = [0._default, 0.5_default]
        pb= [1._default, 0.5_default]
        call mapping%check (u, p, pb, FMT_16)

        write (u, *)
        write (u, "(A)")  "Probe at (0.5,0.5):"
        p = [0.5_default, 0.5_default]
        pb= [0.5_default, 0.5_default]
        call mapping%check (u, p, pb, FMT_16)

        write (u, *)
        write (u, "(A)")  "Probe at (0.9,0.5):"
        p = [0.9_default, 0.5_default]
        pb= [0.1_default, 0.5_default]

```

```

call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
pb= [0.3_default, 0.8_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.8):"
p = [0.7_default, 0.8_default]
pb= [0.3_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.99,0.02):"
p = [0.99_default, 0.02_default]
pb= [0.01_default, 0.98_default]
call mapping%check (u, p, pb, FMT_14, FMT_12)

write (u, *)
write (u, "(A)") "Probe at (0.99,0.98):"
p = [0.99_default, 0.98_default]
pb= [0.01_default, 0.02_default]
call mapping%check (u, p, pb, FMT_14, FMT_12)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_8"

end subroutine sf_mappings_8

```

Check resonant power mapping

Probe the power mapping of the unit square, adapted for an s-channel resonance, for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_9, "sf_mappings_9", &
    "power resonance mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_9

<SF mappings: tests>+≡
  subroutine sf_mappings_9 (u)

```

```

integer, intent(in) :: u
class(sf_mapping_t), allocatable :: mapping
real(default), dimension(2) :: p, pb

write (u, "(A)")  "* Test output: sf_mappings_9"
write (u, "(A)")  "* Purpose: probe power resonant pair mapping"
write (u, "(A)")

allocate (sf_ipr_mapping_t :: mapping)
select type (mapping)
type is (sf_ipr_mapping_t)
    call mapping%init (eps = 0.1_default, m = 0.5_default, w = 0.1_default)
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)")  "Probe at (0,0.5):"
p = [0._default, 0.5_default]
pb= [1._default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
pb= [0.5_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.9,0.5):"
p = [0.9_default, 0.5_default]
pb= [0.1_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
pb= [0.3_default, 0.8_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.7,0.8):"
p = [0.7_default, 0.8_default]
pb= [0.3_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.9999,0.02):"
p = [0.9999_default, 0.02_default]
pb= [0.0001_default, 0.98_default]
call mapping%check (u, p, pb, FMT_11, FMT_12)

```

```

write (u, *)
write (u, "(A)") "Probe at (0.9999,0.98):"
p = [0.9999_default, 0.98_default]
pb= [0.0001_default, 0.02_default]
call mapping%check (u, p, pb, FMT_11, FMT_12)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Same mapping without resonance:"
write (u, "(A)")

allocate (sf_ipr_mapping_t :: mapping)
select type (mapping)
type is (sf_ipr_mapping_t)
    call mapping%init (eps = 0.1_default)
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0,0.5):"
p = [0._default, 0.5_default]
pb= [1._default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.5,0.5):"
p = [0.5_default, 0.5_default]
pb= [0.5_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.9,0.5):"
p = [0.9_default, 0.5_default]
pb= [0.1_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.2):"
p = [0.7_default, 0.2_default]
pb= [0.3_default, 0.8_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7,0.8):"
p = [0.7_default, 0.8_default]
pb= [0.3_default, 0.2_default]

```



```

call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_9"

end subroutine sf_mappings_9

```

Check on-shell power mapping

Probe the power mapping of the unit square, adapted for single-particle production, for different parameter values. Also calculates integrals. For a finite number of bins, they differ slightly from 1, but the result is well-defined because we are not using random points.

```

<SF mappings: execute tests>+≡
call test (sf_mappings_10, "sf_mappings_10", &
  "power on-shell mapping", &
  u, results)

<SF mappings: test declarations>+≡
public :: sf_mappings_10

<SF mappings: tests>+≡
subroutine sf_mappings_10 (u)
  integer, intent(in) :: u
  class(sf_mapping_t), allocatable :: mapping
  real(default), dimension(2) :: p, pb

  write (u, "(A)") "* Test output: sf_mappings_10"
  write (u, "(A)") "* Purpose: probe power on-shell mapping"
  write (u, "(A)")

  allocate (sf_ipo_mapping_t :: mapping)
  select type (mapping)
  type is (sf_ipo_mapping_t)
    call mapping%init (eps = 0.1_default, m = 0.5_default)
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
  end select

  call mapping%write (u)

  write (u, *)
  write (u, "(A)") "Probe at (0,0.5):"
  p = [0._default, 0.5_default]
  pb= [1._default, 0.5_default]
  call mapping%check (u, p, pb, FMT_16)

```

```

write (u, *)
write (u, "(A)") "Probe at (0,0.02):"
p = [0._default, 0.02_default]
pb= [1._default, 0.98_default]
call mapping%check (u, p, pb, FMT_15, FMT_12)

write (u, *)
write (u, "(A)") "Probe at (0,0.98):"
p = [0._default, 0.98_default]
pb= [1._default, 0.02_default]
call mapping%check (u, p, pb, FMT_15, FMT_12)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_10"

end subroutine sf_mappings_10

```

Check combined endpoint-power mapping

Probe the mapping for the beamstrahlung/ISR combination.

```

<SF mappings: execute tests>+≡
call test (sf_mappings_11, "sf_mappings_11", &
  "endpoint/power combined mapping", &
  u, results)

<SF mappings: test declarations>+≡
public :: sf_mappings_11

<SF mappings: tests>+≡
subroutine sf_mappings_11 (u)
  integer, intent(in) :: u
  class(sf_mapping_t), allocatable :: mapping
  real(default), dimension(4) :: p, pb

  write (u, "(A)") "* Test output: sf_mappings_11"
  write (u, "(A)") "* Purpose: probe power pair mapping"
  write (u, "(A)")

  allocate (sf_ei_mapping_t :: mapping)
  select type (mapping)
  type is (sf_ei_mapping_t)
    call mapping%init (eps = 0.1_default)
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
    call mapping%set_index (3, 3)
    call mapping%set_index (4, 4)
  end select

```

```

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0.5, 0.5, 0.5, 0.5):"
p = [0.5_default, 0.5_default, 0.5_default, 0.5_default]
pb= [0.5_default, 0.5_default, 0.5_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7, 0.2, 0.4, 0.8):"
p = [0.7_default, 0.2_default, 0.4_default, 0.8_default]
pb= [0.3_default, 0.8_default, 0.6_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.9, 0.06, 0.95, 0.1):"
p = [0.9_default, 0.06_default, 0.95_default, 0.1_default]
pb= [0.1_default, 0.94_default, 0.05_default, 0.9_default]
call mapping%check (u, p, pb, FMT_13, FMT_12)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_11"

end subroutine sf_mappings_11

```

Check resonant endpoint-power mapping

Probe the mapping for the beamstrahlung/ISR combination.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_12, "sf_mappings_12", &
    "endpoint/power resonant combined mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_12

<SF mappings: tests>+≡
  subroutine sf_mappings_12 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(4) :: p, pb

    write (u, "(A)") "* Test output: sf_mappings_12"
    write (u, "(A)") "* Purpose: probe resonant combined mapping"
    write (u, "(A)")

    allocate (sf_eir_mapping_t :: mapping)
    select type (mapping)

```

```

type is (sf_eir_mapping_t)
  call mapping%init (a = 1._default, &
    eps = 0.1_default, m = 0.5_default, w = 0.1_default)
  call mapping%set_index (1, 1)
  call mapping%set_index (2, 2)
  call mapping%set_index (3, 3)
  call mapping%set_index (4, 4)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)") "Probe at (0.5, 0.5, 0.5, 0.5):"
p = [0.5_default, 0.5_default, 0.5_default, 0.5_default]
pb= [0.5_default, 0.5_default, 0.5_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.7, 0.2, 0.4, 0.8):"
p = [0.7_default, 0.2_default, 0.4_default, 0.8_default]
pb= [0.3_default, 0.8_default, 0.6_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)") "Probe at (0.9, 0.06, 0.95, 0.1):"
p = [0.9_default, 0.06_default, 0.95_default, 0.1_default]
pb= [0.1_default, 0.94_default, 0.05_default, 0.9_default]
call mapping%check (u, p, pb, FMT_15, FMT_12)

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_12"

end subroutine sf_mappings_12

```

Check on-shell endpoint-power mapping

Probe the mapping for the beamstrahlung/ISR combination.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_13, "sf_mappings_13", &
    "endpoint/power on-shell combined mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_13

<SF mappings: tests>+≡
  subroutine sf_mappings_13 (u)
    integer, intent(in) :: u

```

```

class(sf_mapping_t), allocatable :: mapping
real(default), dimension(4) :: p, pb

write (u, "(A)")  "* Test output: sf_mappings_13"
write (u, "(A)")  "* Purpose: probe on-shell combined mapping"
write (u, "(A)")

allocate (sf_eio_mapping_t :: mapping)
select type (mapping)
type is (sf_eio_mapping_t)
    call mapping%init (a = 1._default, eps = 0.1_default, m = 0.5_default)
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
    call mapping%set_index (3, 3)
    call mapping%set_index (4, 4)
end select

call mapping%write (u)

write (u, *)
write (u, "(A)")  "Probe at (0.5, 0.5, 0.5, 0.5):"
p = [0.5_default, 0.5_default, 0.5_default, 0.5_default]
pb= [0.5_default, 0.5_default, 0.5_default, 0.5_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.7, 0.2, 0.4, 0.8):"
p = [0.7_default, 0.2_default, 0.4_default, 0.8_default]
pb= [0.3_default, 0.8_default, 0.6_default, 0.2_default]
call mapping%check (u, p, pb, FMT_16)

write (u, *)
write (u, "(A)")  "Probe at (0.9, 0.06, 0.95, 0.1):"
p = [0.9_default, 0.06_default, 0.95_default, 0.1_default]
pb= [0.1_default, 0.94_default, 0.05_default, 0.9_default]
call mapping%check (u, p, pb, FMT_14, FMT_12)

write (u, *)
write (u, "(A)")  "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_13"

end subroutine sf_mappings_13

```

Check rescaling

Check the rescaling factor in on-shell basic mapping.

<SF mappings: execute tests>+≡

```

call test (sf_mappings_14, "sf_mappings_14", &
          "rescaled on-shell mapping", &
          u, results)

<SF mappings: test declarations>+≡
public :: sf_mappings_14

<SF mappings: tests>+≡
subroutine sf_mappings_14 (u)
  integer, intent(in) :: u
  real(default), dimension(2) :: p2, r2
  real(default), dimension(1) :: p1, r1
  real(default) :: f, x_free, m2

  write (u, "(A)")  "* Test output: sf_mappings_14"
  write (u, "(A)")  "* Purpose: probe rescaling in os mapping"
  write (u, "(A)")

  x_free = 0.9_default
  m2 = 0.5_default

  write (u, "(A)")  "* Two parameters"
  write (u, "(A)")

  p2 = [0.1_default, 0.2_default]

  call map_on_shell (r2, f, p2, -log (m2), x_free)

  write (u, "(A,9(1x," // FMT_14 // "))") "p =", p2
  write (u, "(A,9(1x," // FMT_14 // "))") "r =", r2
  write (u, "(A,9(1x," // FMT_14 // "))") "f =", f
  write (u, "(A,9(1x," // FMT_14 // "))") "*r=", x_free * product (r2)

  write (u, *)

  call map_on_shell_inverse (r2, f, p2, -log (m2), x_free)

  write (u, "(A,9(1x," // FMT_14 // "))") "p =", p2
  write (u, "(A,9(1x," // FMT_14 // "))") "r =", r2
  write (u, "(A,9(1x," // FMT_14 // "))") "f =", f
  write (u, "(A,9(1x," // FMT_14 // "))") "*r=", x_free * product (r2)

  write (u, "(A)")
  write (u, "(A)")  "* One parameter"
  write (u, "(A)")

  p1 = [0.1_default]

  call map_on_shell_single (r1, f, p1, -log (m2), x_free)

  write (u, "(A,9(1x," // FMT_14 // "))") "p =", p1
  write (u, "(A,9(1x," // FMT_14 // "))") "r =", r1
  write (u, "(A,9(1x," // FMT_14 // "))") "f =", f
  write (u, "(A,9(1x," // FMT_14 // "))") "*r=", x_free * product (r1)

```

```

write (u, *)

call map_on_shell_single_inverse (r1, f, p1, -log (m2), x_free)

write (u, "(A,9(1x," // FMT_14 // "))") "p =", p1
write (u, "(A,9(1x," // FMT_14 // "))") "r =", r1
write (u, "(A,9(1x," // FMT_14 // "))") "f =", f
write (u, "(A,9(1x," // FMT_14 // "))") "*r=", x_free * product (r1)

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_mappings_14"

end subroutine sf_mappings_14

```

Check single parameter resonance mapping

Probe the resonance mapping of the unit interval for different parameter values.
Also calculates integrals.

The resonance mass is at $1/2$ the energy, the width is $1/10$.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_15, "sf_mappings_15", &
    "resonant single mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_15

<SF mappings: tests>+≡
  subroutine sf_mappings_15 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(1) :: p

    write (u, "(A)")  "* Test output: sf_mappings_15"
    write (u, "(A)")  "* Purpose: probe resonance single mapping"
    write (u, "(A)")

    allocate (sf_res_mapping_single_t :: mapping)
    select type (mapping)
    type is (sf_res_mapping_single_t)
      call mapping%init (0.5_default, 0.1_default)
      call mapping%set_index (1, 1)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)")  "Probe at (0):"
    p = [0._default]
    call mapping%check (u, p, 1-p, "F7.5")

    write (u, *)
    write (u, "(A)")  "Probe at (0.5):"

```

```

p = [0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.1):"
p = [0.1_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)")  "** Test output end: sf_mappings_15"

end subroutine sf_mappings_15

```

Check single parameter on-shell mapping

Probe the on-shell (pseudo) mapping of the unit interval for different parameter values. Also calculates integrals.

The resonance mass is at $1/2$ the energy.

```

<SF mappings: execute tests>+≡
  call test (sf_mappings_16, "sf_mappings_16", &
    "on-shell single mapping", &
    u, results)

<SF mappings: test declarations>+≡
  public :: sf_mappings_16

<SF mappings: tests>+≡
  subroutine sf_mappings_16 (u)
    integer, intent(in) :: u
    class(sf_mapping_t), allocatable :: mapping
    real(default), dimension(1) :: p

    write (u, "(A)")  "** Test output: sf_mappings_16"
    write (u, "(A)")  "** Purpose: probe on-shell single mapping"
    write (u, "(A)")

    allocate (sf_os_mapping_single_t :: mapping)
    select type (mapping)
    type is (sf_os_mapping_single_t)
      call mapping%init (0.5_default)
      call mapping%set_index (1, 1)
    end select

    call mapping%write (u)

    write (u, *)
    write (u, "(A)") "Probe at (0):"

```



```

p = [0._default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Probe at (0.5):"
p = [0.5_default]
call mapping%check (u, p, 1-p, "F7.5")

write (u, *)
write (u, "(A)") "Compute integral:"
write (u, "(3x,A,1x,F7.5)") "I =", mapping%integral (100000)

deallocate (mapping)

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_mappings_16"

end subroutine sf_mappings_16

```

16.5 Structure function base

```

<sf_base.f90>≡
  <File header>

  module sf_base

    <Use kinds>
    <Use strings>
    use io_units
    use format_utils, only: write_separator
    use format_defs, only: FMT_17, FMT_19
    use diagnostics
    use lorentz
    use quantum_numbers
    use interactions
    use evaluators
    use pdg_arrays
    use beams
    use sf_aux
    use sf_mappings
    use constants, only: one, two
    use physics_defs, only: n_beams_rescaled

    <Standard module head>

    <SF base: public>

    <SF base: parameters>

    <SF base: types>

    <SF base: interfaces>

```

```

contains

<SF base: procedures>

end module sf_base

```

16.5.1 Abstract rescale data-type

NLO calculations require the treatment of initial state parton radiation. The radiation of a parton rescales the energy fraction which enters the hard process. We allow for different rescale settings by extending the abstract. `sf_rescale_t` data type.

```

<SF base: public>≡
    public :: sf_rescale_t
<SF base: types>≡
    type, abstract :: sf_rescale_t
        integer :: i_beam = 0
    contains
    <SF base: rescaling function: TBP>
    end type sf_rescale_t

<SF base: rescaling function: TBP>≡
    procedure (sf_rescale_apply), deferred :: apply
<SF base: interfaces>≡
    abstract interface
        subroutine sf_rescale_apply (func, x)
            import
            class(sf_rescale_t), intent(in) :: func
            real(default), intent(inout) :: x
        end subroutine sf_rescale_apply
    end interface

<SF base: rescaling function: TBP>+≡
    procedure :: set_i_beam => sf_rescale_set_i_beam
<SF base: procedures>≡
    subroutine sf_rescale_set_i_beam (func, i_beam)
        class(sf_rescale_t), intent(inout) :: func
        integer, intent(in) :: i_beam
        func%i_beam = i_beam
    end subroutine sf_rescale_set_i_beam

<SF base: public>+≡
    public :: sf_rescale_collinear_t
<SF base: types>+≡
    type, extends (sf_rescale_t) :: sf_rescale_collinear_t
        real(default) :: xi_tilde
    contains
    <SF base: rescale collinear: TBP>
    end type sf_rescale_collinear_t

```

For the subtraction terms we need to rescale the Born x of both beams in the collinear limit. This leaves one beam unaffected and rescales the other according to

$$x = \frac{\bar{x}}{1 - \xi} \quad (16.27)$$

which is the collinear limit of `sf_rescale_real_apply`.

```

<SF base: rescale collinear: TBP>≡
  procedure :: apply => sf_rescale_collinear_apply

<SF base: procedures>+≡
  subroutine sf_rescale_collinear_apply (func, x)
    class(sf_rescale_collinear_t), intent(in) :: func
    real(default), intent(inout) :: x
    real(default) :: xi
    if (debug2_active (D_BEAMS)) then
      print *, 'Rescaling function - Collinear: '
      print *, 'Input, unscaled x: ', x
      print *, 'xi_tilde: ', func%xi_tilde
    end if
    xi = func%xi_tilde * (one - x)
    x = x / (one - xi)
    if (debug2_active (D_BEAMS)) print *, 'rescaled x: ', x
  end subroutine sf_rescale_collinear_apply

<SF base: rescale collinear: TBP>+≡
  procedure :: set => sf_rescale_collinear_set

<SF base: procedures>+≡
  subroutine sf_rescale_collinear_set (func, xi_tilde)
    class(sf_rescale_collinear_t), intent(inout) :: func
    real(default), intent(in) :: xi_tilde
    func%xi_tilde = xi_tilde
  end subroutine sf_rescale_collinear_set

<SF base: public>+≡
  public :: sf_rescale_real_t

<SF base: types>+≡
  type, extends (sf_rescale_t) :: sf_rescale_real_t
    real(default) :: xi, y
  contains
    <SF base: rescale real: TBP>
  end type sf_rescale_real_t

```

In case of IS Splittings, the beam x changes from Born to real and thus needs to be rescaled according to

$$x_{\oplus} = \frac{\bar{x}_{\oplus}}{\sqrt{1 - \xi}} \sqrt{\frac{2 - \xi(1 - y)}{2 - \xi(1 + y)}}, \quad x_{\ominus} = \frac{\bar{x}_{\ominus}}{\sqrt{1 - \xi}} \sqrt{\frac{2 - \xi(1 + y)}{2 - \xi(1 - y)}} \quad (16.28)$$

Refs:

- [0709.2092] Eq. (5.7).

- [0907.4076] Eq. (2.21).
- Christian Weiss' PhD Thesis (DESY-THESIS-2017-025), Eq. (A.2.3).

```

<SF base: rescale real: TBP>≡
  procedure :: apply => sf_rescale_real_apply

<SF base: procedures>+≡
  subroutine sf_rescale_real_apply (func, x)
    class(sf_rescale_real_t), intent(in) :: func
    real(default), intent(inout) :: x
    real(default) :: onepy, onemy
    if (debug2_active (D_BEAMS)) then
      print *, 'Rescaling function - Real: '
      print *, 'Input, unscaled: ', x
      print *, 'Beam index: ', func%i_beam
      print *, 'xi: ', func%xi, 'y: ', func%y
    end if
    x = x / sqrt (one - func%xi)
    onepy = one + func%y; onemy = one - func%y
    if (func%i_beam == 1) then
      x = x * sqrt ((two - func%xi * onemy) / (two - func%xi * onepy))
    else if (func%i_beam == 2) then
      x = x * sqrt ((two - func%xi * onemy) / (two - func%xi * onemy))
    else
      call msg_fatal ("sf_rescale_real_apply - invalid beam index")
    end if
    if (debug2_active (D_BEAMS)) print *, 'rescaled x: ', x
  end subroutine sf_rescale_real_apply

<SF base: rescale real: TBP>+≡
  procedure :: set => sf_rescale_real_set

<SF base: procedures>+≡
  subroutine sf_rescale_real_set (func, xi, y)
    class(sf_rescale_real_t), intent(inout) :: func
    real(default), intent(in) :: xi, y
    func%xi = xi; func%y = y
  end subroutine sf_rescale_real_set

<SF base: public>+≡
  public :: sf_rescale_dglap_t

<SF base: types>+≡
  type, extends(sf_rescale_t) :: sf_rescale_dglap_t
    real(default), dimension(:), allocatable :: z
    contains
    <SF base: rescale dglap: TBP>
  end type sf_rescale_dglap_t

<SF base: rescale dglap: TBP>≡
  procedure :: apply => sf_rescale_dglap_apply

```

```

<SF base: procedures>+=
  subroutine sf_rescale_dglap_apply (func, x)
    class(sf_rescale_dglap_t), intent(in) :: func
    real(default), intent(inout) :: x
    if (debug2_active (D_BEAMS)) then
      print *, "Rescaling function - DGLAP:"
      print *, "Input: ", x
      print *, "Beam index: ", func%i_beam
      print *, "z: ", func%z
    end if
    x = x / func%z(func%i_beam)
    if (debug2_active (D_BEAMS)) print *, "scaled x: ", x
  end subroutine sf_rescale_dglap_apply

<SF base: rescale dglap: TBP>+=
  procedure :: set => sf_rescale_dglap_set

<SF base: procedures>+=
  subroutine sf_rescale_dglap_set (func, z)
    class(sf_rescale_dglap_t), intent(inout) :: func
    real(default), dimension(:), intent(in) :: z
    ! allocate-on-assginment
    func%z = z
  end subroutine sf_rescale_dglap_set

```

16.5.2 Abstract structure-function data type

This type should hold all configuration data for a specific type of structure function. The base object is empty; the implementations will fill it.

```

<SF base: public>+=
  public :: sf_data_t

<SF base: types>+=
  type, abstract :: sf_data_t
    contains
    <SF base: sf data: TBP>
  end type sf_data_t

```

Output.

```

<SF base: sf data: TBP>=
  procedure (sf_data_write), deferred :: write

<SF base: interfaces>+=
  abstract interface
    subroutine sf_data_write (data, unit, verbose)
      import
      class(sf_data_t), intent(in) :: data
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: verbose
    end subroutine sf_data_write
  end interface

```

Return true if this structure function is in generator mode. In that case, all parameters are free, otherwise bound. (We do not support mixed cases.) Default is: no generator.

```

<SF base: sf data: TBP>+≡
  procedure :: is_generator => sf_data_is_generator

<SF base: procedures>+≡
  function sf_data_is_generator (data) result (flag)
    class(sf_data_t), intent(in) :: data
    logical :: flag
    flag = .false.
  end function sf_data_is_generator

```

Return the number of input parameters that determine the structure function.

```

<SF base: sf data: TBP>+≡
  procedure (sf_data_get_int), deferred :: get_n_par

<SF base: interfaces>+≡
  abstract interface
    function sf_data_get_int (data) result (n)
      import
      class(sf_data_t), intent(in) :: data
      integer :: n
    end function sf_data_get_int
  end interface

```

Return the outgoing particle PDG codes for the current setup. The codes can be an array of particles, for each beam.

```

<SF base: sf data: TBP>+≡
  procedure (sf_data_get_pdg_out), deferred :: get_pdg_out

<SF base: interfaces>+≡
  abstract interface
    subroutine sf_data_get_pdg_out (data, pdg_out)
      import
      class(sf_data_t), intent(in) :: data
      type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    end subroutine sf_data_get_pdg_out
  end interface

```

Allocate a matching structure function interaction object and properly initialize it.

```

<SF base: sf data: TBP>+≡
  procedure (sf_data_allocate_sf_int), deferred :: allocate_sf_int

<SF base: interfaces>+≡
  abstract interface
    subroutine sf_data_allocate_sf_int (data, sf_int)
      import
      class(sf_data_t), intent(in) :: data
      class(sf_int_t), intent(inout), allocatable :: sf_int
    end subroutine sf_data_allocate_sf_int
  end interface

```

Return the PDF set index, if applicable. We implement a default method which returns zero. The PDF (builtin and LHA) implementations will override this.

```

<SF base: sf data: TBP>+≡
  procedure :: get_pdf_set => sf_data_get_pdf_set

<SF base: procedures>+≡
  elemental function sf_data_get_pdf_set (data) result (pdf_set)
    class(sf_data_t), intent(in) :: data
    integer :: pdf_set
    pdf_set = 0
  end function sf_data_get_pdf_set

```

Return the spectrum file, if applicable. We implement a default method which returns zero. CIRCE1, CIRCE2 and the beam spectrum will override this.

```

<SF base: sf data: TBP>+≡
  procedure :: get_beam_file => sf_data_get_beam_file

<SF base: procedures>+≡
  function sf_data_get_beam_file (data) result (file)
    class(sf_data_t), intent(in) :: data
    type(string_t) :: file
    file = ""
  end function sf_data_get_beam_file

```

16.5.3 Structure-function chain configuration

This is the data type that the `process` module uses for setting up its structure-function chain. For each structure function described by the beam data, there is an entry. The `i` array indicates the beam(s) to which this structure function applies, and the `data` object contains the actual configuration data.

```

<SF base: public>+≡
  public :: sf_config_t

<SF base: types>+≡
  type :: sf_config_t
    integer, dimension(:), allocatable :: i
    class(sf_data_t), allocatable :: data
  contains
    <SF base: sf config: TBP>
  end type sf_config_t

```

Output:

```

<SF base: sf config: TBP>≡
  procedure :: write => sf_config_write

<SF base: procedures>+≡
  subroutine sf_config_write (object, unit, verbose)
    class(sf_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)

```

```

    if (allocated (object%i)) then
        write (u, "(1x,A,2(1x,I0))") "Structure-function configuration: &
            &beam(s)", object%i
        if (allocated (object%data)) &
            call object%data%write (u, verbose = verbose)
    else
        write (u, "(1x,A)") "Structure-function configuration: [undefined]"
    end if
end subroutine sf_config_write

```

Initialize.

```

<SF base: sf config: TBP>+≡
    procedure :: init => sf_config_init

<SF base: procedures>+≡
    subroutine sf_config_init (sf_config, i_beam, sf_data)
        class(sf_config_t), intent(out) :: sf_config
        integer, dimension(:), intent(in) :: i_beam
        class(sf_data_t), intent(in) :: sf_data
        allocate (sf_config%i (size (i_beam)), source = i_beam)
        allocate (sf_config%data, source = sf_data)
    end subroutine sf_config_init

```

Return the PDF set, if any.

```

<SF base: sf config: TBP>+≡
    procedure :: get_pdf_set => sf_config_get_pdf_set

<SF base: procedures>+≡
    elemental function sf_config_get_pdf_set (sf_config) result (pdf_set)
        class(sf_config_t), intent(in) :: sf_config
        integer :: pdf_set
        pdf_set = sf_config%data%get_pdf_set ()
    end function sf_config_get_pdf_set

```

Return the beam spectrum file, if any.

```

<SF base: sf config: TBP>+≡
    procedure :: get_beam_file => sf_config_get_beam_file

<SF base: procedures>+≡
    function sf_config_get_beam_file (sf_config) result (file)
        class(sf_config_t), intent(in) :: sf_config
        type(string_t) :: file
        file = sf_config%data%get_beam_file ()
    end function sf_config_get_beam_file

```

16.5.4 Structure-function instance

The `sf_int_t` data type contains an `interaction_t` object (it is an extension of this type) and a pointer to the `sf_data_t` configuration data. This interaction, or copies of it, is used to implement structure-function kinematics and dynamics in the context of process evaluation.

The status code `status` tells whether the interaction is undefined, has defined kinematics (but matrix elements invalid), or is completely defined. There is also a status code for failure. The implementation is responsible for updating the status.

The entries `mi2`, `mr2`, and `mo2` hold the squared invariant masses of the incoming, radiated, and outgoing particle, respectively. They are supposed to be set upon initialization, but could also be varied event by event.

If the radiated or outgoing mass is nonzero, we may need to apply an on-shell projection. The projection mode is stored as `on_shell_mode`.

The array `beam_index` is the list of beams on which this structure function applies (1, 2, or both). The arrays `incoming`, `radiated`, and `outgoing` contain the indices of the respective particle sets within the interaction, for convenient lookup. The array `par_index` indicates the MC input parameters that this entry will use up in the structure-function chain. The first parameter (or the first two, for a spectrum) in this array determines the momentum fraction and is thus subject to global mappings.

In the abstract base type, we do not implement the data pointer. This allows us to restrict its type in the implementations.

```

<SF base: public>+≡
  public :: sf_int_t

<SF base: types>+≡
  type, abstract, extends (interaction_t) :: sf_int_t
    integer :: status = SF_UNDEFINED
    real(default), dimension(:), allocatable :: mi2
    real(default), dimension(:), allocatable :: mr2
    real(default), dimension(:), allocatable :: mo2
    integer :: on_shell_mode = KEEP_ENERGY
    logical :: qmin_defined = .false.
    logical :: qmax_defined = .false.
    real(default), dimension(:), allocatable :: qmin
    real(default), dimension(:), allocatable :: qmax
    integer, dimension(:), allocatable :: beam_index
    integer, dimension(:), allocatable :: incoming
    integer, dimension(:), allocatable :: radiated
    integer, dimension(:), allocatable :: outgoing
    integer, dimension(:), allocatable :: par_index
    integer, dimension(:), allocatable :: par_primary
  contains
    <SF base: sf_int: TBP>
  end type sf_int_t

```

Status codes. The codes that refer to links, masks, and connections, apply to structure-function chains only.

The status codes are public.

```

<SF base: parameters>≡
  integer, parameter, public :: SF_UNDEFINED = 0
  integer, parameter, public :: SF_INITIAL = 1
  integer, parameter, public :: SF_DONE_LINKS = 2
  integer, parameter, public :: SF_FAILED_MASK = 3
  integer, parameter, public :: SF_DONE_MASK = 4
  integer, parameter, public :: SF_FAILED_CONNECTIONS = 5

```

```

integer, parameter, public :: SF_DONE_CONNECTIONS = 6
integer, parameter, public :: SF_SEED_KINEMATICS = 10
integer, parameter, public :: SF_FAILED_KINEMATICS = 11
integer, parameter, public :: SF_DONE_KINEMATICS = 12
integer, parameter, public :: SF_FAILED_EVALUATION = 13
integer, parameter, public :: SF_EVALUATED = 20

```

Write a string version of the status code:

```

<SF base: procedures>+=
subroutine write_sf_status (status, u)
  integer, intent(in) :: status
  integer, intent(in) :: u
  select case (status)
  case (SF_UNDEFINED)
    write (u, "(1x,'[',A,']')") "undefined"
  case (SF_INITIAL)
    write (u, "(1x,'[',A,']')") "initialized"
  case (SF_DONE_LINKS)
    write (u, "(1x,'[',A,']')") "links set"
  case (SF_FAILED_MASK)
    write (u, "(1x,'[',A,']')") "mask mismatch"
  case (SF_DONE_MASK)
    write (u, "(1x,'[',A,']')") "mask set"
  case (SF_FAILED_CONNECTIONS)
    write (u, "(1x,'[',A,']')") "connections failed"
  case (SF_DONE_CONNECTIONS)
    write (u, "(1x,'[',A,']')") "connections set"
  case (SF_SEED_KINEMATICS)
    write (u, "(1x,'[',A,']')") "incoming momenta set"
  case (SF_FAILED_KINEMATICS)
    write (u, "(1x,'[',A,']')") "kinematics failed"
  case (SF_DONE_KINEMATICS)
    write (u, "(1x,'[',A,']')") "kinematics set"
  case (SF_FAILED_EVALUATION)
    write (u, "(1x,'[',A,']')") "evaluation failed"
  case (SF_EVALUATED)
    write (u, "(1x,'[',A,']')") "evaluated"
  end select
end subroutine write_sf_status

```

This is the basic output routine. Display status and interaction.

```

<SF base: sf int: TBP>=
procedure :: base_write => sf_int_base_write

<SF base: procedures>+=
subroutine sf_int_base_write (object, unit, testflag)
  class(sf_int_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)", advance="no") "SF instance:"
  call write_sf_status (object%status, u)
  if (allocated (object%beam_index)) &

```

```

        write (u, "(3x,A,2(1x,I0))") "beam      =", object%beam_index
if (allocated (object%incoming)) &
    write (u, "(3x,A,2(1x,I0))") "incoming  =", object%incoming
if (allocated (object%radiated)) &
    write (u, "(3x,A,2(1x,I0))") "radiated  =", object%radiated
if (allocated (object%outgoing)) &
    write (u, "(3x,A,2(1x,I0))") "outgoing  =", object%outgoing
if (allocated (object%par_index)) &
    write (u, "(3x,A,2(1x,I0))") "parameter =", object%par_index
if (object%qmin_defined) &
    write (u, "(3x,A,1x," // FMT_19 // ")") "q_min     =", object%qmin
if (object%qmax_defined) &
    write (u, "(3x,A,1x," // FMT_19 // ")") "q_max     =", object%qmax
call object%interaction_t%basic_write (u, testflag = testflag)
end subroutine sf_int_base_write

```

The type string identifies the structure function class, and possibly more details about the structure function.

```

<SF base: sf_int: TBP>+≡
  procedure (sf_int_type_string), deferred :: type_string

<SF base: interfaces>+≡
  abstract interface
    function sf_int_type_string (object) result (string)
      import
      class(sf_int_t), intent(in) :: object
      type(string_t) :: string
    end function sf_int_type_string
  end interface

```

Output of the concrete object. We should not forget to call the output routine for the base type.

```

<SF base: sf_int: TBP>+≡
  procedure (sf_int_write), deferred :: write

<SF base: interfaces>+≡
  abstract interface
    subroutine sf_int_write (object, unit, testflag)
      import
      class(sf_int_t), intent(in) :: object
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: testflag
    end subroutine sf_int_write
  end interface

```

Basic initialization: set the invariant masses for the particles and initialize the interaction. The caller should then add states to the interaction and freeze it.

The dimension of the mask should be equal to the sum of the dimensions of the mass-squared arrays, which determine incoming, radiated, and outgoing particles, respectively.

Optionally, we can define minimum and maximum values for the momentum transfer to the outgoing particle(s). If all masses are zero, this is actually

required for non-collinear splitting.

```

<SF base: sf_int: TBP>+=
  procedure :: base_init => sf_int_base_init

<SF base: procedures>+=
  subroutine sf_int_base_init &
    (sf_int, mask, mi2, mr2, mo2, qmin, qmax, hel_lock)
    class(sf_int_t), intent(out) :: sf_int
    type (quantum_numbers_mask_t), dimension(:), intent(in) :: mask
    real(default), dimension(:), intent(in) :: mi2, mr2, mo2
    real(default), dimension(:), intent(in), optional :: qmin, qmax
    integer, dimension(:), intent(in), optional :: hel_lock
    allocate (sf_int%mi2 (size (mi2)))
    sf_int%mi2 = mi2
    allocate (sf_int%mr2 (size (mr2)))
    sf_int%mr2 = mr2
    allocate (sf_int%mo2 (size (mo2)))
    sf_int%mo2 = mo2
    if (present (qmin)) then
      sf_int%qmin_defined = .true.
      allocate (sf_int%qmin (size (qmin)))
      sf_int%qmin = qmin
    end if
    if (present (qmax)) then
      sf_int%qmax_defined = .true.
      allocate (sf_int%qmax (size (qmax)))
      sf_int%qmax = qmax
    end if
    call sf_int%interaction_t%basic_init &
      (size (mi2), 0, size (mr2) + size (mo2), &
       mask = mask, hel_lock = hel_lock, set_relations = .true.)
  end subroutine sf_int_base_init

```

Set the indices of the incoming, radiated, and outgoing particles, respectively.

```

<SF base: sf_int: TBP>+=
  procedure :: set_incoming => sf_int_set_incoming
  procedure :: set_radiated => sf_int_set_radiated
  procedure :: set_outgoing => sf_int_set_outgoing

<SF base: procedures>+=
  subroutine sf_int_set_incoming (sf_int, incoming)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: incoming
    allocate (sf_int%incoming (size (incoming)))
    sf_int%incoming = incoming
  end subroutine sf_int_set_incoming

  subroutine sf_int_set_radiated (sf_int, radiated)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: radiated
    allocate (sf_int%radiated (size (radiated)))
    sf_int%radiated = radiated
  end subroutine sf_int_set_radiated

```

```

subroutine sf_int_set_outgoing (sf_int, outgoing)
  class(sf_int_t), intent(inout) :: sf_int
  integer, dimension(:), intent(in) :: outgoing
  allocate (sf_int%outgoing (size (outgoing)))
  sf_int%outgoing = outgoing
end subroutine sf_int_set_outgoing

```

Initialization. This proceeds via an abstract data object, which for the actual implementation should have the matching concrete type. Since all implementations have the same signature, we can prepare a deferred procedure. The data object will become the target of a corresponding pointer within the `sf_int_t` implementation.

This should call the previous procedure.

```

⟨SF base: sf_int: TBP⟩+≡
  procedure (sf_int_init), deferred :: init

⟨SF base: interfaces⟩+≡
  abstract interface
    subroutine sf_int_init (sf_int, data)
      import
      class(sf_int_t), intent(out) :: sf_int
      class(sf_data_t), intent(in), target :: data
    end subroutine sf_int_init
  end interface

```

Complete initialization. This routine contains initializations that can only be performed after the interaction object got its final shape, i.e., redundant helicities have been eliminated by matching with beams and process.

The default implementation does nothing.

The `target` attribute is formally required since some overriding implementations use a temporary pointer (iterator) to the state-matrix component. It doesn't appear to make a real difference, though.

```

⟨SF base: sf_int: TBP⟩+≡
  procedure :: setup_constants => sf_int_setup_constants

⟨SF base: procedures⟩+≡
  subroutine sf_int_setup_constants (sf_int)
    class(sf_int_t), intent(inout), target :: sf_int
  end subroutine sf_int_setup_constants

```

Set beam indices, i.e., the beam(s) on which this structure function applies.

```

⟨SF base: sf_int: TBP⟩+≡
  procedure :: set_beam_index => sf_int_set_beam_index

⟨SF base: procedures⟩+≡
  subroutine sf_int_set_beam_index (sf_int, beam_index)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: beam_index
    allocate (sf_int%beam_index (size (beam_index)))
    sf_int%beam_index = beam_index
  end subroutine sf_int_set_beam_index

```

Set parameter indices, indicating which MC input parameters are to be used for evaluating this structure function.

```

<SF base: sf_int: TBP>+=
  procedure :: set_par_index => sf_int_set_par_index

<SF base: procedures>+=
  subroutine sf_int_set_par_index (sf_int, par_index)
    class(sf_int_t), intent(inout) :: sf_int
    integer, dimension(:), intent(in) :: par_index
    allocate (sf_int%par_index (size (par_index)))
    sf_int%par_index = par_index
  end subroutine sf_int_set_par_index

```

Initialize the structure-function kinematics, setting incoming momenta. We assume that array shapes match.

Three versions. The first version relies on the momenta being linked to another interaction. The second version sets the momenta explicitly. In the third version, we first compute momenta for the specified energies and store those.

```

<SF base: sf_int: TBP>+=
  generic :: seed_kinematics => sf_int_receive_momenta
  generic :: seed_kinematics => sf_int_seed_momenta
  generic :: seed_kinematics => sf_int_seed_energies
  procedure :: sf_int_receive_momenta
  procedure :: sf_int_seed_momenta
  procedure :: sf_int_seed_energies

<SF base: procedures>+=
  subroutine sf_int_receive_momenta (sf_int)
    class(sf_int_t), intent(inout) :: sf_int
    if (sf_int%status >= SF_INITIAL) then
      call sf_int%receive_momenta ()
      sf_int%status = SF_SEED_KINEMATICS
    end if
  end subroutine sf_int_receive_momenta

  subroutine sf_int_seed_momenta (sf_int, k)
    class(sf_int_t), intent(inout) :: sf_int
    type(vector4_t), dimension(:), intent(in) :: k
    if (sf_int%status >= SF_INITIAL) then
      call sf_int%set_momenta (k, outgoing=.false.)
      sf_int%status = SF_SEED_KINEMATICS
    end if
  end subroutine sf_int_seed_momenta

  subroutine sf_int_seed_energies (sf_int, E)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: E
    type(vector4_t), dimension(:), allocatable :: k
    integer :: j
    if (sf_int%status >= SF_INITIAL) then
      allocate (k (size (E)))
      if (all (E**2 >= sf_int%mi2)) then
        do j = 1, size (E)

```

```

        k(j) = vector4_moving (E(j), &
            (3-2*j) * sqrt (E(j)**2 - sf_int%mi2(j)), 3)
    end do
    call sf_int%seed_kinematics (k)
end if
end if
end subroutine sf_int_seed_energies

```

Tell if in generator mode. By default, this is false. To be overridden where appropriate; we may refer to the `is_generator` method of the `data` component in the concrete type.

```

⟨SF base: sf_int: TBP⟩+=
    procedure :: is_generator => sf_int_is_generator

⟨SF base: procedures⟩+=
    function sf_int_is_generator (sf_int) result (flag)
        class(sf_int_t), intent(in) :: sf_int
        logical :: flag
        flag = .false.
    end function sf_int_is_generator

```

Generate free parameters `r`. Parameters are free if they do not correspond to integration parameters (i.e., are bound), but are generated by the structure function object itself. By default, all parameters are bound, and the output values of this procedure will be discarded. With free parameters, we have to override this procedure.

The value `x_free` is the renormalization factor of the total energy that corresponds to the free parameters. If there are no free parameters, the procedure will not change its value, which starts as unity. Otherwise, the fraction is typically decreased, but may also be increased in some cases.

```

⟨SF base: sf_int: TBP⟩+=
    procedure :: generate_free => sf_int_generate_free

⟨SF base: procedures⟩+=
    subroutine sf_int_generate_free (sf_int, r, rb, x_free)
        class(sf_int_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
        r = 0
        rb = 1
    end subroutine sf_int_generate_free

```

Complete the structure-function kinematics, derived from an input parameter (array) `r` between 0 and 1. The interaction momenta are calculated, and we return `x` (the momentum fraction), and `f` (the Jacobian factor for the map $r \rightarrow x$), if `map` is set.

If the `map` flag is unset, `r` and `x` values will coincide, and `f` will become unity. If it is set, the structure-function implementation chooses a convenient mapping from `r` to `x` with Jacobian `f`.

In the `inverse_kinematics` variant, we exchange the intent of `x` and `r`. The momenta are calculated only if the optional flag `set_momenta` is present and set.

Internal parameters of `sf_int` are calculated only if the optional flag `set_x` is present and set.

Update 2018-08-22: Throughout this algorithm, we now carry $xb=1-x$ together with x values, as we did for r before. This allows us to handle unstable endpoint numerics wherever necessary. The only place where the changes actually did matter was for inverse kinematics in the ISR setup, with a very soft photon, but it might be most sensible to apply the extension with xb everywhere.

```

(SF base: sf_int: TBP)+≡
  procedure (sf_int_complete_kinematics), deferred :: complete_kinematics
  procedure (sf_int_inverse_kinematics), deferred :: inverse_kinematics

(SF base: interfaces)+≡
  abstract interface
    subroutine sf_int_complete_kinematics (sf_int, x, xb, f, r, rb, map)
      import
      class(sf_int_t), intent(inout) :: sf_int
      real(default), dimension(:), intent(out) :: x
      real(default), dimension(:), intent(out) :: xb
      real(default), intent(out) :: f
      real(default), dimension(:), intent(in) :: r
      real(default), dimension(:), intent(in) :: rb
      logical, intent(in) :: map
    end subroutine sf_int_complete_kinematics
  end interface

  abstract interface
    subroutine sf_int_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
      import
      class(sf_int_t), intent(inout) :: sf_int
      real(default), dimension(:), intent(in) :: x
      real(default), dimension(:), intent(in) :: xb
      real(default), intent(out) :: f
      real(default), dimension(:), intent(out) :: r
      real(default), dimension(:), intent(out) :: rb
      logical, intent(in) :: map
      logical, intent(in), optional :: set_momenta
    end subroutine sf_int_inverse_kinematics
  end interface

```

Single splitting: compute momenta, given x input parameters. We assume that the incoming momentum is set. The status code is set to `SF_FAILED_KINEMATICS` if the x array does not correspond to a valid momentum configuration. Otherwise, it is updated to `SF_DONE_KINEMATICS`.

We force the outgoing particle on-shell. The on-shell projection is determined by the `on_shell_mode`. The radiated particle should already be on shell.

```

(SF base: sf_int: TBP)+≡
  procedure :: split_momentum => sf_int_split_momentum

(SF base: procedures)+≡
  subroutine sf_int_split_momentum (sf_int, x, xb)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb

```



```

type(vector4_t) :: k
type(vector4_t), dimension(2) :: q
type(splitting_data_t) :: sd
real(default) :: E1, E2
logical :: fail
if (sf_int%status >= SF_SEED_KINEMATICS) then
  k = sf_int%get_momentum (1)
  call sd%init (k, &
    sf_int%mi2(1), sf_int%mr2(1), sf_int%mo2(1), &
    collinear = size (x) == 1)
  call sd%set_t_bounds (x(1), xb(1))
  select case (size (x))
  case (1)
  case (3)
    if (sf_int%qmax_defined) then
      if (sf_int%qmin_defined) then
        call sd%sample_t (x(2), &
          t0 = - sf_int%qmax(1) ** 2, t1 = - sf_int%qmin(1) ** 2)
      else
        call sd%sample_t (x(2), &
          t0 = - sf_int%qmax(1) ** 2)
      end if
    else
      if (sf_int%qmin_defined) then
        call sd%sample_t (x(2), t1 = - sf_int%qmin(1) ** 2)
      else
        call sd%sample_t (x(2))
      end if
    end if
    call sd%sample_phi (x(3))
  case default
    call msg_bug ("Structure function: impossible number of parameters")
  end select
  q = sd%split_momentum (k)
  call on_shell (q, [sf_int%mr2, sf_int%mo2], &
    sf_int%on_shell_mode)
  call sf_int%set_momenta (q, outgoing=.true.)
  E1 = energy (q(1))
  E2 = energy (q(2))
  fail = E1 < 0 .or. E2 < 0 &
    .or. E1 ** 2 < sf_int%mr2(1) &
    .or. E2 ** 2 < sf_int%mo2(1)
  if (fail) then
    sf_int%status = SF_FAILED_KINEMATICS
  else
    sf_int%status = SF_DONE_KINEMATICS
  end if
end if
end subroutine sf_int_split_momentum

```

Pair splitting: two incoming momenta, two radiated, two outgoing. This is simple because we insist on all momenta being collinear.

$\langle SF \text{ base: } sf \text{ int: } TBP \rangle + \equiv$

```

    procedure :: split_momenta => sf_int_split_momenta
  (SF base: procedures)+≡
  subroutine sf_int_split_momenta (sf_int, x, xb)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    type(vector4_t), dimension(2) :: k
    type(vector4_t), dimension(4) :: q
    real(default), dimension(4) :: E
    logical :: fail
    if (sf_int%status >= SF_SEED_KINEMATICS) then
      select case (size (x))
      case (2)
      case default
        call msg_bug ("Pair structure function: recoil requested &
          &but not implemented yet")
      end select
      k(1) = sf_int%get_momentum (1)
      k(2) = sf_int%get_momentum (2)
      q(1:2) = xb * k
      q(3:4) = x * k
      select case (size (sf_int%mr2))
      case (2)
        call on_shell (q, &
          [sf_int%mr2(1), sf_int%mr2(2), &
            sf_int%mo2(1), sf_int%mo2(2)], &
          sf_int%on_shell_mode)
        call sf_int%set_momenta (q, outgoing=.true.)
        E = energy (q)
        fail = any (E < 0) &
          .or. any (E(1:2) ** 2 < sf_int%mr2) &
          .or. any (E(3:4) ** 2 < sf_int%mo2)
      case default; call msg_bug ("split momenta: incorrect use")
      end select
      if (fail) then
        sf_int%status = SF_FAILED_KINEMATICS
      else
        sf_int%status = SF_DONE_KINEMATICS
      end if
    end if
  end subroutine sf_int_split_momenta

```

Pair spectrum: the reduced version of the previous splitting, without radiated momenta.

```

  (SF base: sf_int: TBP)+≡
  procedure :: reduce_momenta => sf_int_reduce_momenta
  (SF base: procedures)+≡
  subroutine sf_int_reduce_momenta (sf_int, x)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    type(vector4_t), dimension(2) :: k
    type(vector4_t), dimension(2) :: q
    real(default), dimension(2) :: E

```

```

logical :: fail
if (sf_int%status >= SF_SEED_KINEMATICS) then
  select case (size (x))
  case (2)
  case default
    call msg_bug ("Pair spectrum: recoil requested &
      &but not implemented yet")
  end select
  k(1) = sf_int%get_momentum (1)
  k(2) = sf_int%get_momentum (2)
  q = x * k
  call on_shell (q, &
    [sf_int%mo2(1), sf_int%mo2(2)], &
    sf_int%on_shell_mode)
  call sf_int%set_momenta (q, outgoing=.true.)
  E = energy (q)
  fail = any (E < 0) &
    .or. any (E ** 2 < sf_int%mo2)
  if (fail) then
    sf_int%status = SF_FAILED_KINEMATICS
  else
    sf_int%status = SF_DONE_KINEMATICS
  end if
end if
end subroutine sf_int_reduce_momenta

```

The inverse procedure: we compute the x array from the momentum configuration. In an overriding TBP, we may also set internal data that depend on this, for convenience.

NOTE: Here and above, the single-particle case is treated in detail, allowing for non-collinearity and non-vanishing masses and nontrivial momentum-transfer bounds. For the pair case, we currently implement only collinear splitting and assume massless particles. This should be improved.

Update 2017-08-22: recover also xb , using the updated `recover` method of the `splitting-data` object. Th

```

⟨SF base: sf_int: TBP⟩+=
  procedure :: recover_x => sf_int_recover_x
  procedure :: base_recover_x => sf_int_recover_x

⟨SF base: procedures⟩+=
  subroutine sf_int_recover_x (sf_int, x, xb, x_free)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    type(vector4_t), dimension(:), allocatable :: k
    type(vector4_t), dimension(:), allocatable :: q
    type(splitting_data_t) :: sd
    if (sf_int%status >= SF_SEED_KINEMATICS) then
      allocate (k (sf_int%interaction_t%get_n_in ()))
      allocate (q (sf_int%interaction_t%get_n_out ()))
      k = sf_int%get_momenta (outgoing=.false.)
      q = sf_int%get_momenta (outgoing=.true.)
    end if
  end subroutine

```

```

select case (size (k))
case (1)
  call sd%init (k(1), &
    sf_int%mi2(1), sf_int%mr2(1), sf_int%mo2(1), &
    collinear = size (x) == 1)
  call sd%recover (k(1), q, sf_int%on_shell_mode)
  x(1) = sd%get_x ()
  xb(1) = sd%get_xb ()
  select case (size (x))
  case (1)
  case (3)
    if (sf_int%qmax_defined) then
      if (sf_int%qmin_defined) then
        call sd%inverse_t (x(2), &
          t0 = - sf_int%qmax(1) ** 2, t1 = - sf_int%qmin(1) ** 2)
      else
        call sd%inverse_t (x(2), &
          t0 = - sf_int%qmax(1) ** 2)
      end if
    else
      if (sf_int%qmin_defined) then
        call sd%inverse_t (x(2), t1 = - sf_int%qmin(1) ** 2)
      else
        call sd%inverse_t (x(2))
      end if
    end if
    call sd%inverse_phi (x(3))
    xb(2:3) = 1 - x(2:3)
  case default
    call msg_bug ("Structure function: impossible number &
      &of parameters")
  end select
case (2)
  select case (size (x))
  case (2)
  case default
    call msg_bug ("Pair structure function: recoil requested &
      &but not implemented yet")
  end select
  select case (sf_int%on_shell_mode)
  case (KEEP_ENERGY)
    select case (size (q))
    case (4)
      x = energy (q(3:4)) / energy (k)
      xb= energy (q(1:2)) / energy (k)
    case (2)
      x = energy (q) / energy (k)
      xb= 1 - x
    end select
  case (KEEP_MOMENTUM)
    select case (size (q))
    case (4)
      x = longitudinal_part (q(3:4)) / longitudinal_part (k)
      xb= longitudinal_part (q(1:2)) / longitudinal_part (k)

```

```

        case (2)
            x = longitudinal_part (q) / longitudinal_part (k)
            xb= 1 - x
        end select
    end select
end select
end if
end subroutine sf_int_recover_x

```

Apply the structure function, i.e., evaluate the interaction. For the calculation, we may use the stored momenta, any further information stored inside the `sf_int` implementation during kinematics setup, and the given energy scale. It may happen that for the given kinematics the value is not defined. This should be indicated by the status code.

```

<SF base: sf_int: TBP>+=
    procedure (sf_int_apply), deferred :: apply

<SF base: interfaces>+=
    abstract interface
        subroutine sf_int_apply (sf_int, scale, negative_sf, rescale, i_sub)
            import
            class(sf_int_t), intent(inout) :: sf_int
            real(default), intent(in) :: scale
            logical, intent(in), optional :: negative_sf
            class(sf_rescale_t), intent(in), optional :: rescale
            integer, intent(in), optional :: i_sub
        end subroutine sf_int_apply
    end interface

```

16.5.5 Accessing the structure function

Return metadata. Once `interaction_t` is rewritten in OO, some of this will be inherited.

The number of outgoing particles is equal to the number of incoming particles. The radiated particles are the difference.

```

<SF base: sf_int: TBP>+=
    procedure :: get_n_in => sf_int_get_n_in
    procedure :: get_n_rad => sf_int_get_n_rad
    procedure :: get_n_out => sf_int_get_n_out

<SF base: procedures>+=
    pure function sf_int_get_n_in (object) result (n_in)
        class(sf_int_t), intent(in) :: object
        integer :: n_in
        n_in = object%interaction_t%get_n_in ()
    end function sf_int_get_n_in

    pure function sf_int_get_n_rad (object) result (n_rad)
        class(sf_int_t), intent(in) :: object
        integer :: n_rad
        n_rad = object%interaction_t%get_n_out () &
            - object%interaction_t%get_n_in ()

```

```

end function sf_int_get_n_rad

pure function sf_int_get_n_out (object) result (n_out)
  class(sf_int_t), intent(in) :: object
  integer :: n_out
  n_out = object%interaction_t%get_n_in ()
end function sf_int_get_n_out

```

Number of matrix element entries in the interaction:

```

<SF base: sf_int: TBP>+≡
  procedure :: get_n_states => sf_int_get_n_states

<SF base: procedures>+≡
  function sf_int_get_n_states (sf_int) result (n_states)
    class(sf_int_t), intent(in) :: sf_int
    integer :: n_states
    n_states = sf_int%get_n_matrix_elements ()
  end function sf_int_get_n_states

```

Return a specific state as a quantum-number array.

```

<SF base: sf_int: TBP>+≡
  procedure :: get_state => sf_int_get_state

<SF base: procedures>+≡
  function sf_int_get_state (sf_int, i) result (qn)
    class(sf_int_t), intent(in) :: sf_int
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    integer, intent(in) :: i
    allocate (qn (sf_int%get_n_tot ()))
    qn = sf_int%get_quantum_numbers (i)
  end function sf_int_get_state

```

Return the matrix-element values for all states. We can assume that the matrix elements are real, so we take the real part.

```

<SF base: sf_int: TBP>+≡
  procedure :: get_values => sf_int_get_values

<SF base: procedures>+≡
  subroutine sf_int_get_values (sf_int, value)
    class(sf_int_t), intent(in) :: sf_int
    real(default), dimension(:), intent(out) :: value
    integer :: i
    if (sf_int%status >= SF_EVALUATED) then
      do i = 1, size (value)
        value(i) = real (sf_int%get_matrix_element (i))
      end do
    else
      value = 0
    end if
  end subroutine sf_int_get_values

```

16.5.6 Direct calculations

Compute a structure function value (array) directly, given an array of x values and a scale. If the energy is also given, we initialize the kinematics for that energy, otherwise take it from a previous run.

We assume that the E array has dimension n_in , and the x array has n_par .

Note: the output x values (xx and xxb) are unused in this use case.

```

<SF base: sf_int: TBP>+=
  procedure :: compute_values => sf_int_compute_values

<SF base: procedures>+=
  subroutine sf_int_compute_values (sf_int, value, x, xb, scale, E)
    class(sf_int_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: value
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(in) :: scale
    real(default), dimension(:), intent(in), optional :: E
    real(default), dimension(size (x)) :: xx, xxb
    real(default) :: f
    if (present (E)) call sf_int%seed_kinematics (E)
    if (sf_int%status >= SF_SEED_KINEMATICS) then
      call sf_int%complete_kinematics (xx, xxb, f, x, xb, map=.false.)
      call sf_int%apply (scale)
      call sf_int%get_values (value)
      value = value * f
    else
      value = 0
    end if
  end subroutine sf_int_compute_values

```

Compute just a single value for one of the states, i.e., throw the others away.

```

<SF base: sf_int: TBP>+=
  procedure :: compute_value => sf_int_compute_value

<SF base: procedures>+=
  subroutine sf_int_compute_value &
    (sf_int, i_state, value, x, xb, scale, E)
    class(sf_int_t), intent(inout) :: sf_int
    integer, intent(in) :: i_state
    real(default), intent(out) :: value
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(in) :: scale
    real(default), dimension(:), intent(in), optional :: E
    real(default), dimension(:), allocatable :: value_array
    if (sf_int%status >= SF_INITIAL) then
      allocate (value_array (sf_int%get_n_states ()))
      call sf_int%compute_values (value_array, x, xb, scale, E)
      value = value_array(i_state)
    else
      value = 0
    end if
  end subroutine sf_int_compute_value

```

16.5.7 Structure-function instance

This is a wrapper for `sf_int_t` objects, such that we can build an array with different structure-function types. The structure-function contains an array (a sequence) of `sf_int_t` objects.

The object, it holds the evaluator that connects the preceding part of the structure-function chain to the current interaction.

It also stores the input and output parameter values for the contained structure function. The `r` array has a second dimension, corresponding to the mapping channels in a multi-channel configuration. There is a Jacobian entry `f` for each channel. The corresponding logical array `mapping` tells whether we apply the mapping appropriate for the current structure function in this channel. The `x` parameter values (energy fractions) are common to all channels.

```

⟨SF base: types⟩+≡
  type :: sf_instance_t
    class(sf_int_t), allocatable :: int
    type(enumerator_t) :: eval
    real(default), dimension(:,:), allocatable :: r
    real(default), dimension(:,:), allocatable :: rb
    real(default), dimension(:), allocatable :: f
    logical, dimension(:), allocatable :: m
    real(default), dimension(:), allocatable :: x
    real(default), dimension(:), allocatable :: xb
  end type sf_instance_t

```

16.5.8 Structure-function chain

A chain is an array of structure functions `sf`, initiated by a beam setup. We do not use this directly for evaluation, but create instances with copies of the contained interactions.

`n_par` is the total number of parameters that is necessary for completely determining the structure-function chain. `n_bound` is the number of MC input parameters that are requested from the integrator. The difference of `n_par` and `n_bound` is the number of free parameters, which are generated by a structure-function object in generator mode.

```

⟨SF base: public⟩+≡
  public :: sf_chain_t

⟨SF base: types⟩+≡
  type, extends (beam_t) :: sf_chain_t
    type(beam_data_t), pointer :: beam_data => null ()
    integer :: n_in = 0
    integer :: n_strfun = 0
    integer :: n_par = 0
    integer :: n_bound = 0
    type(sf_instance_t), dimension(:), allocatable :: sf
    logical :: trace_enable = .false.
    integer :: trace_unit = 0
  contains
    ⟨SF base: sf chain: TBP⟩
  end type sf_chain_t

```


Finalizer.

```

<SF base: sf chain: TBP>≡
  procedure :: final => sf_chain_final

<SF base: procedures>+≡
  subroutine sf_chain_final (object)
    class(sf_chain_t), intent(inout) :: object
    integer :: i
    call object%final_tracing ()
    if (allocated (object%sf)) then
      do i = 1, size (object%sf, 1)
        associate (sf => object%sf(i))
          if (allocated (sf%int)) then
            call sf%int%final ()
          end if
        end associate
      end do
    end if
    call beam_final (object%beam_t)
  end subroutine sf_chain_final

```

Output.

```

<SF base: sf chain: TBP>+≡
  procedure :: write => sf_chain_write

<SF base: procedures>+≡
  subroutine sf_chain_write (object, unit)
    class(sf_chain_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Incoming particles / structure-function chain:"
    if (associated (object%beam_data)) then
      write (u, "(3x,A,I0)") "n_in      = ", object%n_in
      write (u, "(3x,A,I0)") "n_strfun  = ", object%n_strfun
      write (u, "(3x,A,I0)") "n_par     = ", object%n_par
      if (object%n_par /= object%n_bound) then
        write (u, "(3x,A,I0)") "n_bound   = ", object%n_bound
      end if
      call object%beam_data%write (u)
      call write_separator (u)
      call beam_write (object%beam_t, u)
      if (allocated (object%sf)) then
        do i = 1, object%n_strfun
          associate (sf => object%sf(i))
            call write_separator (u)
            if (allocated (sf%int)) then
              call sf%int%write (u)
            else
              write (u, "(1x,A)") "SF instance: [undefined]"
            end if
          end associate
        end do
      end if
    end if
  end subroutine sf_chain_write

```

```

else
  write (u, "(3x,A)") "[undefined]"
end if
end subroutine sf_chain_write

```

Initialize: setup beams. The `beam_data` target must remain valid for the lifetime of the chain, since we just establish a pointer. The structure-function configuration array is used to initialize the individual structure-function entries. The target attribute is needed because the `sf_int` entries establish pointers to the configuration data.

```

<SF base: sf chain: TBP>+≡
  procedure :: init => sf_chain_init

<SF base: procedures>+≡
  subroutine sf_chain_init (sf_chain, beam_data, sf_config)
    class(sf_chain_t), intent(out) :: sf_chain
    type(beam_data_t), intent(in), target :: beam_data
    type(sf_config_t), dimension(:), intent(in), optional, target :: sf_config
    integer :: i
    sf_chain%beam_data => beam_data
    sf_chain%n_in = beam_data%get_n_in ()
    call beam_init (sf_chain%beam_t, beam_data)
    if (present (sf_config)) then
      sf_chain%n_strfun = size (sf_config)
      allocate (sf_chain%sf (sf_chain%n_strfun))
      do i = 1, sf_chain%n_strfun
        call sf_chain%set_strfun (i, sf_config(i)%i, sf_config(i)%data)
      end do
    end if
  end subroutine sf_chain_init

```

Receive the beam momenta from a source to which the beam interaction is linked.

```

<SF base: sf chain: TBP>+≡
  procedure :: receive_beam_momenta => sf_chain_receive_beam_momenta

<SF base: procedures>+≡
  subroutine sf_chain_receive_beam_momenta (sf_chain)
    class(sf_chain_t), intent(inout), target :: sf_chain
    type(interaction_t), pointer :: beam_int
    beam_int => sf_chain%get_beam_int_ptr ()
    call beam_int%receive_momenta ()
  end subroutine sf_chain_receive_beam_momenta

```

Explicitly set the beam momenta.

```

<SF base: sf chain: TBP>+≡
  procedure :: set_beam_momenta => sf_chain_set_beam_momenta

<SF base: procedures>+≡
  subroutine sf_chain_set_beam_momenta (sf_chain, p)
    class(sf_chain_t), intent(inout) :: sf_chain
    type(vector4_t), dimension(:), intent(in) :: p
    call beam_set_momenta (sf_chain%beam_t, p)

```

```
end subroutine sf_chain_set_beam_momenta
```

Set a structure-function entry. We use the `data` input to allocate the `int` structure-function instance with appropriate type, then initialize the entry. The entry establishes a pointer to `data`.

The index `i` is the structure-function index in the chain.

```
<SF base: sf chain: TBP>+≡
  procedure :: set_strfun => sf_chain_set_strfun

<SF base: procedures>+≡
  subroutine sf_chain_set_strfun (sf_chain, i, beam_index, data)
    class(sf_chain_t), intent(inout) :: sf_chain
    integer, intent(in) :: i
    integer, dimension(:), intent(in) :: beam_index
    class(sf_data_t), intent(in), target :: data
    integer :: n_par, j
    n_par = data%get_n_par ()
    call data%allocate_sf_int (sf_chain%sf(i)%int)
    associate (sf_int => sf_chain%sf(i)%int)
      call sf_int%init (data)
      call sf_int%set_beam_index (beam_index)
      call sf_int%set_par_index &
        ([ (j, j = sf_chain%n_par + 1, sf_chain%n_par + n_par)])
      sf_chain%n_par = sf_chain%n_par + n_par
      if (.not. data%is_generator ()) then
        sf_chain%n_bound = sf_chain%n_bound + n_par
      end if
    end associate
  end subroutine sf_chain_set_strfun
```

Return the number of structure-function parameters.

```
<SF base: sf chain: TBP>+≡
  procedure :: get_n_par => sf_chain_get_n_par
  procedure :: get_n_bound => sf_chain_get_n_bound

<SF base: procedures>+≡
  function sf_chain_get_n_par (sf_chain) result (n)
    class(sf_chain_t), intent(in) :: sf_chain
    integer :: n
    n = sf_chain%n_par
  end function sf_chain_get_n_par

  function sf_chain_get_n_bound (sf_chain) result (n)
    class(sf_chain_t), intent(in) :: sf_chain
    integer :: n
    n = sf_chain%n_bound
  end function sf_chain_get_n_bound
```

Return a pointer to the beam interaction.

```
<SF base: sf chain: TBP>+≡
  procedure :: get_beam_int_ptr => sf_chain_get_beam_int_ptr
```

```

<SF base: procedures>+=
function sf_chain_get_beam_int_ptr (sf_chain) result (int)
    type(interaction_t), pointer :: int
    class(sf_chain_t), intent(in), target :: sf_chain
    int => beam_get_int_ptr (sf_chain%beam_t)
end function sf_chain_get_beam_int_ptr

```

Enable the trace feature: record structure function data (input parameters, x values, evaluation result) to an external file.

```

<SF base: sf chain: TBP>+=
procedure :: setup_tracing => sf_chain_setup_tracing
procedure :: final_tracing => sf_chain_final_tracing

<SF base: procedures>+=
subroutine sf_chain_setup_tracing (sf_chain, file)
    class(sf_chain_t), intent(inout) :: sf_chain
    type(string_t), intent(in) :: file
    if (sf_chain%n_strfun > 0) then
        sf_chain%trace_enable = .true.
        sf_chain%trace_unit = free_unit ()
        open (sf_chain%trace_unit, file = char (file), action = "write", &
            status = "replace")
        call sf_chain%write_trace_header ()
    else
        call msg_error ("Beam structure: no structure functions, tracing &
            &disabled")
    end if
end subroutine sf_chain_setup_tracing

subroutine sf_chain_final_tracing (sf_chain)
    class(sf_chain_t), intent(inout) :: sf_chain
    if (sf_chain%trace_enable) then
        close (sf_chain%trace_unit)
        sf_chain%trace_enable = .false.
    end if
end subroutine sf_chain_final_tracing

```

Write the header for the tracing file.

```

<SF base: sf chain: TBP>+=
procedure :: write_trace_header => sf_chain_write_trace_header

<SF base: procedures>+=
subroutine sf_chain_write_trace_header (sf_chain)
    class(sf_chain_t), intent(in) :: sf_chain
    integer :: u
    if (sf_chain%trace_enable) then
        u = sf_chain%trace_unit
        write (u, "('# ',A)") "WHIZARD output: &
            &structure-function sampling data"
        write (u, "('# ',A,1x,I0)") "Number of sf records:", sf_chain%n_strfun
        write (u, "('# ',A,1x,I0)") "Number of parameters:", sf_chain%n_par
        write (u, "('# ',A)") "Columns: channel, p(n_par), x(n_par), f, Jac * f"
    end if
end subroutine sf_chain_write_trace_header

```

Write a record which collects the structure function data for the current data point. For the selected channel, we print first the input integration parameters, then the x values, then the structure-function value summed over all quantum numbers, then the structure function value times the mapping Jacobian.

```

<SF base: sf chain: TBP>+≡
  procedure :: trace => sf_chain_trace

<SF base: procedures>+≡
  subroutine sf_chain_trace (sf_chain, c_sel, p, x, f, sf_sum)
    class(sf_chain_t), intent(in) :: sf_chain
    integer, intent(in) :: c_sel
    real(default), dimension(:,:), intent(in) :: p
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: f
    real(default), intent(in) :: sf_sum
    real(default) :: sf_sum_pac, f_sf_sum_pac
    integer :: u, i
    if (sf_chain%trace_enable) then
      u = sf_chain%trace_unit
      write (u, "(1x,I0)", advance="no") c_sel
      write (u, "(2x)", advance="no")
      do i = 1, sf_chain%n_par
        write (u, "(1x," // FMT_17 // ")", advance="no") p(i,c_sel)
      end do
      write (u, "(2x)", advance="no")
      do i = 1, sf_chain%n_par
        write (u, "(1x," // FMT_17 // ")", advance="no") x(i)
      end do
      write (u, "(2x)", advance="no")
      sf_sum_pac = sf_sum
      f_sf_sum_pac = f(c_sel) * sf_sum
      call pacify (sf_sum_pac, 1.E-28_default)
      call pacify (f_sf_sum_pac, 1.E-28_default)
      write (u, "(2(1x," // FMT_17 // "))" sf_sum_pac, f_sf_sum_pac
    end if
  end subroutine sf_chain_trace

```

16.5.9 Chain instances

A structure-function chain instance contains copies of the interactions in the configuration chain, suitably linked to each other and connected by evaluators.

After initialization, `out_sf` should point, for each beam, to the last structure function that affects this beam. `out_sf_i` should indicate the index of the corresponding outgoing particle within that structure-function interaction.

Analogously, `out_eval` is the last evaluator in the structure-function chain, which contains the complete set of outgoing particles. `out_eval_i` should indicate the index of the outgoing particles, within that evaluator, which will initiate the collision.

When calculating actual kinematics, we fill the `p`, `r`, and `x` arrays and the `f` factor. The `p` array denotes the MC input parameters as they come from the

random-number generator. The **r** array results from applying global mappings. The **x** array results from applying structure-function local mappings. The x values can be interpreted directly as momentum fractions (or angle fractions, where recoil is involved). The **f** factor is the Jacobian that results from applying all mappings.

Update 2017-08-22: carry and output all complements (**pb**, **rb**, **xb**). Previously, **xb** was not included in the record, and the output did not contain either. It does become more verbose, however.

The **mapping** entry may store a global mapping that is applied to a combination of x values and structure functions, as opposed to mappings that affect only a single structure function. It is applied before the latter mappings, in the transformation from the **p** array to the **r** array. For parameters affected by this mapping, we should ensure that they are not involved in a local mapping.

```

<SF base: public>+≡
    public :: sf_chain_instance_t

<SF base: types>+≡
    type, extends (beam_t) :: sf_chain_instance_t
        type(sf_chain_t), pointer :: config => null ()
        integer :: status = SF_UNDEFINED
        type(sf_instance_t), dimension(:), allocatable :: sf
        integer, dimension(:), allocatable :: out_sf
        integer, dimension(:), allocatable :: out_sf_i
        integer :: out_eval = 0
        integer, dimension(:), allocatable :: out_eval_i
        integer :: selected_channel = 0
        real(default), dimension(:, :), allocatable :: p, pb
        real(default), dimension(:, :), allocatable :: r, rb
        real(default), dimension(:), allocatable :: f
        real(default), dimension(:), allocatable :: x, xb
        logical, dimension(:), allocatable :: bound
        real(default) :: x_free = 1
        type(sf_channel_t), dimension(:), allocatable :: channel
    contains
        <SF base: sf chain instance: TBP>
    end type sf_chain_instance_t

```

Finalizer.

```

<SF base: sf chain instance: TBP>≡
    procedure :: final => sf_chain_instance_final

<SF base: procedures>+≡
    subroutine sf_chain_instance_final (object)
        class(sf_chain_instance_t), intent(inout) :: object
        integer :: i
        if (allocated (object%sf)) then
            do i = 1, size (object%sf, 1)
                associate (sf => object%sf(i))
                    if (allocated (sf%int)) then
                        call sf%eval%final ()
                        call sf%int%final ()
                    end if
                end associate
            end do
        end if
    end subroutine sf_chain_instance_final

```

```

        end do
    end if
    call beam_final (object%beam_t)
end subroutine sf_chain_instance_final

```

Output.

```

<SF base: sf chain instance: TBP>+=
    procedure :: write => sf_chain_instance_write

<SF base: procedures>+=
subroutine sf_chain_instance_write (object, unit, col_verbose)
    class(sf_chain_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: col_verbose
    integer :: u, i, c
    u = given_output_unit (unit)
    write (u, "(1x,A)", advance="no") "Structure-function chain instance:"
    call write_sf_status (object%status, u)
    if (allocated (object%out_sf)) then
        write (u, "(3x,A)", advance="no") "outgoing (interactions) ="
        do i = 1, size (object%out_sf)
            write (u, "(1x,I0,':',I0)", advance="no") &
                object%out_sf(i), object%out_sf_i(i)
        end do
        write (u, *)
    end if
    if (object%out_eval /= 0) then
        write (u, "(3x,A)", advance="no") "outgoing (evaluators) ="
        do i = 1, size (object%out_sf)
            write (u, "(1x,I0,':',I0)", advance="no") &
                object%out_eval, object%out_eval_i(i)
        end do
        write (u, *)
    end if
    if (allocated (object%sf)) then
        if (size (object%sf) /= 0) then
            write (u, "(1x,A)") "Structure-function parameters:"
            do c = 1, size (object%f)
                write (u, "(1x,A,I0,A)", advance="no") "Channel #", c, ":"
                if (c == object%selected_channel) then
                    write (u, "(1x,A)") "[selected]"
                else
                    write (u, *)
                end if
                write (u, "(3x,A,9(1x,F9.7))") "p =", object%p(:,c)
                write (u, "(3x,A,9(1x,F9.7))") "pb=", object%pb(:,c)
                write (u, "(3x,A,9(1x,F9.7))") "r =", object%r(:,c)
                write (u, "(3x,A,9(1x,F9.7))") "rb=", object%rb(:,c)
                write (u, "(3x,A,9(1x,ES13.7))") "f =", object%f(c)
                write (u, "(3x,A)", advance="no") "m ="
                call object%channel(c)%write (u)
            end do
            write (u, "(3x,A,9(1x,F9.7))") "x =", object%x
            write (u, "(3x,A,9(1x,F9.7))") "xb=", object%xb

```

```

        if (.not. all (object%bound)) then
            write (u, "(3x,A,9(1x,L1))" ) "bound =", object%bound
        end if
    end if
end if
call write_separator (u)
call beam_write (object%beam_t, u, col_verbose = col_verbose)
if (allocated (object%sf)) then
    do i = 1, size (object%sf)
        associate (sf => object%sf(i))
            call write_separator (u)
            if (allocated (sf%int)) then
                if (allocated (sf%r)) then
                    write (u, "(1x,A)" ) "Structure-function parameters:"
                    do c = 1, size (sf%f)
                        write (u, "(1x,A,I0,A)", advance="no") "Channel #", c, ":"
                        if (c == object%selected_channel) then
                            write (u, "(1x,A)" ) "[selected]"
                        else
                            write (u, *)
                        end if
                        write (u, "(3x,A,9(1x,F9.7))" ) "r =", sf%r(:,c)
                        write (u, "(3x,A,9(1x,F9.7))" ) "rb=", sf%rb(:,c)
                        write (u, "(3x,A,9(1x,ES13.7))" ) "f =", sf%f(c)
                        write (u, "(3x,A,9(1x,L1,7x))" ) "m =", sf%m(c)
                    end do
                    write (u, "(3x,A,9(1x,F9.7))" ) "x =", sf%x
                    write (u, "(3x,A,9(1x,F9.7))" ) "xb=", sf%xb
                end if
                call sf%int%write(u)
                if (.not. sf%eval%is_empty ()) then
                    call sf%eval%write (u, col_verbose = col_verbose)
                end if
            end if
        end associate
    end do
end if
end subroutine sf_chain_instance_write

```

Initialize. This creates a copy of the interactions in the configuration chain, assumed to be properly initialized. In the copy, we allocate the `p` etc. arrays.

The brute-force assignment of the `sf` component would be straightforward, but we provide a more fine-grained copy. In any case, the copy is deep as far as allocatables are concerned, but for the contained `interaction_t` objects the copy is shallow, as long as we do not bind defined assignment to the type. Therefore, we have to re-assign the `interaction_t` components explicitly, this time calling the proper defined assignment. Furthermore, we allocate the parameter arrays for each structure function.

(SF base: sf chain instance: TBP)+≡

```
procedure :: init => sf_chain_instance_init
```

(SF base: procedures)+≡

```
subroutine sf_chain_instance_init (chain, config, n_channel)
```



```

class(sf_chain_instance_t), intent(out), target :: chain
type(sf_chain_t), intent(in), target :: config
integer, intent(in) :: n_channel
integer :: i, j
integer :: n_par_tot, n_par, n_strfun
chain%config => config
n_strfun = config%n_strfun
chain%beam_t = config%beam_t
allocate (chain%out_sf (config%n_in), chain%out_sf_i (config%n_in))
allocate (chain%out_eval_i (config%n_in))
chain%out_sf = 0
chain%out_sf_i = [(i, i = 1, config%n_in)]
chain%out_eval_i = chain%out_sf_i
n_par_tot = 0
if (n_strfun /= 0) then
  allocate (chain%sf (n_strfun))
  do i = 1, n_strfun
    associate (sf => chain%sf(i))
      allocate (sf%int, source=config%sf(i)%int)
      sf%int%interaction_t = config%sf(i)%int%interaction_t
      n_par = size (sf%int%par_index)
      allocate (sf%r (n_par, n_channel)); sf%r = 0
      allocate (sf%rb(n_par, n_channel)); sf%rb= 0
      allocate (sf%f (n_channel)); sf%f = 0
      allocate (sf%m (n_channel)); sf%m = .false.
      allocate (sf%x (n_par)); sf%x = 0
      allocate (sf%xb(n_par)); sf%xb= 0
      n_par_tot = n_par_tot + n_par
    end associate
  end do
  allocate (chain%p (n_par_tot, n_channel)); chain%p = 0
  allocate (chain%pb(n_par_tot, n_channel)); chain%pb= 0
  allocate (chain%r (n_par_tot, n_channel)); chain%r = 0
  allocate (chain%rb(n_par_tot, n_channel)); chain%rb= 0
  allocate (chain%f (n_channel)); chain%f = 0
  allocate (chain%x (n_par_tot)); chain%x = 0
  allocate (chain%xb(n_par_tot)); chain%xb= 0
  call allocate_sf_channels &
    (chain%channel, n_channel=n_channel, n_strfun=n_strfun)
end if
allocate (chain%bound (n_par_tot), source = .true.)
do i = 1, n_strfun
  associate (sf => chain%sf(i))
    if (sf%int%is_generator ()) then
      do j = 1, size (sf%int%par_index)
        chain%bound(sf%int%par_index(j)) = .false.
      end do
    end if
  end associate
end do
chain%status = SF_INITIAL
end subroutine sf_chain_instance_init

```

Manually select a channel.

```

<SF base: sf chain instance: TBP>+=
  procedure :: select_channel => sf_chain_instance_select_channel

<SF base: procedures>+=
  subroutine sf_chain_instance_select_channel (chain, channel)
    class(sf_chain_instance_t), intent(inout) :: chain
    integer, intent(in), optional :: channel
    if (present (channel)) then
      chain%selected_channel = channel
    else
      chain%selected_channel = 0
    end if
  end subroutine sf_chain_instance_select_channel

```

Copy a channel-mapping object to the structure-function chain instance. We assume that assignment is sufficient, i.e., any non-static components of the `channel` object are allocatable und thus recursively copied.

After the copy, we extract the single-entry mappings and activate them for the individual structure functions. If there is a multi-entry mapping, we obtain the corresponding MC parameter indices and set them in the copy of the channel object.

```

<SF base: sf chain instance: TBP>+=
  procedure :: set_channel => sf_chain_instance_set_channel

<SF base: procedures>+=
  subroutine sf_chain_instance_set_channel (chain, c, channel)
    class(sf_chain_instance_t), intent(inout) :: chain
    integer, intent(in) :: c
    type(sf_channel_t), intent(in) :: channel
    integer :: i, j, k
    if (chain%status >= SF_INITIAL) then
      chain%channel(c) = channel
      j = 0
      do i = 1, chain%config%n_strfun
        associate (sf => chain%sf(i))
          sf%m(c) = channel%is_single_mapping (i)
          if (channel%is_multi_mapping (i)) then
            do k = 1, size (sf%int%beam_index)
              j = j + 1
              call chain%channel(c)%set_par_index &
                (j, sf%int%par_index(k))
            end do
          end if
        end associate
      end do
      if (j /= chain%channel(c)%get_multi_mapping_n_par ()) then
        print *, "index last filled      = ", j
        print *, "number of parameters = ", &
          chain%channel(c)%get_multi_mapping_n_par ()
        call msg_bug ("Structure-function setup: mapping index mismatch")
      end if
      chain%status = SF_INITIAL
    end if
  end subroutine sf_chain_instance_set_channel

```

Link the interactions in the chain. First, link the beam instance to its template in the configuration chain, which should have the appropriate momenta fixed.

Then, we follow the chain via the arrays `out_sf` and `out_sf_i`. The arrays are (up to) two-dimensional, the entries correspond to the beam particle(s). For each beam, the entry `out_sf` points to the last interaction that affected this beam, and `out_sf_i` is the out-particle index within that interaction. For the initial beam, `out_sf` is zero by definition.

For each entry in the chain, we scan the affected beams (one or two). We look for `out_sf` and link the out-particle there to the corresponding in-particle in the current interaction. Then, we update the entry in `out_sf` and `out_sf_i` to point to the current interaction.

```

<SF base: sf chain instance: TBP>+≡
  procedure :: link_interactions => sf_chain_instance_link_interactions

<SF base: procedures>+≡
  subroutine sf_chain_instance_link_interactions (chain)
    class(sf_chain_instance_t), intent(inout), target :: chain
    type(interaction_t), pointer :: int
    integer :: i, j, b
    if (chain%status >= SF_INITIAL) then
      do b = 1, chain%config%n_in
        int => beam_get_int_ptr (chain%beam_t)
        call interaction_set_source_link (int, b, &
          chain%config%beam_t, b)
      end do
      if (allocated (chain%sf)) then
        do i = 1, size (chain%sf)
          associate (sf_int => chain%sf(i)%int)
            do j = 1, size (sf_int%beam_index)
              b = sf_int%beam_index(j)
              call link (sf_int%interaction_t, b, sf_int%incoming(j))
              chain%out_sf(b) = i
              chain%out_sf_i(b) = sf_int%outgoing(j)
            end do
          end associate
        end do
      end if
      chain%status = SF_DONE_LINKS
    end if
  contains
    subroutine link (int, b, in_index)
      type(interaction_t), intent(inout) :: int
      integer, intent(in) :: b, in_index
      integer :: i
      i = chain%out_sf(b)
      select case (i)
      case (0)
        call interaction_set_source_link (int, in_index, &
          chain%beam_t, chain%out_sf_i(b))
      case default
        call int%set_source_link (in_index, &
          chain%sf(i)%int, chain%out_sf_i(b))
      end select
    end subroutine link
  end subroutine sf_chain_instance_link_interactions

```

```

        end select
    end subroutine link
end subroutine sf_chain_instance_link_interactions

```

Exchange the quantum-number masks between the interactions in the chain, so we can combine redundant entries and detect any obvious mismatch.

We proceed first in the forward direction and then backwards again.

After this is finished, we finalize initialization by calling the `setup_constants` method, which prepares constant data that depend on the matrix element structure.

```

<SF base: sf chain instance: TBP>+=
    procedure :: exchange_mask => sf_chain_exchange_mask

<SF base: procedures>+=
    subroutine sf_chain_exchange_mask (chain)
        class(sf_chain_instance_t), intent(inout), target :: chain
        type(interaction_t), pointer :: int
        type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
        integer :: i
        if (chain%status >= SF_DONE_LINKS) then
            if (allocated (chain%sf)) then
                int => beam_get_int_ptr (chain%beam_t)
                allocate (mask (int%get_n_out ()))
                mask = int%get_mask ()
                if (size (chain%sf) /= 0) then
                    do i = 1, size (chain%sf) - 1
                        call interaction_exchange_mask (chain%sf(i)%int%interaction_t)
                    end do
                    do i = size (chain%sf), 1, -1
                        call interaction_exchange_mask (chain%sf(i)%int%interaction_t)
                    end do
                    if (any (mask .neqv. int%get_mask ())) then
                        chain%status = SF_FAILED_MASK
                        return
                    end if
                    do i = 1, size (chain%sf)
                        call chain%sf(i)%int%setup_constants ()
                    end do
                end if
            end if
            chain%status = SF_DONE_MASK
        end if
    end subroutine sf_chain_exchange_mask

```

Initialize the evaluators that connect the interactions in the chain.

```

<SF base: sf chain instance: TBP>+=
    procedure :: init_evaluators => sf_chain_instance_init_evaluators

<SF base: procedures>+=
    subroutine sf_chain_instance_init_evaluators (chain, extended_sf)
        class(sf_chain_instance_t), intent(inout), target :: chain
        logical, intent(in), optional :: extended_sf
        type(interaction_t), pointer :: int

```

```

type(quantum_numbers_mask_t) :: mask
integer :: i
logical :: yorn
yorn = .false.; if (present (extended_sf)) yorn = extended_sf
if (chain%status >= SF_DONE_MASK) then
  if (allocated (chain%sf)) then
    if (size (chain%sf) /= 0) then
      mask = quantum_numbers_mask (.false., .false., .true.)
      int => beam_get_int_ptr (chain%beam_t)
      do i = 1, size (chain%sf)
        associate (sf => chain%sf(i))
          if (yorn) then
            if (int%get_n_sub () == 0) then
              call int%declare_subtraction (n_beams_rescaled)
            end if
            if (sf%int%interaction_t%get_n_sub () == 0) then
              call sf%int%interaction_t%declare_subtraction (n_beams_rescaled)
            end if
          end if
          call sf%eval%init_product (int, sf%int%interaction_t, mask, &
            & ignore_sub_for_qn = .true.)
          if (sf%eval%is_empty ()) then
            chain%status = SF_FAILED_CONNECTIONS
            return
          end if
          int => sf%eval%interaction_t
        end associate
      end do
      call find_outgoing_particles ()
    end if
  else if (chain%out_eval == 0) then
    int => beam_get_int_ptr (chain%beam_t)
    call int%tag_hard_process ()
  end if
  chain%status = SF_DONE_CONNECTIONS
end if
contains
<SF base: init evaluators: find outgoing particles>
end subroutine sf_chain_instance_init_evaluators

```

For debug purposes

```

<SF base: sf chain instance: TBP>+≡
  procedure :: write_interaction => sf_chain_instance_write_interaction

<SF base: procedures>+≡
  subroutine sf_chain_instance_write_interaction (chain, i_sf, i_int, unit)
    class(sf_chain_instance_t), intent(in) :: chain
    integer, intent(in) :: i_sf, i_int
    integer, intent(in) :: unit
    class(interaction_t), pointer :: int_in1 => null ()
    class(interaction_t), pointer :: int_in2 => null ()
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    if (chain%status >= SF_DONE_MASK) then

```

```

    if (allocated (chain%sf)) then
      int_in1 => evaluator_get_int_in_ptr (chain%sf(i_sf)%eval, 1)
      int_in2 => evaluator_get_int_in_ptr (chain%sf(i_sf)%eval, 2)
      if (int_in1%get_tag () == i_int) then
        call int_in1%basic_write (u)
      else if (int_in2%get_tag () == i_int) then
        call int_in2%basic_write (u)
      else
        write (u, "(A,1x,I0,1x,A,1x,I0)") 'No tag of sf', i_sf, 'matches' , i_int
      end if
    else
      write (u, "(A)") 'No sf_chain allocated!'
    end if
  else
    write (u, "(A)") 'sf_chain not ready!'
  end if
end subroutine sf_chain_instance_write_interaction

```

This is an internal subroutine of the previous one: After evaluators are set, trace the outgoing particles to the last evaluator. We only need the first channel, all channels are equivalent for this purpose.

For each beam, the outgoing particle is located by `out_sf` (the structure-function object where it originates) and `out_sf_i` (the index within that object). This particle is referenced by the corresponding evaluator, which in turn is referenced by the next evaluator, until we are at the end of the chain. We can trace back references by `interaction_find_link`. Knowing that `out_eval` is the index of the last evaluator, we thus determine `out_eval_i`, the index of the outgoing particle within that evaluator.

```

(SF base: init evaluators: find outgoing particles)≡
subroutine find_outgoing_particles ()
  type(interaction_t), pointer :: int, int_next
  integer :: i, j, out_sf, out_i
  chain%out_eval = size (chain%sf)
  do j = 1, size (chain%out_eval_i)
    out_sf = chain%out_sf(j)
    out_i = chain%out_sf_i(j)
    if (out_sf == 0) then
      int => beam_get_int_ptr (chain%beam_t)
      out_sf = 1
    else
      int => chain%sf(out_sf)%int%interaction_t
    end if
    do i = out_sf, chain%out_eval
      int_next => chain%sf(i)%eval%interaction_t
      out_i = interaction_find_link (int_next, int, out_i)
      int => int_next
    end do
    chain%out_eval_i(j) = out_i
  end do
  call int%tag_hard_process (chain%out_eval_i)
end subroutine find_outgoing_particles

```

Compute the kinematics in the chain instance. We can assume that the seed momenta are set in the configuration beams. Scanning the chain, we first transfer the incoming momenta. Then, we use up the MC input parameter array \mathbf{p} to compute the radiated and outgoing momenta.

In the multi-channel case, c_sel is the channel which we use for computing the kinematics and the \mathbf{x} values. In the other channels, we invert the kinematics in order to recover the corresponding rows in the \mathbf{r} array, and the Jacobian \mathbf{f} .

We first apply any global mapping to transform the input \mathbf{p} into the array \mathbf{r} . This is then given to the structure functions which compute the final array \mathbf{x} and Jacobian factors \mathbf{f} , which we multiply to obtain the overall Jacobian.

```

<SF base: sf chain instance: TBP>+=
  procedure :: compute_kinematics => sf_chain_instance_compute_kinematics

<SF base: procedures>+=
  subroutine sf_chain_instance_compute_kinematics (chain, c_sel, p_in)
    class(sf_chain_instance_t), intent(inout), target :: chain
    integer, intent(in) :: c_sel
    real(default), dimension(:), intent(in) :: p_in
    type(interaction_t), pointer :: int
    real(default) :: f_mapping
    integer :: i, j, c
    if (chain%status >= SF_DONE_CONNECTIONS) then
      call chain%select_channel (c_sel)
      int => beam_get_int_ptr (chain%beam_t)
      call int%receive_momenta ()
      if (allocated (chain%sf)) then
        if (size (chain%sf) /= 0) then
          forall (i = 1:size (chain%sf)) chain%sf(i)%int%status = SF_INITIAL
          chain%p (:,c_sel) = unpack (p_in, chain%bound, 0._default)
          chain%pb(:,c_sel) = 1 - chain%p(:,c_sel)
          chain%f = 1
          chain%x_free = 1
          do i = 1, size (chain%sf)
            associate (sf => chain%sf(i))
              call sf%int%generate_free (sf%r(:,c_sel), sf%rb(:,c_sel), &
                chain%x_free)
              do j = 1, size (sf%x)
                if (.not. chain%bound(sf%int%par_index(j))) then
                  chain%p (sf%int%par_index(j),c_sel) = sf%r (j,c_sel)
                  chain%pb(sf%int%par_index(j),c_sel) = sf%rb(j,c_sel)
                end if
              end do
            end associate
          end do
          if (allocated (chain%channel(c_sel)%multi_mapping)) then
            call chain%channel(c_sel)%multi_mapping%compute &
              (chain%r(:,c_sel), chain%rb(:,c_sel), &
                f_mapping, &
                chain%p(:,c_sel), chain%pb(:,c_sel), &
                chain%x_free)
            chain%f(c_sel) = f_mapping
          else
            chain%r (:,c_sel) = chain%p (:,c_sel)
            chain%rb(:,c_sel) = chain%pb(:,c_sel)
          end if
        end if
      end if
    end if
  end subroutine

```

```

        chain%f(c_sel) = 1
    end if
    do i = 1, size (chain%sf)
        associate (sf => chain%sf(i))
            call sf%int%seed_kinematics ()
            do j = 1, size (sf%x)
                sf%r (j,c_sel) = chain%r (sf%int%par_index(j),c_sel)
                sf%rb(j,c_sel) = chain%rb(sf%int%par_index(j),c_sel)
            end do
            call sf%int%complete_kinematics &
                (sf%x, sf%xb, sf%f(c_sel), sf%r(:,c_sel), sf%rb(:,c_sel), &
                sf%m(c_sel))
            do j = 1, size (sf%x)
                chain%x(sf%int%par_index(j)) = sf%x(j)
                chain%xb(sf%int%par_index(j)) = sf%xb(j)
            end do
            if (sf%int%status <= SF_FAILED_KINEMATICS) then
                chain%status = SF_FAILED_KINEMATICS
                return
            end if
            do c = 1, size (sf%f)
                if (c /= c_sel) then
                    call sf%int%inverse_kinematics &
                        (sf%x, sf%xb, sf%f(c), sf%r(:,c), sf%rb(:,c), sf%m(c))
                    do j = 1, size (sf%x)
                        chain%r (sf%int%par_index(j),c) = sf%r (j,c)
                        chain%rb(sf%int%par_index(j),c) = sf%rb(j,c)
                    end do
                end if
                chain%f(c) = chain%f(c) * sf%f(c)
            end do
            if (.not. sf%eval%is_empty ()) then
                call sf%eval%receive_momenta ()
            end if
        end associate
    end do
    do c = 1, size (chain%f)
        if (c /= c_sel) then
            if (allocated (chain%channel(c)%multi_mapping)) then
                call chain%channel(c)%multi_mapping%inverse &
                    (chain%r(:,c), chain%rb(:,c), &
                    f_mapping, &
                    chain%p(:,c), chain%pb(:,c), &
                    chain%x_free)
                chain%f(c) = chain%f(c) * f_mapping
            else
                chain%p (:,c) = chain%r (:,c)
                chain%pb(:,c) = chain%rb(:,c)
            end if
        end if
    end do
end if
end if
chain%status = SF_DONE_KINEMATICS

```



```

end if
end subroutine sf_chain_instance_compute_kinematics

```

This is a variant of the previous procedure. We know the x parameters and reconstruct the momenta and the MC input parameters p . We do not need to select a channel.

Note: this is probably redundant, since the method we actually want starts from the momenta, recovers all x parameters, and then inverts mappings. See below `recover_kinematics`.

```

<SF base: sf chain instance: TBP>+=
  procedure :: inverse_kinematics => sf_chain_instance_inverse_kinematics

<SF base: procedures>+=
  subroutine sf_chain_instance_inverse_kinematics (chain, x, xb)
    class(sf_chain_instance_t), intent(inout), target :: chain
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    type(interaction_t), pointer :: int
    real(default) :: f_mapping
    integer :: i, j, c
    if (chain%status >= SF_DONE_CONNECTIONS) then
      call chain%select_channel ()
      int => beam_get_int_ptr (chain%beam_t)
      call int%receive_momenta ()
      if (allocated (chain%sf)) then
        chain%f = 1
        if (size (chain%sf) /= 0) then
          forall (i = 1:size (chain%sf)) chain%sf(i)%int%status = SF_INITIAL
          chain%x = x
          chain%xb= xb
          do i = 1, size (chain%sf)
            associate (sf => chain%sf(i))
              call sf%int%seed_kinematics ()
              do j = 1, size (sf%x)
                sf%x(j) = chain%x(sf%int%par_index(j))
                sf%xb(j) = chain%xb(sf%int%par_index(j))
              end do
              do c = 1, size (sf%f)
                call sf%int%inverse_kinematics &
                  (sf%x, sf%xb, sf%f(c), sf%r(:,c), sf%rb(:,c), sf%m(c), &
                    set_momenta = c==1)
                chain%f(c) = chain%f(c) * sf%f(c)
                do j = 1, size (sf%x)
                  chain%r (sf%int%par_index(j),c) = sf%r (j,c)
                  chain%rb(sf%int%par_index(j),c) = sf%rb(j,c)
                end do
              end do
              if (.not. sf%eval%is_empty ()) then
                call sf%eval%receive_momenta ()
              end if
            end associate
          end do
          do c = 1, size (chain%f)
            if (allocated (chain%channel(c)%multi_mapping)) then

```

```

        call chain%channel(c)%multi_mapping%inverse &
            (chain%r(:,c), chain%rb(:,c), &
             f_mapping, &
             chain%p(:,c), chain%pb(:,c), &
             chain%x_free)
        chain%f(c) = chain%f(c) * f_mapping
    else
        chain%p(:,c) = chain%r(:,c)
        chain%pb(:,c) = chain%rb(:,c)
    end if
end do
end if
chain%status = SF_DONE_KINEMATICS
end if
end subroutine sf_chain_instance_inverse_kinematics

```

Recover the kinematics: assuming that the last evaluator has been filled with a valid set of momenta, we travel the momentum links backwards and fill the preceding evaluators and, as a side effect, interactions. We stop at the beam interaction.

After all momenta are set, apply the `inverse_kinematics` procedure above, suitably modified, to recover the x and p parameters and the Jacobian factors.

The `c_sel` (channel) argument is just used to mark a selected channel for the records, otherwise the recovery procedure is independent of this.

(SF base: sf chain instance: TBP)+≡

```

    procedure :: recover_kinematics => sf_chain_instance_recover_kinematics

```

(SF base: procedures)+≡

```

subroutine sf_chain_instance_recover_kinematics (chain, c_sel)
    class(sf_chain_instance_t), intent(inout), target :: chain
    integer, intent(in) :: c_sel
    real(default) :: f_mapping
    integer :: i, j, c
    if (chain%status >= SF_DONE_CONNECTIONS) then
        call chain%select_channel (c_sel)
        if (allocated (chain%sf)) then
            do i = size (chain%sf), 1, -1
                associate (sf => chain%sf(i))
                    if (.not. sf%eval%is_empty ()) then
                        call interaction_send_momenta (sf%eval%interaction_t)
                    end if
                end associate
            end do
            chain%f = 1
            if (size (chain%sf) /= 0) then
                forall (i = 1:size (chain%sf)) chain%sf(i)%int%status = SF_INITIAL
                chain%x_free = 1
                do i = 1, size (chain%sf)
                    associate (sf => chain%sf(i))
                        call sf%int%seed_kinematics ()
                        call sf%int%recover_x (sf%x, sf%xb, chain%x_free)
                        do j = 1, size (sf%x)

```

```

        chain%x(sf%int%par_index(j)) = sf%x(j)
        chain%xb(sf%int%par_index(j)) = sf%xb(j)
    end do
    do c = 1, size (sf%f)
        call sf%int%inverse_kinematics &
            (sf%x, sf%xb, sf%f(c), sf%r(:,c), sf%rb(:,c), sf%m(c), &
            set_momenta = .false.)
        chain%f(c) = chain%f(c) * sf%f(c)
        do j = 1, size (sf%x)
            chain%r (sf%int%par_index(j),c) = sf%r (j,c)
            chain%rb(sf%int%par_index(j),c) = sf%rb(j,c)
        end do
    end do
end associate
end do
do c = 1, size (chain%f)
    if (allocated (chain%channel(c)%multi_mapping)) then
        call chain%channel(c)%multi_mapping%inverse &
            (chain%r(:,c), chain%rb(:,c), &
            f_mapping, &
            chain%p(:,c), chain%pb(:,c), &
            chain%x_free)
        chain%f(c) = chain%f(c) * f_mapping
    else
        chain%p (:,c) = chain%r (:,c)
        chain%pb(:,c) = chain%rb(:,c)
    end if
end do
end if
chain%status = SF_DONE_KINEMATICS
end if
end subroutine sf_chain_instance_recover_kinematics

```

Return the initial beam momenta to their source, thus completing kinematics recovery. Obviously, this works as a side effect.

(SF base: sf chain instance: TBP)+≡

```

    procedure :: return_beam_momenta => sf_chain_instance_return_beam_momenta

```

(SF base: procedures)+≡

```

    subroutine sf_chain_instance_return_beam_momenta (chain)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(interaction_t), pointer :: int
        if (chain%status >= SF_DONE_KINEMATICS) then
            int => beam_get_int_ptr (chain%beam_t)
            call interaction_send_momenta (int)
        end if
    end subroutine sf_chain_instance_return_beam_momenta

```

Evaluate all interactions in the chain and the product evaluators. We provide a **scale** argument that is given to all structure functions in the chain.

Hadronic NLO calculations involve rescaled fractions of the original beam momentum. In particular, we have to handle the following cases:

- normal evaluation (where `i_sub = 0`) for all terms except the real non-subtracted,
- rescaled momentum fraction for both beams in the case of the real non-subtracted term (`i_sub = 0`),
- and rescaled momentum fraction for one of both beams in the case of the subtraction and DGLAP component (`i_sub = 1,2`).

For the collinear final or initial state counter terms, we apply a rescaling to one beam, and keep the other beam as is. We redo it then vice versa having now two subtractions.

```

(SF base: sf chain instance: TBP)+≡
  procedure :: evaluate => sf_chain_instance_evaluate

(SF base: procedures)+≡
  subroutine sf_chain_instance_evaluate (chain, scale, negative_sf, sf_rescale)
    class(sf_chain_instance_t), intent(inout), target :: chain
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(inout), optional :: sf_rescale
    type(interaction_t), pointer :: out_int
    real(default) :: sf_sum
    integer :: i_beam, i_sub, n_sub
    logical :: rescale
    n_sub = 0
    rescale = .false.; if (present (sf_rescale)) rescale = .true.
    if (rescale) then
      n_sub = chain%get_n_sub ()
    end if
    if (chain%status >= SF_DONE_KINEMATICS) then
      if (allocated (chain%sf)) then
        if (size (chain%sf) /= 0) then
          do i_beam = 1, size (chain%sf)
            associate (sf => chain%sf(i_beam))
              if (rescale) then
                call sf_rescale%set_i_beam (i_beam)
                do i_sub = 0, n_sub
                  select case (i_sub)
                    case (0)
                      if (n_sub == 0) then
                        call sf%int%apply (scale, negative_sf, sf_rescale, i_sub = i_sub)
                      else
                        call sf%int%apply (scale, negative_sf, i_sub = i_sub)
                      end if
                    case default
                      if (i_beam == i_sub) then
                        call sf%int%apply (scale, negative_sf, sf_rescale, i_sub = i_sub)
                      else
                        call sf%int%apply (scale, negative_sf, i_sub = i_sub)
                      end if
                    end select
                  end do
                end do
              end if
            end do
          end do
        else
          call sf%int%apply (scale, negative_sf, i_sub = n_sub)
        end if
      end if
    end if
  end subroutine

```

```

        end if
        if (sf%int%status <= SF_FAILED_EVALUATION) then
            chain%status = SF_FAILED_EVALUATION
            return
        end if
        if (.not. sf%eval%is_empty ()) call sf%eval%evaluate ()
    end associate
end do
out_int => chain%get_out_int_ptr ()
sf_sum = real (out_int%sum ())
call chain%config%trace &
    (chain%selected_channel, chain%p, chain%x, chain%f, sf_sum)
end if
end if
chain%status = SF_EVALUATED
end if
end subroutine sf_chain_instance_evaluate

```

16.5.10 Access to the chain instance

Transfer the outgoing momenta to the array p. We assume that array sizes match.

```

<SF base: sf chain instance: TBP>+≡
    procedure :: get_out_momenta => sf_chain_instance_get_out_momenta

<SF base: procedures>+≡
    subroutine sf_chain_instance_get_out_momenta (chain, p)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(vector4_t), dimension(:), intent(out) :: p
        type(interaction_t), pointer :: int
        integer :: i, j
        if (chain%status >= SF_DONE_KINEMATICS) then
            do j = 1, size (chain%out_sf)
                i = chain%out_sf(j)
                select case (i)
                    case (0)
                        int => beam_get_int_ptr (chain%beam_t)
                    case default
                        int => chain%sf(i)%int%interaction_t
                end select
                p(j) = int%get_momentum (chain%out_sf_i(j))
            end do
        end if
    end subroutine sf_chain_instance_get_out_momenta

```

Return a pointer to the last evaluator in the chain (to the interaction).

```

<SF base: sf chain instance: TBP>+≡
    procedure :: get_out_int_ptr => sf_chain_instance_get_out_int_ptr

<SF base: procedures>+≡
    function sf_chain_instance_get_out_int_ptr (chain) result (int)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(interaction_t), pointer :: int

```

```

    if (chain%out_eval == 0) then
        int => beam_get_int_ptr (chain%beam_t)
    else
        int => chain%sf(chain%out_eval)%eval%interaction_t
    end if
end function sf_chain_instance_get_out_int_ptr

```

Return the index of the j-th outgoing particle, within the last evaluator.

```

⟨SF base: sf chain instance: TBP⟩+≡
    procedure :: get_out_i => sf_chain_instance_get_out_i

⟨SF base: procedures⟩+≡
    function sf_chain_instance_get_out_i (chain, j) result (i)
        class(sf_chain_instance_t), intent(in) :: chain
        integer, intent(in) :: j
        integer :: i
        i = chain%out_eval_i(j)
    end function sf_chain_instance_get_out_i

```

Return the mask for the outgoing particle(s), within the last evaluator.

```

⟨SF base: sf chain instance: TBP⟩+≡
    procedure :: get_out_mask => sf_chain_instance_get_out_mask

⟨SF base: procedures⟩+≡
    function sf_chain_instance_get_out_mask (chain) result (mask)
        class(sf_chain_instance_t), intent(in), target :: chain
        type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
        type(interaction_t), pointer :: int
        allocate (mask (chain%config%n_in))
        int => chain%get_out_int_ptr ()
        mask = int%get_mask (chain%out_eval_i)
    end function sf_chain_instance_get_out_mask

```

Return the array of MC input parameters that corresponds to channel c. This is the p array, the parameters before all mappings.

The p array may be deallocated. This should correspond to a zero-size r argument, so nothing to do then.

```

⟨SF base: sf chain instance: TBP⟩+≡
    procedure :: get_mcpair => sf_chain_instance_get_mcpair

⟨SF base: procedures⟩+≡
    subroutine sf_chain_instance_get_mcpair (chain, c, r)
        class(sf_chain_instance_t), intent(in) :: chain
        integer, intent(in) :: c
        real(default), dimension(:), intent(out) :: r
        if (allocated (chain%p)) r = pack (chain%p(:,c), chain%bound)
    end subroutine sf_chain_instance_get_mcpair

```

Return the Jacobian factor that corresponds to channel c.

```

⟨SF base: sf chain instance: TBP⟩+≡
    procedure :: get_f => sf_chain_instance_get_f

```

```

<SF base: procedures>+≡
function sf_chain_instance_get_f (chain, c) result (f)
  class(sf_chain_instance_t), intent(in) :: chain
  integer, intent(in) :: c
  real(default) :: f
  if (allocated (chain%f)) then
    f = chain%f(c)
  else
    f = 1
  end if
end function sf_chain_instance_get_f

```

Return the evaluation status.

```

<SF base: sf chain instance: TBP>+≡
procedure :: get_status => sf_chain_instance_get_status

```

```

<SF base: procedures>+≡
function sf_chain_instance_get_status (chain) result (status)
  class(sf_chain_instance_t), intent(in) :: chain
  integer :: status
  status = chain%status
end function sf_chain_instance_get_status

```

```

<SF base: sf chain instance: TBP>+≡
procedure :: get_matrix_elements => sf_chain_instance_get_matrix_elements

```

```

<SF base: procedures>+≡
subroutine sf_chain_instance_get_matrix_elements (chain, i, ff)
  class(sf_chain_instance_t), intent(in) :: chain
  integer, intent(in) :: i
  real(default), intent(out), dimension(:), allocatable :: ff

  associate (sf => chain%sf(i))
    ff = real (sf%int%get_matrix_element ())
  end associate
end subroutine sf_chain_instance_get_matrix_elements

```

```

<SF base: sf chain instance: TBP>+≡
procedure :: get_beam_int_ptr => sf_chain_instance_get_beam_int_ptr

```

```

<SF base: procedures>+≡
function sf_chain_instance_get_beam_int_ptr (chain) result (int)
  type(interaction_t), pointer :: int
  class(sf_chain_instance_t), intent(in), target :: chain
  int => beam_get_int_ptr (chain%beam_t)
end function sf_chain_instance_get_beam_int_ptr

```

```

<SF base: sf chain instance: TBP>+≡
procedure :: get_n_sub => sf_chain_instance_get_n_sub

```

```

⟨SF base: procedures⟩+=
  integer function sf_chain_instance_get_n_sub (chain) result (n_sub)
    type(interaction_t), pointer :: int
    class(sf_chain_instance_t), intent(in), target :: chain
    int => beam_get_int_ptr (chain%beam_t)
    n_sub = int%get_n_sub ()
  end function sf_chain_instance_get_n_sub

```

16.5.11 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sf_base.ut.f90⟩≡
  ⟨File header⟩

  module sf_base_ut
    use unit_tests
    use sf_base_uti

    ⟨Standard module head⟩

    ⟨SF base: public test auxiliary⟩

    ⟨SF base: public test⟩

    contains

    ⟨SF base: test driver⟩

  end module sf_base_ut

⟨sf_base.uti.f90⟩≡
  ⟨File header⟩

  module sf_base_uti

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use io_units
    use format_defs, only: FMT_19
    use format_utils, only: write_separator
    use diagnostics
    use lorentz
    use pdg_arrays
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices, only: FM_IGNORE_HELICITY
    use interactions
    use particles
    use model_data
    use beams
    use sf_aux

```



```

    use sf_mappings

    use sf_base

    <Standard module head>

    <SF base: test declarations>

    <SF base: public test auxiliary>

    <SF base: test types>

    contains

    <SF base: tests>

    <SF base: test auxiliary>

    end module sf_base_util

API: driver for the unit tests below.
<SF base: public test>≡
    public :: sf_base_test
<SF base: test driver>≡
    subroutine sf_base_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <SF base: execute tests>
    end subroutine sf_base_test

```

16.5.12 Test implementation: structure function

This is a template for the actual structure-function implementation which will be defined in separate modules.

Configuration data

The test structure function uses the **Test** model. It describes a scalar within an arbitrary initial particle, which is given in the initialization. The radiated particle is also a scalar, the same one, but we set its mass artificially to zero.

```

<SF base: public test auxiliary>≡
    public :: sf_test_data_t
<SF base: test types>≡
    type, extends (sf_data_t) :: sf_test_data_t
        class(model_data_t), pointer :: model => null ()
        integer :: mode = 0
        type(flavor_t) :: flv_in
        type(flavor_t) :: flv_out
        type(flavor_t) :: flv_rad
        real(default) :: m = 0
        logical :: collinear = .true.

```

```

    real(default), dimension(:), allocatable :: qbounds
contains
  <SF base: sf test data: TBP>
end type sf_test_data_t

```

Output.

```

<SF base: sf test data: TBP>≡
  procedure :: write => sf_test_data_write

<SF base: test auxiliary>≡
  subroutine sf_test_data_write (data, unit, verbose)
    class(sf_test_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "SF test data:"
    write (u, "(3x,A,A)") "model      = ", char (data%model%get_name ())
    write (u, "(3x,A)", advance="no") "incoming  = "
    call data%flv_in%write (u); write (u, *)
    write (u, "(3x,A)", advance="no") "outgoing  = "
    call data%flv_out%write (u); write (u, *)
    write (u, "(3x,A)", advance="no") "radiated  = "
    call data%flv_rad%write (u); write (u, *)
    write (u, "(3x,A," // FMT_19 // ")") "mass      = ", data%m
    write (u, "(3x,A,L1)") "collinear = ", data%collinear
    if (.not. data%collinear .and. allocated (data%qbounds)) then
      write (u, "(3x,A," // FMT_19 // ")") "qmin      = ", data%qbounds(1)
      write (u, "(3x,A," // FMT_19 // ")") "qmax      = ", data%qbounds(2)
    end if
  end subroutine sf_test_data_write

```

Initialization.

```

<SF base: sf test data: TBP>+≡
  procedure :: init => sf_test_data_init

<SF base: test auxiliary>+≡
  subroutine sf_test_data_init (data, model, pdg_in, collinear, qbounds, mode)
    class(sf_test_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    logical, intent(in), optional :: collinear
    real(default), dimension(2), intent(in), optional :: qbounds
    integer, intent(in), optional :: mode
    data%model => model
    if (present (mode)) data%mode = mode
    if (pdg_array_get (pdg_in, 1) /= 25) then
      call msg_fatal ("Test spectrum function: input flavor must be 's'")
    end if
    call data%flv_in%init (25, model)
    data%m = data%flv_in%get_mass ()
    if (present (collinear)) data%collinear = collinear
    call data%flv_out%init (25, model)
    call data%flv_rad%init (25, model)

```

```

    if (present (qbounds)) then
        allocate (data%qbounds (2))
        data%qbounds = qbounds
    end if
end subroutine sf_test_data_init

```

Return the number of parameters: 1 if only consider collinear splitting, 3 otherwise.

```

<SF base: sf test data: TBP>+≡
    procedure :: get_n_par => sf_test_data_get_n_par

<SF base: test auxiliary>+≡
    function sf_test_data_get_n_par (data) result (n)
        class(sf_test_data_t), intent(in) :: data
        integer :: n
        if (data%collinear) then
            n = 1
        else
            n = 3
        end if
    end function sf_test_data_get_n_par

```

Return the outgoing particle PDG code: 25

```

<SF base: sf test data: TBP>+≡
    procedure :: get_pdg_out => sf_test_data_get_pdg_out

<SF base: test auxiliary>+≡
    subroutine sf_test_data_get_pdg_out (data, pdg_out)
        class(sf_test_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        pdg_out(1) = 25
    end subroutine sf_test_data_get_pdg_out

```

Allocate the matching interaction.

```

<SF base: sf test data: TBP>+≡
    procedure :: allocate_sf_int => sf_test_data_allocate_sf_int

<SF base: test auxiliary>+≡
    subroutine sf_test_data_allocate_sf_int (data, sf_int)
        class(sf_test_data_t), intent(in) :: data
        class(sf_int_t), intent(inout), allocatable :: sf_int
        if (allocated (sf_int)) deallocate (sf_int)
        allocate (sf_test_t :: sf_int)
    end subroutine sf_test_data_allocate_sf_int

```

Interaction

```

<SF base: test types>+≡
    type, extends (sf_int_t) :: sf_test_t
        type(sf_test_data_t), pointer :: data => null ()
        real(default) :: x = 0
    contains

```

```

    <SF base: sf test int: TBP>
end type sf_test_t

```

Type string: constant

```

<SF base: sf test int: TBP>≡
    procedure :: type_string => sf_test_type_string

<SF base: test auxiliary>+≡
    function sf_test_type_string (object) result (string)
        class(sf_test_t), intent(in) :: object
        type(string_t) :: string
        string = "Test"
    end function sf_test_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF base: sf test int: TBP>+≡
    procedure :: write => sf_test_write

<SF base: test auxiliary>+≡
    subroutine sf_test_write (object, unit, testflag)
        class(sf_test_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%data)) then
            call object%data%write (u)
            call object%base_write (u, testflag)
        else
            write (u, "(1x,A)") "SF test data: [undefined]"
        end if
    end subroutine sf_test_write

```

Initialize. We know that data will be of concrete type `sf_test_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass, but keep the radiated mass zero.

Optionally, we can provide minimum and maximum values for the momentum transfer.

```

<SF base: sf test int: TBP>+≡
    procedure :: init => sf_test_init

<SF base: test auxiliary>+≡
    subroutine sf_test_init (sf_int, data)
        class(sf_test_t), intent(out) :: sf_int
        class(sf_data_t), intent(in), target :: data
        type(quantum_numbers_mask_t), dimension(3) :: mask
        type(helicity_t) :: hel0
        type(color_t) :: col0
        type(quantum_numbers_t), dimension(3) :: qn
        mask = quantum_numbers_mask (.false., .false., .false.)
        select type (data)
        type is (sf_test_data_t)

```

```

    if (allocated (data%qbounds)) then
      call sf_int%base_init (mask, &
        [data%m**2], [0._default], [data%m**2], &
        [data%qbounds(1)], [data%qbounds(2)])
    else
      call sf_int%base_init (mask, &
        [data%m**2], [0._default], [data%m**2])
    end if
    sf_int%data => data
    call hel0%init (0)
    call col0%init ()
    call qn(1)%init (data%flv_in, col0, hel0)
    call qn(2)%init (data%flv_rad, col0, hel0)
    call qn(3)%init (data%flv_out, col0, hel0)
    call sf_int%add_state (qn)
    call sf_int%freeze ()
    call sf_int%set_incoming ([1])
    call sf_int%set_radiated ([2])
    call sf_int%set_outgoing ([3])
  end select
  sf_int%status = SF_INITIAL
end subroutine sf_test_init

```

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, we are asked to provide an efficient mapping. For the test case, we set $x = r^2$ and consequently $f(r) = 2r$.

(SF base: sf test int: TBP)+≡

```

  procedure :: complete_kinematics => sf_test_complete_kinematics

```

(SF base: test auxiliary)+≡

```

  subroutine sf_test_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(sf_test_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    if (map) then
      x(1) = r(1)**2
      f = 2 * r(1)
    else
      x(1) = r(1)
      f = 1
    end if
    xb(1) = 1 - x(1)
    if (size (x) == 3) then
      x(2:3) = r(2:3)
      xb(2:3) = rb(2:3)
    end if
    call sf_int%split_momentum (x, xb)
    sf_int%x = x(1)
    select case (sf_int%status)

```

```

        case (SF_FAILED_KINEMATICS); f = 0
    end select
end subroutine sf_test_complete_kinematics

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

<SF base: sf test int: TBP>+≡

```

    procedure :: inverse_kinematics => sf_test_inverse_kinematics

```

<SF base: test auxiliary>+≡

```

subroutine sf_test_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(sf_test_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    if (map) then
        r(1) = sqrt (x(1))
        f = 2 * r(1)
    else
        r(1) = x(1)
        f = 1
    end if
    if (size (x) == 3) r(2:3) = x(2:3)
    rb = 1 - r
    sf_int%x = x(1)
    if (set_mom) then
        call sf_int%split_momentum (x, xb)
        select case (sf_int%status)
            case (SF_FAILED_KINEMATICS); f = 0
        end select
    end if
end subroutine sf_test_inverse_kinematics

```

Apply the structure function. The matrix element becomes unity and the application always succeeds.

If the `mode` indicator is one, the matrix element is equal to the parameter x .

<SF base: sf test int: TBP>+≡

```

    procedure :: apply => sf_test_apply

```

<SF base: test auxiliary>+≡

```

subroutine sf_test_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(sf_test_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub

```

```

select case (sf_int%data%mode)
case (0)
  call sf_int%set_matrix_element &
    (cmplx (1._default, kind=default))
case (1)
  call sf_int%set_matrix_element &
    (cmplx (sf_int%x, kind=default))
end select
sf_int%status = SF_EVALUATED
end subroutine sf_test_apply

```

16.5.13 Test implementation: pair spectrum

Another template, this time for a incoming particle pair, splitting into two radiated and two outgoing particles.

Configuration data

For simplicity, the spectrum contains two mirror images of the previous structure-function configuration: the incoming and all outgoing particles are test scalars.

We have two versions, one with radiated particles, one without.

```

<SF base: test types>+≡
type, extends (sf_data_t) :: sf_test_spectrum_data_t
  class(model_data_t), pointer :: model => null ()
  type(flavor_t) :: flv_in
  type(flavor_t) :: flv_out
  type(flavor_t) :: flv_rad
  logical :: with_radiation = .true.
  real(default) :: m = 0
contains
  <SF base: sf test spectrum data: TBP>
end type sf_test_spectrum_data_t

```

Output.

```

<SF base: sf test spectrum data: TBP>≡
  procedure :: write => sf_test_spectrum_data_write

<SF base: test auxiliary>+≡
subroutine sf_test_spectrum_data_write (data, unit, verbose)
  class(sf_test_spectrum_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "SF test spectrum data:"
  write (u, "(3x,A,A)") "model      = ", char (data%model%get_name ())
  write (u, "(3x,A)", advance="no") "incoming  = "
  call data%flv_in%write (u); write (u, *)
  write (u, "(3x,A)", advance="no") "outgoing  = "
  call data%flv_out%write (u); write (u, *)
  write (u, "(3x,A)", advance="no") "radiated  = "
  call data%flv_rad%write (u); write (u, *)

```

```

        write (u, "(3x,A," // FMT_19 // ")") "mass      = ", data%m
    end subroutine sf_test_spectrum_data_write

```

Initialization.

```

<SF base: sf test spectrum data: TBP>+≡
    procedure :: init => sf_test_spectrum_data_init

<SF base: test auxiliary>+≡
    subroutine sf_test_spectrum_data_init (data, model, pdg_in, with_radiation)
        class(sf_test_spectrum_data_t), intent(out) :: data
        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), intent(in) :: pdg_in
        logical, intent(in) :: with_radiation
        data%model => model
        data%with_radiation = with_radiation
        if (pdg_array_get (pdg_in, 1) /= 25) then
            call msg_fatal ("Test structure function: input flavor must be 's'")
        end if
        call data%flv_in%init (25, model)
        data%m = data%flv_in%get_mass ()
        call data%flv_out%init (25, model)
        if (with_radiation) then
            call data%flv_rad%init (25, model)
        end if
    end subroutine sf_test_spectrum_data_init

```

Return the number of parameters: 2, since we have only collinear splitting here.

```

<SF base: sf test spectrum data: TBP>+≡
    procedure :: get_n_par => sf_test_spectrum_data_get_n_par

<SF base: test auxiliary>+≡
    function sf_test_spectrum_data_get_n_par (data) result (n)
        class(sf_test_spectrum_data_t), intent(in) :: data
        integer :: n
        n = 2
    end function sf_test_spectrum_data_get_n_par

```

Return the outgoing particle PDG codes: 25

```

<SF base: sf test spectrum data: TBP>+≡
    procedure :: get_pdg_out => sf_test_spectrum_data_get_pdg_out

<SF base: test auxiliary>+≡
    subroutine sf_test_spectrum_data_get_pdg_out (data, pdg_out)
        class(sf_test_spectrum_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        pdg_out(1) = 25
        pdg_out(2) = 25
    end subroutine sf_test_spectrum_data_get_pdg_out

```

Allocate the matching interaction.

```

<SF base: sf test spectrum data: TBP>+≡
    procedure :: allocate_sf_int => &
        sf_test_spectrum_data_allocate_sf_int

```



```

<SF base: test auxiliary>+=
  subroutine sf_test_spectrum_data_allocate_sf_int (data, sf_int)
    class(sf_test_spectrum_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (sf_test_spectrum_t :: sf_int)
  end subroutine sf_test_spectrum_data_allocate_sf_int

```

Interaction

```

<SF base: test types>+=
  type, extends (sf_int_t) :: sf_test_spectrum_t
    type(sf_test_spectrum_data_t), pointer :: data => null ()
    contains
    <SF base: sf test spectrum: TBP>
  end type sf_test_spectrum_t

<SF base: sf test spectrum: TBP>=
  procedure :: type_string => sf_test_spectrum_type_string

<SF base: test auxiliary>+=
  function sf_test_spectrum_type_string (object) result (string)
    class(sf_test_spectrum_t), intent(in) :: object
    type(string_t) :: string
    string = "Test Spectrum"
  end function sf_test_spectrum_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF base: sf test spectrum: TBP>+=
  procedure :: write => sf_test_spectrum_write

<SF base: test auxiliary>+=
  subroutine sf_test_spectrum_write (object, unit, testflag)
    class(sf_test_spectrum_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "SF test spectrum data: [undefined]"
    end if
  end subroutine sf_test_spectrum_write

```

Initialize. We know that `data` will be of concrete type `sf_test_spectrum_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass, but keep the radiated mass zero.

Optionally, we can provide minimum and maximum values for the momentum transfer.

```

<SF base: sf test spectrum: TBP>+=

```

```

procedure :: init => sf_test_spectrum_init
(SF base: test auxiliary)+≡
subroutine sf_test_spectrum_init (sf_int, data)
  class(sf_test_spectrum_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
  type(quantum_numbers_mask_t), dimension(6) :: mask
  type(helicity_t) :: hel0
  type(color_t) :: col0
  type(quantum_numbers_t), dimension(6) :: qn
  mask = quantum_numbers_mask (.false., .false., .false.)
  select type (data)
  type is (sf_test_spectrum_data_t)
    if (data%with_radiation) then
      call sf_int%base_init (mask(1:6), &
        [data%m**2, data%m**2], &
        [0._default, 0._default], &
        [data%m**2, data%m**2])
      sf_int%data => data
      call hel0%init (0)
      call col0%init ()
      call qn(1)%init (data%flv_in, col0, hel0)
      call qn(2)%init (data%flv_in, col0, hel0)
      call qn(3)%init (data%flv_rad, col0, hel0)
      call qn(4)%init (data%flv_rad, col0, hel0)
      call qn(5)%init (data%flv_out, col0, hel0)
      call qn(6)%init (data%flv_out, col0, hel0)
      call sf_int%add_state (qn(1:6))
      call sf_int%set_incoming ([1,2])
      call sf_int%set_radiated ([3,4])
      call sf_int%set_outgoing ([5,6])
    else
      call sf_int%base_init (mask(1:4), &
        [data%m**2, data%m**2], &
        [real(default) :: ], &
        [data%m**2, data%m**2])
      sf_int%data => data
      call hel0%init (0)
      call col0%init ()
      call qn(1)%init (data%flv_in, col0, hel0)
      call qn(2)%init (data%flv_in, col0, hel0)
      call qn(3)%init (data%flv_out, col0, hel0)
      call qn(4)%init (data%flv_out, col0, hel0)
      call sf_int%add_state (qn(1:4))
      call sf_int%set_incoming ([1,2])
      call sf_int%set_outgoing ([3,4])
    end if
    call sf_int%freeze ()
  end select
  sf_int%status = SF_INITIAL
end subroutine sf_test_spectrum_init

```

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, we are asked to provide an efficient mapping. For the test case, we set $x = r^2$ (as above) for both x parameters and consequently $f(r) = 4r_1r_2$.

```

(SF base: sf test spectrum: TBP)+≡
  procedure :: complete_kinematics => sf_test_spectrum_complete_kinematics

(SF base: test auxiliary)+≡
  subroutine sf_test_spectrum_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(sf_test_spectrum_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    real(default), dimension(2) :: xb1
    if (map) then
      x = r**2
      f = 4 * r(1) * r(2)
    else
      x = r
      f = 1
    end if
    xb = 1 - x
    if (sf_int%data%with_radiation) then
      call sf_int%split_momenta (x, xb)
    else
      call sf_int%reduce_momenta (x)
    end if
    select case (sf_int%status)
    case (SF_FAILED_KINEMATICS); f = 0
    end select
  end subroutine sf_test_spectrum_complete_kinematics

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

(SF base: sf test spectrum: TBP)+≡
  procedure :: inverse_kinematics => sf_test_spectrum_inverse_kinematics

(SF base: test auxiliary)+≡
  subroutine sf_test_spectrum_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(sf_test_spectrum_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    real(default), dimension(2) :: xb1
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    if (map) then

```

```

        r = sqrt (x)
        f = 4 * r(1) * r(2)
    else
        r = x
        f = 1
    end if
    rb = 1 - r
    if (set_mom) then
        if (sf_int%data%with_radiation) then
            call sf_int%split_momenta (x, xb)
        else
            call sf_int%reduce_momenta (x)
        end if
        select case (sf_int%status)
        case (SF_FAILED_KINEMATICS); f = 0
        end select
    end if
end subroutine sf_test_spectrum_inverse_kinematics

```

Apply the structure function. The matrix element becomes unity and the application always succeeds.

<SF base: sf test spectrum: TBP>+≡

```

    procedure :: apply => sf_test_spectrum_apply

```

<SF base: test auxiliary>+≡

```

subroutine sf_test_spectrum_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(sf_test_spectrum_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    call sf_int%set_matrix_element &
        (cmplx (1._default, kind=default))
    sf_int%status = SF_EVALUATED
end subroutine sf_test_spectrum_apply

```

16.5.14 Test implementation: generator spectrum

A generator for two beams, no radiation (for simplicity).

Configuration data

For simplicity, the spectrum contains two mirror images of the previous structure-function configuration: the incoming and all outgoing particles are test scalars.

We have two versions, one with radiated particles, one without.

<SF base: test types>+≡

```

type, extends (sf_data_t) :: sf_test_generator_data_t
    class(model_data_t), pointer :: model => null ()
    type(flavor_t) :: flv_in
    type(flavor_t) :: flv_out
    type(flavor_t) :: flv_rad
    real(default) :: m = 0

```

```

contains
  <SF base: sf test generator data: TBP>
end type sf_test_generator_data_t

```

Output.

```

<SF base: sf test generator data: TBP>≡
  procedure :: write => sf_test_generator_data_write

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_data_write (data, unit, verbose)
    class(sf_test_generator_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "SF test generator data:"
    write (u, "(3x,A,A)") "model      = ", char (data%model%get_name ())
    write (u, "(3x,A)", advance="no") "incoming  = "
    call data%flv_in%write (u); write (u, *)
    write (u, "(3x,A)", advance="no") "outgoing  = "
    call data%flv_out%write (u); write (u, *)
    write (u, "(3x,A," // FMT_19 // ")") "mass      = ", data%m
  end subroutine sf_test_generator_data_write

```

Initialization.

```

<SF base: sf test generator data: TBP>+≡
  procedure :: init => sf_test_generator_data_init

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_data_init (data, model, pdg_in)
    class(sf_test_generator_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    data%model => model
    if (pdg_array_get (pdg_in, 1) /= 25) then
      call msg_fatal ("Test generator: input flavor must be 's'")
    end if
    call data%flv_in%init (25, model)
    data%m = data%flv_in%get_mass ()
    call data%flv_out%init (25, model)
  end subroutine sf_test_generator_data_init

```

This structure function is a generator.

```

<SF base: sf test generator data: TBP>+≡
  procedure :: is_generator => sf_test_generator_data_is_generator

<SF base: test auxiliary>+≡
  function sf_test_generator_data_is_generator (data) result (flag)
    class(sf_test_generator_data_t), intent(in) :: data
    logical :: flag
    flag = .true.
  end function sf_test_generator_data_is_generator

```

Return the number of parameters: 2, since we have only collinear splitting here.

```

<SF base: sf test generator data: TBP>+≡
  procedure :: get_n_par => sf_test_generator_data_get_n_par
<SF base: test auxiliary>+≡
  function sf_test_generator_data_get_n_par (data) result (n)
    class(sf_test_generator_data_t), intent(in) :: data
    integer :: n
    n = 2
  end function sf_test_generator_data_get_n_par

```

Return the outgoing particle PDG codes: 25

```

<SF base: sf test generator data: TBP>+≡
  procedure :: get_pdg_out => sf_test_generator_data_get_pdg_out
<SF base: test auxiliary>+≡
  subroutine sf_test_generator_data_get_pdg_out (data, pdg_out)
    class(sf_test_generator_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    pdg_out(1) = 25
    pdg_out(2) = 25
  end subroutine sf_test_generator_data_get_pdg_out

```

Allocate the matching interaction.

```

<SF base: sf test generator data: TBP>+≡
  procedure :: allocate_sf_int => &
    sf_test_generator_data_allocate_sf_int
<SF base: test auxiliary>+≡
  subroutine sf_test_generator_data_allocate_sf_int (data, sf_int)
    class(sf_test_generator_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (sf_test_generator_t :: sf_int)
  end subroutine sf_test_generator_data_allocate_sf_int

```

Interaction

```

<SF base: test types>+≡
  type, extends (sf_int_t) :: sf_test_generator_t
    type(sf_test_generator_data_t), pointer :: data => null ()
  contains
    <SF base: sf test generator: TBP>
  end type sf_test_generator_t

<SF base: sf test generator: TBP>≡
  procedure :: type_string => sf_test_generator_type_string
<SF base: test auxiliary>+≡
  function sf_test_generator_type_string (object) result (string)
    class(sf_test_generator_t), intent(in) :: object
    type(string_t) :: string
    string = "Test Generator"
  end function sf_test_generator_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF base: sf test generator: TBP>+≡
  procedure :: write => sf_test_generator_write

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_write (object, unit, testflag)
    class(sf_test_generator_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "SF test generator data: [undefined]"
    end if
  end subroutine sf_test_generator_write

```

Initialize. We know that data will be of concrete type `sf_test_generator_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass. No radiation.

```

<SF base: sf test generator: TBP>+≡
  procedure :: init => sf_test_generator_init

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_init (sf_int, data)
    class(sf_test_generator_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(4) :: mask
    type(helicity_t) :: hel0
    type(color_t) :: col0
    type(quantum_numbers_t), dimension(4) :: qn
    mask = quantum_numbers_mask (.false., .false., .false.)
    select type (data)
    type is (sf_test_generator_data_t)
      call sf_int%base_init (mask(1:4), &
        [data%m**2, data%m**2], &
        [real(default) :: ], &
        [data%m**2, data%m**2])
      sf_int%data => data
      call hel0%init (0)
      call col0%init ()
      call qn(1)%init (data%flv_in, col0, hel0)
      call qn(2)%init (data%flv_in, col0, hel0)
      call qn(3)%init (data%flv_out, col0, hel0)
      call qn(4)%init (data%flv_out, col0, hel0)
      call sf_int%add_state (qn(1:4))
      call sf_int%set_incoming ([1,2])
      call sf_int%set_outgoing ([3,4])
      call sf_int%freeze ()
    end select
    sf_int%status = SF_INITIAL
  end subroutine sf_test_generator_init

```

```
end subroutine sf_test_generator_init
```

This structure function is a generator.

```
<SF base: sf test generator: TBP>+≡
  procedure :: is_generator => sf_test_generator_is_generator

<SF base: test auxiliary>+≡
  function sf_test_generator_is_generator (sf_int) result (flag)
    class(sf_test_generator_t), intent(in) :: sf_int
    logical :: flag
    flag = sf_int%data%is_generator ()
  end function sf_test_generator_is_generator
```

Generate free parameters. This mock generator always produces the nubmers 0.8 and 0.5.

```
<SF base: sf test generator: TBP>+≡
  procedure :: generate_free => sf_test_generator_generate_free

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_generate_free (sf_int, r, rb, x_free)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(inout) :: x_free
    r = [0.8, 0.5]
    rb= 1 - r
    x_free = x_free * product (r)
  end subroutine sf_test_generator_generate_free
```

Recover momentum fractions. Since the x values are free, we also set the x_free parameter.

```
<SF base: sf test generator: TBP>+≡
  procedure :: recover_x => sf_test_generator_recover_x

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_recover_x (sf_int, x, xb, x_free)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb)
    if (present (x_free)) x_free = x_free * product (x)
  end subroutine sf_test_generator_recover_x
```

Set kinematics. Since this is a generator, just transfer input to output.

```
<SF base: sf test generator: TBP>+≡
  procedure :: complete_kinematics => sf_test_generator_complete_kinematics

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
```



```

real(default), dimension(:), intent(in) :: r
real(default), dimension(:), intent(in) :: rb
logical, intent(in) :: map
x = r
xb= rb
f = 1
call sf_int%reduce_momenta (x)
end subroutine sf_test_generator_complete_kinematics

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF base: sf test generator: TBP>+≡
  procedure :: inverse_kinematics => sf_test_generator_inverse_kinematics

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    r = x
    rb= xb
    f = 1
    if (set_mom) call sf_int%reduce_momenta (x)
  end subroutine sf_test_generator_inverse_kinematics

```

Apply the structure function. The matrix element becomes unity and the application always succeeds.

```

<SF base: sf test generator: TBP>+≡
  procedure :: apply => sf_test_generator_apply

<SF base: test auxiliary>+≡
  subroutine sf_test_generator_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(sf_test_generator_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    call sf_int%set_matrix_element &
      (cmplx (1._default, kind=default))
    sf_int%status = SF_EVALUATED
  end subroutine sf_test_generator_apply

```

Test structure function data

Construct and display a test structure function data object.

```
<SF base: execute tests>≡
  call test (sf_base_1, "sf_base_1", &
    "structure function configuration", &
    u, results)

<SF base: test declarations>≡
  public :: sf_base_1

<SF base: tests>≡
  subroutine sf_base_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(pdg_array_t), dimension(1) :: pdg_out
    integer, dimension(:), allocatable :: pdg1
    class(sf_data_t), allocatable :: data

    write (u, "(A)")  "* Test output: sf_base_1"
    write (u, "(A)")  "*   Purpose: initialize and display &
      &test structure function data"
    write (u, "(A)")

    call model%init_test ()
    pdg_in = 25

    allocate (sf_test_data_t :: data)
    select type (data)
    type is (sf_test_data_t)
      call data%init (model, pdg_in)
    end select

    call data%write (u)

    write (u, "(A)")

    write (u, "(1x,A)") "Outgoing particle code:"
    call data%get_pdg_out (pdg_out)
    pdg1 = pdg_out(1)
    write (u, "(2x,99(1x,I0))")  pdg1

    call model%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: sf_base_1"

  end subroutine sf_base_1
```

Test and probe structure function

Construct and display a structure function object based on the test structure function.

```

<SF base: execute tests>+≡
  call test (sf_base_2, "sf_base_2", &
    "structure function instance", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_2

<SF base: tests>+≡
  subroutine sf_base_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_base_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    pdg_in = 25
    call flv%init (25, model)

    call reset_interaction_counter ()

    allocate (sf_test_data_t :: data)
    select type (data)
    type is (sf_test_data_t)
      call data%init (model, pdg_in)
    end select

    write (u, "(A)")  "* Initialize structure-function object"
    write (u, "(A)")

    call data%allocate_sf_int (sf_int)
    call sf_int%init (data)
    call sf_int%set_beam_index ([1])

    call sf_int%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize incoming momentum with E=500"
    write (u, "(A)")
    E = 500

```

```

k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=1"
write (u, "(A)")

r = 1
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Set kinematics with mapping for r=0.8"
write (u, "(A)")

```

```

r = 0.8_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)") "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)") "* Compute inverse kinematics for x=0.64 and evaluate"
write (u, "(A)")

x = 0.64_default
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%apply (scale=0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_base_2"

end subroutine sf_base_2

```

Collinear kinematics

Scan over the possibilities for mass assignment and on-shell projections, collinear case.

```
<SF base: execute tests>+≡
  call test (sf_base_3, "sf_base_3", &
    "alternatives for collinear kinematics", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_3

<SF base: tests>+≡
  subroutine sf_base_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_base_3"
    write (u, "(A)")  "*   Purpose: check various kinematical setups"
    write (u, "(A)")  "*               for collinear structure-function splitting."
    write (u, "(A)")  "               (two masses equal, one zero)"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    pdg_in = 25
    call flv%init (25, model)

    call reset_interaction_counter ()

    allocate (sf_test_data_t :: data)
    select type (data)
    type is (sf_test_data_t)
      call data%init (model, pdg_in)
    end select

    write (u, "(A)")  "* Initialize structure-function object"
    write (u, "(A)")

    call data%allocate_sf_int (sf_int)
    call sf_int%init (data)
```

```

call sf_int%write (u)

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"

E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set radiated mass to zero"

sf_int%mr2 = 0
sf_int%mo2 = sf_int%mi2

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping energy"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping momentum"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

```

```

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set outgoing mass to zero"

sf_int%mr2 = sf_int%mi2
sf_int%mo2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping energy"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping momentum"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r

```



```

write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set incoming mass to zero"

k = vector4_moving (E, E, 3)
call sf_int%seed_kinematics ([k])

sf_int%mr2 = sf_int%mi2
sf_int%mo2 = sf_int%mi2
sf_int%mi2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping energy"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping momentum"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

```

```

write (u, "(A)")
write (u, "(A)")  "* Set all masses to zero"

sf_int%mr2 = 0
sf_int%mo2 = 0
sf_int%mi2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping energy"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5, keeping momentum"
write (u, "(A)")

r = 0.5_default
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_3"

end subroutine sf_base_3

```

Non-collinear kinematics

Scan over the possibilities for mass assignment and on-shell projections, non-collinear case.

```

<SF base: execute tests>+≡
  call test (sf_base_4, "sf_base_4", &
    "alternatives for non-collinear kinematics", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_4

<SF base: tests>+≡
  subroutine sf_base_4 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_base_4"
    write (u, "(A)")  "* Purpose: check various kinematical setups"
    write (u, "(A)")  "*           for free structure-function splitting."
    write (u, "(A)")  "           (two masses equal, one zero)"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    pdg_in = 25
    call flv%init (25, model)

    call reset_interaction_counter ()

    allocate (sf_test_data_t :: data)
    select type (data)
    type is (sf_test_data_t)
      call data%init (model, pdg_in, collinear=.false.)
    end select

    write (u, "(A)")  "* Initialize structure-function object"

```

```

write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%write (u)

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"

E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ( )**2), 3)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set radiated mass to zero"

sf_int%mr2 = 0
sf_int%mo2 = sf_int%mi2

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping energy"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping momentum"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

```

```

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set outgoing mass to zero"

sf_int%mr2 = sf_int%mi2
sf_int%mo2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping energy"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping momentum"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

```

```

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set incoming mass to zero"

k = vector4_moving (E, E, 3)
call sf_int%seed_kinematics ([k])

sf_int%mr2 = sf_int%mi2
sf_int%mo2 = sf_int%mi2
sf_int%mi2 = 0

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping energy"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping momentum"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)

```

```

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set all masses to zero"

sf_int%mr2 = 0
sf_int%mo2 = 0
sf_int%mi2 = 0

write (u, "(A)")
write (u, "(A)")  "* Re-Initialize structure-function object with Q bounds"

call reset_interaction_counter ()

select type (data)
type is (sf_test_data_t)
    call data%init (model, pdg_in, collinear=.false., &
        qbounds = [1._default, 100._default])
end select

call sf_int%init (data)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping energy"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.125, keeping momentum"
write (u, "(A)")

r = [0.5_default, 0.5_default, 0.125_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_MOMENTUM

```

```

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recover x and r"
write (u, "(A)")

call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_4"

end subroutine sf_base_4

```

Pair spectrum

Construct and display a structure function object for a pair spectrum (a structure function involving two particles simultaneously).

```

<SF base: execute tests>+≡
call test (sf_base_5, "sf_base_5", &
    "pair spectrum with radiation", &
    u, results)

<SF base: test declarations>+≡
public :: sf_base_5

<SF base: tests>+≡
subroutine sf_base_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(pdg_array_t), dimension(2) :: pdg_out
    integer, dimension(:), allocatable :: pdg1, pdg2
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t), dimension(2) :: k
    type(vector4_t), dimension(4) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

```



```

write (u, "(A)")  "* Test output: sf_base_5"
write (u, "(A)")  "* Purpose: initialize and fill &
    &a pair spectrum object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)
pdg_in = 25

call reset_interaction_counter ()

allocate (sf_test_spectrum_data_t :: data)
select type (data)
type is (sf_test_spectrum_data_t)
    call data%init (model, pdg_in, with_radiation=.true.)
end select

write (u, "(1x,A)")  "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
pdg2 = pdg_out(2)
write (u, "(2x,99(1x,I0))")  pdg1, pdg2

write (u, "(A)")
write (u, "(A)")  "* Initialize spectrum object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momenta with sqrts=1000"

E = 500
k(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
k(2) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call sf_int%seed_kinematics (k)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.4,0.8"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.4_default, 0.8_default]
rb = 1 - r

```

```

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)") "* Set kinematics with mapping for r=0.6,0.8"
write (u, "(A)")

r = [0.6_default, 0.8_default]
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)") "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call reset_interaction_counter ()
call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%seed_kinematics (k)
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)") "* Compute inverse kinematics for x=0.36,0.64 &
&and evaluate"
write (u, "(A)")

x = [0.36_default, 0.64_default]
xb = 1 - x
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true.)
call sf_int%apply (scale=0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb

```

```

write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_5"

end subroutine sf_base_5

```

Pair spectrum without radiation

Construct and display a structure function object for a pair spectrum (a structure function involving two particles simultaneously).

```

<SF base: execute tests>+≡
  call test (sf_base_6, "sf_base_6", &
    "pair spectrum without radiation", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_6

<SF base: tests>+≡
  subroutine sf_base_6 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(flavor_t) :: flv
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t), dimension(2) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_base_6"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &a pair spectrum object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

```

```

allocate (sf_test_spectrum_data_t :: data)
select type (data)
type is (sf_test_spectrum_data_t)
    call data%init (model, pdg_in, with_radiation=.false.)
end select

write (u, "(A)")  "* Initialize spectrum object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

write (u, "(A)")  "* Initialize incoming momenta with sqrts=1000"

E = 500
k(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
k(2) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call sf_int%seed_kinematics (k)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.4,0.8"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.4_default, 0.8_default]
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call reset_interaction_counter ()
call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%seed_kinematics (k)
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
write (u, "(A,9(1x,F10.7))")  "x =", x

```

```

write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)")  "* Compute inverse kinematics for x=0.4,0.8 &
    &and evaluate"
write (u, "(A)")

x = [0.4_default, 0.8_default]
xb = 1 - x
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale=0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_6"

end subroutine sf_base_6

```

Direct access to structure function

Probe a structure function directly.

```

<SF base: execute tests>+≡
    call test (sf_base_7, "sf_base_7", &
        "direct access", &
        u, results)

<SF base: test declarations>+≡
    public :: sf_base_7

<SF base: tests>+≡
    subroutine sf_base_7 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(pdg_array_t) :: pdg_in
        type(flavor_t) :: flv
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        real(default), dimension(:), allocatable :: value

        write (u, "(A)")  "* Test output: sf_base_7"
        write (u, "(A)")  "* Purpose: check direct access method"
        write (u, "(A)")

```

```

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)
pdg_in = 25

call reset_interaction_counter ()

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (model, pdg_in)
end select

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

write (u, "(A)")  "* Probe structure function: states"
write (u, "(A)")

write (u, "(A,I0)")  "n_states = ", sf_int%get_n_states ()
write (u, "(A,I0)")  "n_in      = ", sf_int%get_n_in ()
write (u, "(A,I0)")  "n_rad     = ", sf_int%get_n_rad ()
write (u, "(A,I0)")  "n_out     = ", sf_int%get_n_out ()
write (u, "(A)")
write (u, "(A)", advance="no")  "state(1) = "
call quantum_numbers_write (sf_int%get_state (1), u)
write (u, *)

allocate (value (sf_int%get_n_states ()))
call sf_int%compute_values (value, &
    E=[500._default], x=[0.5_default], xb=[0.5_default], scale=0._default)

write (u, "(A)")
write (u, "(A)", advance="no")  "value (E=500, x=0.5) ="
write (u, "(9(1x," // FMT_19 // "))" value

call sf_int%compute_values (value, &
    x=[0.1_default], xb=[0.9_default], scale=0._default)

write (u, "(A)")
write (u, "(A)", advance="no")  "value (E=500, x=0.1) ="
write (u, "(9(1x," // FMT_19 // "))" value

write (u, "(A)")
write (u, "(A)")  "* Initialize spectrum object"
write (u, "(A)")

deallocate (value)

```

```

call sf_int%final ()
deallocate (sf_int)
deallocate (data)

allocate (sf_test_spectrum_data_t :: data)
select type (data)
type is (sf_test_spectrum_data_t)
  call data%init (model, pdg_in, with_radiation=.false.)
end select

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

write (u, "(A)")  "* Probe spectrum: states"
write (u, "(A)")

write (u, "(A,I0)")  "n_states = ", sf_int%get_n_states ()
write (u, "(A,I0)")  "n_in      = ", sf_int%get_n_in ()
write (u, "(A,I0)")  "n_rad     = ", sf_int%get_n_rad ()
write (u, "(A,I0)")  "n_out     = ", sf_int%get_n_out ()
write (u, "(A)")
write (u, "(A)", advance="no")  "state(1) = "
call quantum_numbers_write (sf_int%get_state (1), u)
write (u, *)

allocate (value (sf_int%get_n_states ()))
call sf_int%compute_value (1, value(1), &
  E = [500._default, 500._default], &
  x = [0.5_default, 0.6_default], &
  xb= [0.5_default, 0.4_default], &
  scale = 0._default)

write (u, "(A)")
write (u, "(A)", advance="no")  "value (E=500,500, x=0.5,0.6) ="
write (u, "(9(1x," // FMT_19 // "))" value

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_7"

end subroutine sf_base_7

```

Structure function chain configuration

```

<SF base: execute tests>+≡
call test (sf_base_8, "sf_base_8", &
  "structure function chain configuration", &
  u, results)

```

```

<SF base: test declarations>+=
  public :: sf_base_8

<SF base: tests>+=
  subroutine sf_base_8 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    type(beam_data_t), target :: beam_data
    class(sf_data_t), allocatable, target :: data_strfun
    class(sf_data_t), allocatable, target :: data_spectrum
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_chain_t) :: sf_chain

    write (u, "(A)")  "* Test output: sf_base_8"
    write (u, "(A)")  "* Purpose: set up a structure-function chain"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

    call beam_data%init_sqrts (1000._default, [flv, flv])

    allocate (sf_test_data_t :: data_strfun)
    select type (data_strfun)
    type is (sf_test_data_t)
      call data_strfun%init (model, pdg_in)
    end select

    allocate (sf_test_spectrum_data_t :: data_spectrum)
    select type (data_spectrum)
    type is (sf_test_spectrum_data_t)
      call data_spectrum%init (model, pdg_in, with_radiation=.true.)
    end select

    write (u, "(A)")  "* Set up chain with beams only"
    write (u, "(A)")

    call sf_chain%init (beam_data)
    call write_separator (u, 2)
    call sf_chain%write (u)
    call write_separator (u, 2)
    call sf_chain%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Set up chain with structure function"
    write (u, "(A)")

```



```

allocate (sf_config (1))
call sf_config(1)%init ([1], data_strfun)
call sf_chain%init (beam_data, sf_config)

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Set up chain with spectrum and structure function"
write (u, "(A)")

deallocate (sf_config)
allocate (sf_config (2))
call sf_config(1)%init ([1,2], data_spectrum)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_8"

end subroutine sf_base_8

```

Structure function instance configuration

We create a structure-function chain instance which implements a configured structure-function chain. We link the momentum entries in the interactions and compute kinematics.

We do not actually connect the interactions and create evaluators. We skip this step and manually advance the status of the chain instead.

```

<SF base: execute tests>+≡
  call test (sf_base_9, "sf_base_9", &
    "structure function chain instance", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_9

<SF base: tests>+≡
  subroutine sf_base_9 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model

```

```

type(flavor_t) :: flv
type(pdg_array_t) :: pdg_in
type(beam_data_t), target :: beam_data
class(sf_data_t), allocatable, target :: data_strfun
class(sf_data_t), allocatable, target :: data_spectrum
type(sf_config_t), dimension(:), allocatable, target :: sf_config
type(sf_chain_t), target :: sf_chain
type(sf_chain_instance_t), target :: sf_chain_instance
type(sf_channel_t), dimension(2) :: sf_channel
type(vector4_t), dimension(2) :: p
integer :: j

write (u, "(A)")  "* Test output: sf_base_9"
write (u, "(A)")  "* Purpose: set up a structure-function chain &
                    &and create an instance"
write (u, "(A)")  "* compute kinematics"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)
pdg_in = 25

call reset_interaction_counter ()

call beam_data%init_sqrts (1000._default, [flv, flv])

allocate (sf_test_data_t :: data_strfun)
select type (data_strfun)
type is (sf_test_data_t)
    call data_strfun%init (model, pdg_in)
end select

allocate (sf_test_spectrum_data_t :: data_spectrum)
select type (data_spectrum)
type is (sf_test_spectrum_data_t)
    call data_spectrum%init (model, pdg_in, with_radiation=.true.)
end select

write (u, "(A)")  "* Set up chain with beams only"
write (u, "(A)")

call sf_chain%init (beam_data)

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%compute_kinematics (1, [real(default) ::])

call write_separator (u, 2)
call sf_chain%write (u)

```

```

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call sf_chain_instance%get_out_momenta (p)

write (u, "(A)")
write (u, "(A)")  "* Outgoing momenta:"

do j = 1, 2
    write (u, "(A)")
    call vector4_write (p(j), u)
end do

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Set up chain with structure function"
write (u, "(A)")

allocate (sf_config (1))
call sf_config(1)%init ([1], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_channel(1)%init (1)
call sf_channel(1)%activate_mapping ([1])
call sf_chain_instance%set_channel (1, sf_channel(1))

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%compute_kinematics (1, [0.8_default])

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call sf_chain_instance%get_out_momenta (p)

write (u, "(A)")
write (u, "(A)")  "* Outgoing momenta:"

do j = 1, 2
    write (u, "(A)")
    call vector4_write (p(j), u)
end do

call sf_chain_instance%final ()
call sf_chain%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Set up chain with spectrum and structure function"
write (u, "(A)")

deallocate (sf_config)
allocate (sf_config (2))
call sf_config(1)%init ([1,2], data_spectrum)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_channel(2)%init (2)
call sf_channel(2)%activate_mapping ([2])
call sf_chain_instance%set_channel (1, sf_channel(2))

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%compute_kinematics &
    (1, [0.5_default, 0.6_default, 0.8_default])

call write_separator (u, 2)
call sf_chain%write (u)
call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call sf_chain_instance%get_out_momenta (p)

write (u, "(A)")
write (u, "(A)")  "* Outgoing momenta:"

do j = 1, 2
    write (u, "(A)")
    call vector4_write (p(j), u)
end do

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_9"

end subroutine sf_base_9

```

Structure function chain mappings

Set up a structure function chain instance with a pair of single-particle structure functions. We test different global mappings for this setup.

Again, we skip evaluators.

```
(SF base: execute tests)+≡
  call test (sf_base_10, "sf_base_10", &
    "structure function chain mapping", &
    u, results)

(SF base: test declarations)+≡
  public :: sf_base_10

(SF base: tests)+≡
  subroutine sf_base_10 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    type(beam_data_t), target :: beam_data
    class(sf_data_t), allocatable, target :: data_strfun
    type(sf_config_t), dimension(:), allocatable, target :: sf_config
    type(sf_chain_t), target :: sf_chain
    type(sf_chain_instance_t), target :: sf_chain_instance
    type(sf_channel_t), dimension(2) :: sf_channel
    real(default), dimension(2) :: x_saved

    write (u, "(A)")  "* Test output: sf_base_10"
    write (u, "(A)")  "*   Purpose: set up a structure-function chain"
    write (u, "(A)")  "*                   and check mappings"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

    call beam_data%init_sqrts (1000._default, [flv, flv])

    allocate (sf_test_data_t :: data_strfun)
    select type (data_strfun)
    type is (sf_test_data_t)
      call data_strfun%init (model, pdg_in)
    end select

    write (u, "(A)")  "* Set up chain with structure function pair &
      &and standard mapping"
    write (u, "(A)")

    allocate (sf_config (2))
    call sf_config(1)%init ([1], data_strfun)
```

```

call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_channel(1)%init (2)
call sf_channel(1)%set_s_mapping ([1,2])
call sf_chain_instance%set_channel (1, sf_channel(1))

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%compute_kinematics (1, [0.8_default, 0.6_default])

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Invert the kinematics calculation"
write (u, "(A)")

x_saved = sf_chain_instance%x

call sf_chain_instance%init (sf_chain, n_channel = 1)

call sf_channel(2)%init (2)
call sf_channel(2)%set_s_mapping ([1, 2])
call sf_chain_instance%set_channel (1, sf_channel(2))

call sf_chain_instance%link_interactions ()
sf_chain_instance%status = SF_DONE_CONNECTIONS
call sf_chain_instance%inverse_kinematics (x_saved, 1 - x_saved)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_10"

end subroutine sf_base_10

```

Structure function chain evaluation

Here, we test the complete workflow for structure-function chains. First, we create the template chain, then initialize an instance. We set up links, mask, and evaluators. Finally, we set kinematics and evaluate the matrix elements and their products.

```
<SF base: execute tests>+≡
  call test (sf_base_11, "sf_base_11", &
    "structure function chain evaluation", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_11

<SF base: tests>+≡
  subroutine sf_base_11 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    type(beam_data_t), target :: beam_data
    class(sf_data_t), allocatable, target :: data_strfun
    class(sf_data_t), allocatable, target :: data_spectrum
    type(sf_config_t), dimension(:), allocatable, target :: sf_config
    type(sf_chain_t), target :: sf_chain
    type(sf_chain_instance_t), target :: sf_chain_instance
    type(sf_channel_t), dimension(2) :: sf_channel
    type(particle_set_t) :: pset
    type(interaction_t), pointer :: int
    logical :: ok

    write (u, "(A)")  "* Test output: sf_base_11"
    write (u, "(A)")  "* Purpose: set up a structure-function chain"
    write (u, "(A)")  "*           create an instance and evaluate"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

    call reset_interaction_counter ()

    call beam_data%init_sqrts (1000._default, [flv, flv])

    allocate (sf_test_data_t :: data_strfun)
    select type (data_strfun)
    type is (sf_test_data_t)
      call data_strfun%init (model, pdg_in)
    end select

    allocate (sf_test_spectrum_data_t :: data_spectrum)
    select type (data_spectrum)
```

```

type is (sf_test_spectrum_data_t)
  call data_spectrum%init (model, pdg_in, with_radiation=.true.)
end select

write (u, "(A)")  "* Set up chain with beams only"
write (u, "(A)")

call sf_chain%init (beam_data)

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

call sf_chain_instance%compute_kinematics (1, [real(default) ::])
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

int => sf_chain_instance%get_out_int_ptr ()
call pset%init (ok, int, int, FM_IGNORE_HELICITY, &
  [0._default, 0._default], .false., .true.)
call sf_chain_instance%final ()

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover chain:"
write (u, "(A)")

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

int => sf_chain_instance%get_out_int_ptr ()
call pset%fill_interaction (int, 2, check_match=.false.)

call sf_chain_instance%recover_kinematics (1)
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call pset%final ()

```



```

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")
write (u, "(A)")
write (u, "(A)")  "* Set up chain with structure function"
write (u, "(A)")

allocate (sf_config (1))
call sf_config(1)%init ([1], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_channel(1)%init (1)
call sf_channel(1)%activate_mapping ([1])
call sf_chain_instance%set_channel (1, sf_channel(1))
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

call sf_chain_instance%compute_kinematics (1, [0.8_default])
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

int => sf_chain_instance%get_out_int_ptr ()
call pset%init (ok, int, int, FM_IGNORE_HELICITY, &
               [0._default, 0._default], .false., .true.)
call sf_chain_instance%final ()

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover chain:"
write (u, "(A)")

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_channel(1)%init (1)
call sf_channel(1)%activate_mapping ([1])
call sf_chain_instance%set_channel (1, sf_channel(1))
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

int => sf_chain_instance%get_out_int_ptr ()

```

```

call pset%fill_interaction (int, 2, check_match=.false.)

call sf_chain_instance%recover_kinematics (1)
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call pset%final ()
call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")
write (u, "(A)")
write (u, "(A)")  "* Set up chain with spectrum and structure function"
write (u, "(A)")

deallocate (sf_config)
allocate (sf_config (2))
call sf_config(1)%init ([1,2], data_spectrum)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_channel(2)%init (2)
call sf_channel(2)%activate_mapping ([2])
call sf_chain_instance%set_channel (1, sf_channel(2))
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

call sf_chain_instance%compute_kinematics &
    (1, [0.5_default, 0.6_default, 0.8_default])
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

int => sf_chain_instance%get_out_int_ptr ()
call pset%init (ok, int, int, FM_IGNORE_HELICITY, &
    [0._default, 0._default], .false., .true.)
call sf_chain_instance%final ()

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Recover chain:"
write (u, "(A)")

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_channel(2)%init (2)
call sf_channel(2)%activate_mapping ([2])
call sf_chain_instance%set_channel (1, sf_channel(2))
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

int => sf_chain_instance%get_out_int_ptr ()
call pset%fill_interaction (int, 2, check_match=.false.)

call sf_chain_instance%recover_kinematics (1)
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

call pset%final ()
call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_11"

end subroutine sf_base_11

```

Multichannel case

We set up a structure-function chain as before, but with three different parameterizations. The first instance is without mappings, the second one with single-particle mappings, and the third one with two-particle mappings.

```

<SF base: execute tests>+≡
  call test (sf_base_12, "sf_base_12", &
    "multi-channel structure function chain", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_12

<SF base: tests>+≡
  subroutine sf_base_12 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model

```

```

type(flavor_t) :: flv
type(pdg_array_t) :: pdg_in
type(beam_data_t), target :: beam_data
class(sf_data_t), allocatable, target :: data
type(sf_config_t), dimension(:), allocatable, target :: sf_config
type(sf_chain_t), target :: sf_chain
type(sf_chain_instance_t), target :: sf_chain_instance
real(default), dimension(2) :: x_saved
real(default), dimension(2,3) :: p_saved
type(sf_channel_t), dimension(:), allocatable :: sf_channel

write (u, "(A)")  "* Test output: sf_base_12"
write (u, "(A)")  "* Purpose: set up and evaluate a multi-channel &
&structure-function chain"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)
pdg_in = 25

call reset_interaction_counter ()

call beam_data%init_sqrts (1000._default, [flv, flv])

allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (model, pdg_in)
end select

write (u, "(A)")  "* Set up chain with structure function pair &
&and three different mappings"
write (u, "(A)")

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call sf_chain%init(beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 3)

call allocate_sf_channels (sf_channel, n_channel = 3, n_strfun = 2)

! channel 1: no mapping
call sf_chain_instance%set_channel (1, sf_channel(1))

! channel 2: single-particle mappings
call sf_channel(2)%activate_mapping ([1,2])
! call sf_chain_instance%activate_mapping (2, [1,2])
call sf_chain_instance%set_channel (2, sf_channel(2))

```

```

! channel 3: two-particle mapping
call sf_channel(3)%set_s_mapping ([1,2])
! call sf_chain_instance%set_s_mapping (3, [1, 2])
call sf_chain_instance%set_channel (3, sf_channel(3))

call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

write (u, "(A)")  "* Compute kinematics in channel 1 and evaluate"
write (u, "(A)")

call sf_chain_instance%compute_kinematics (1, [0.8_default, 0.6_default])
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Invert the kinematics calculation"
write (u, "(A)")

x_saved = sf_chain_instance%x

call sf_chain_instance%inverse_kinematics (x_saved, 1 - x_saved)
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Compute kinematics in channel 2 and evaluate"
write (u, "(A)")

p_saved = sf_chain_instance%p

call sf_chain_instance%compute_kinematics (2, p_saved(:,2))
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Compute kinematics in channel 3 and evaluate"
write (u, "(A)")

call sf_chain_instance%compute_kinematics (3, p_saved(:,3))
call sf_chain_instance%evaluate (scale=0._default)

call write_separator (u, 2)
call sf_chain_instance%write (u)

```

```

call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_chain_instance%final ()
call sf_chain%final ()

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_12"

end subroutine sf_base_12

```

Generated spectrum

Construct and evaluate a structure function object for a pair spectrum which is evaluated as a beam-event generator.

```

<SF base: execute tests>+≡
  call test (sf_base_13, "sf_base_13", &
    "pair spectrum generator", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_13

<SF base: tests>+≡
  subroutine sf_base_13 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t), dimension(2) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, x_free

    write (u, "(A)")  "* Test output: sf_base_13"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &a pair generator object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)
    pdg_in = 25

```

```

call reset_interaction_counter ()

allocate (sf_test_generator_data_t :: data)
select type (data)
type is (sf_test_generator_data_t)
    call data%init (model, pdg_in)
end select

write (u, "(A)")  "* Initialize generator object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

write (u, "(A)")  "* Generate free r values"
write (u, "(A)")

x_free = 1
call sf_int%generate_free (r, rb, x_free)

write (u, "(A)")  "* Initialize incoming momenta with sqrts=1000"

E = 500
k(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
k(2) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call sf_int%seed_kinematics (k)

write (u, "(A)")
write (u, "(A)")  "* Complete kinematics"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call reset_interaction_counter ()

```

```

call data%allocate_sf_int (sf_int)
call sf_int%init (data)

call sf_int%seed_kinematics (k)
call sf_int%set_momenta (q, outgoing=.true.)
x_free = 1
call sf_int%recover_x (x, xb, x_free)
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Compute inverse kinematics &
&and evaluate"
write (u, "(A)")

call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale=0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_base_13"

end subroutine sf_base_13

```

Structure function chain evaluation

Here, we test the complete workflow for a structure-function chain with generator. First, we create the template chain, then initialize an instance. We set up links, mask, and evaluators. Finally, we set kinematics and evaluate the matrix elements and their products.

```

<SF base: execute tests>+≡
  call test (sf_base_14, "sf_base_14", &
    "structure function generator evaluation", &
    u, results)

<SF base: test declarations>+≡
  public :: sf_base_14

<SF base: tests>+≡
  subroutine sf_base_14 (u)
    integer, intent(in) :: u

```



```

type(model_data_t), target :: model
type(flavor_t) :: flv
type(pdg_array_t) :: pdg_in
type(beam_data_t), target :: beam_data
class(sf_data_t), allocatable, target :: data_strfun
class(sf_data_t), allocatable, target :: data_generator
type(sf_config_t), dimension(:), allocatable, target :: sf_config
real(default), dimension(:), allocatable :: p_in
type(sf_chain_t), target :: sf_chain
type(sf_chain_instance_t), target :: sf_chain_instance

write (u, "(A)")  "* Test output: sf_base_14"
write (u, "(A)")  "* Purpose: set up a structure-function chain"
write (u, "(A)")  "*           create an instance and evaluate"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)
pdg_in = 25

call reset_interaction_counter ()

call beam_data%init_sqrts (1000._default, [flv, flv])

allocate (sf_test_data_t :: data_strfun)
select type (data_strfun)
type is (sf_test_data_t)
    call data_strfun%init (model, pdg_in)
end select

allocate (sf_test_generator_data_t :: data_generator)
select type (data_generator)
type is (sf_test_generator_data_t)
    call data_generator%init (model, pdg_in)
end select

write (u, "(A)")  "* Set up chain with generator and structure function"
write (u, "(A)")

allocate (sf_config (2))
call sf_config(1)%init ([1,2], data_generator)
call sf_config(2)%init ([2], data_strfun)
call sf_chain%init (beam_data, sf_config)

call sf_chain_instance%init (sf_chain, n_channel = 1)
call sf_chain_instance%link_interactions ()
call sf_chain_instance%exchange_mask ()
call sf_chain_instance%init_evaluators ()

write (u, "(A)")  "* Inject integration parameter"
write (u, "(A)")

```

```

allocate (p_in (sf_chain%get_n_bound ()), source = 0.9_default)
write (u, "(A,9(1x,F10.7))") "p_in =", p_in

write (u, "(A)")
write (u, "(A)")  "** Evaluate"
write (u, "(A)")

call sf_chain_instance%compute_kinematics (1, p_in)
call sf_chain_instance%evaluate (scale=0._default)

call sf_chain_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "** Extract integration parameter"
write (u, "(A)")

call sf_chain_instance%get_mcpair (1, p_in)
write (u, "(A,9(1x,F10.7))") "p_in =", p_in

call sf_chain_instance%final ()
call sf_chain%final ()

write (u, "(A)")
write (u, "(A)")  "** Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: sf_base_14"

end subroutine sf_base_14

```

16.6 Photon radiation: ISR

```

⟨sf_isr.f90⟩≡
  ⟨File header⟩

module sf_isr

  ⟨Use kinds⟩
  ⟨Use strings⟩
  use io_units
  use constants, only: pi
  use format_defs, only: FMT_15, FMT_19
  use numeric_utils
  use diagnostics
  use physics_defs, only: PHOTON
  use lorentz
  use sm_physics, only: Li2
  use pdg_arrays
  use model_data

```

```

use flavors
use colors
use quantum_numbers
use polarizations
use sf_aux
use sf_mappings
use sf_base
use electron_pdfs

⟨Standard module head⟩

⟨SF isr: public⟩

⟨SF isr: parameters⟩

⟨SF isr: types⟩

contains

⟨SF isr: procedures⟩

end module sf_isr

```

16.6.1 Physics

The ISR structure function is in the most crude approximation (LLA without α corrections, i.e. ϵ^0)

$$f_0(x) = \epsilon(1-x)^{-1+\epsilon} \quad \text{with} \quad \epsilon = \frac{\alpha}{\pi} q_e^2 \ln \frac{s}{m^2}, \quad (16.29)$$

where m is the mass of the incoming (and outgoing) particle, which is initially assumed on-shell.

In $f_0(x)$, there is an integrable singularity at $x = 1$ which does not spoil the integration, but would lead to an unbounded f_{\max} . Therefore, we map this singularity like

$$x = 1 - (1-x')^{1/\epsilon} \quad (16.30)$$

such that

$$\int dx f_0(x) = \int dx' \quad (16.31)$$

For the detailed form of the QED ISR structure function cf. Chap. 10.

16.6.2 Implementation

In the concrete implementation, the zeroth order mapping (16.30) is implemented, and the Jacobian is equal to $f_i(x)/f_0(x)$. This can be written as

$$\frac{f_0(x)}{f_0(x)} = 1 \quad (16.32)$$

$$\frac{f_1(x)}{f_0(x)} = 1 + \frac{3}{4}\epsilon - \frac{1-x^2}{2(1-x')} \quad (16.33)$$

$$\begin{aligned} \frac{f_2(x)}{f_0(x)} = 1 + \frac{3}{4}\epsilon + \frac{27-8\pi^2}{96}\epsilon^2 - \frac{1-x^2}{2(1-x')} \\ - \frac{(1+3x^2)\ln x + (1-x)(4(1+x)\ln(1-x) + 5+x)}{8(1-x')}\epsilon \end{aligned} \quad (16.34)$$

For $x = 1$ (i.e., numerically indistinguishable from 1), this reduces to

$$\frac{f_0(x)}{f_0(x)} = 1 \quad (16.35)$$

$$\frac{f_1(x)}{f_0(x)} = 1 + \frac{3}{4}\epsilon \quad (16.36)$$

$$\frac{f_2(x)}{f_0(x)} = 1 + \frac{3}{4}\epsilon + \frac{27-8\pi^2}{96}\epsilon^2 \quad (16.37)$$

The last line in (16.34) is zero for

$$x_{\min} = 0.00714053329734592839549879772019 \quad (16.38)$$

(Mathematica result), independent of ϵ . For x values less than this we ignore this correction because of the logarithmic singularity which should in principle be resummed.

16.6.3 The ISR data block

```

<SF isr: public>≡
    public :: isr_data_t

<SF isr: types>≡
    type, extends (sf_data_t) :: isr_data_t
    private
    class(model_data_t), pointer :: model => null ()
    type(flavor_t), dimension(:), allocatable :: flv_in
    type(qed_pdf_t) :: pdf
    real(default) :: alpha = 0
    real(default) :: q_max = 0
    real(default) :: real_mass = 0
    real(default) :: mass = 0
    real(default) :: eps = 0
    real(default) :: log = 0
    logical :: recoil = .false.
    logical :: keep_energy = .true.
    integer :: order = 3
    integer :: error = NONE

```

```

contains
  <SF isr: isr data: TBP>
end type isr_data_t

```

Error codes

```

<SF isr: parameters>≡
  integer, parameter :: NONE = 0
  integer, parameter :: ZERO_MASS = 1
  integer, parameter :: Q_MAX_TOO_SMALL = 2
  integer, parameter :: EPS_TOO_LARGE = 3
  integer, parameter :: INVALID_ORDER = 4
  integer, parameter :: CHARGE_MIX = 5
  integer, parameter :: CHARGE_ZERO = 6
  integer, parameter :: MASS_MIX = 7

```

Generate flavor-dependent ISR data:

```

<SF isr: isr data: TBP>≡
  procedure :: init => isr_data_init

<SF isr: procedures>≡
  subroutine isr_data_init (data, model, pdg_in, alpha, q_max, &
    mass, order, recoil, keep_energy)
    class(isr_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    real(default), intent(in) :: alpha
    real(default), intent(in) :: q_max
    real(default), intent(in), optional :: mass
    integer, intent(in), optional :: order
    logical, intent(in), optional :: recoil
    logical, intent(in), optional :: keep_energy
    integer :: i, n_flv
    real(default) :: charge
    data%model => model
    n_flv = pdg_array_get_length (pdg_in)
    allocate (data%flv_in (n_flv))
    do i = 1, n_flv
      call data%flv_in(i)%init (pdg_array_get (pdg_in, i), model)
    end do
    data%alpha = alpha
    data%q_max = q_max
    if (present (order)) then
      call data%set_order (order)
    end if
    if (present (recoil)) then
      data%recoil = recoil
    end if
    if (present (keep_energy)) then
      data%keep_energy = keep_energy
    end if
    data%real_mass = data%flv_in(1)%get_mass ()
    if (present (mass)) then
      if (mass > 0) then
        data%mass = mass
      end if
    end if
  end subroutine

```

```

else
  data%mass = data%real_mass
  if (any (data%flv_in%get_mass () /= data%mass)) then
    data%error = MASS_MIX; return
  end if
end if
else
  data%mass = data%real_mass
  if (any (data%flv_in%get_mass () /= data%mass)) then
    data%error = MASS_MIX; return
  end if
end if
if (vanishes (data%mass)) then
  data%error = ZERO_MASS; return
else if (data%mass >= data%q_max) then
  data%error = Q_MAX_TOO_SMALL; return
end if
data%log = log (1 + (data%q_max / data%mass)**2)
charge = data%flv_in(1)%get_charge ()
if (any (abs (data%flv_in%get_charge ()) /= abs (charge))) then
  data%error = CHARGE_MIX; return
else if (charge == 0) then
  data%error = CHARGE_ZERO; return
end if
data%eps = data%alpha / pi * charge ** 2 &
  * (2 * log (data%q_max / data%mass) - 1)
if (data%eps > 1) then
  data%error = EPS_TOO_LARGE; return
end if
call data%pdf%init &
  (data%mass, data%alpha, charge, data%q_max, data%order)
end subroutine isr_data_init

```

Explicitly set ISR order

```

<SF isr: isr data: TBP>+≡
  procedure :: set_order => isr_data_set_order

<SF isr: procedures>+≡
  elemental subroutine isr_data_set_order (data, order)
    class(isr_data_t), intent(inout) :: data
    integer, intent(in) :: order
    if (order < 0 .or. order > 3) then
      data%error = INVALID_ORDER
    else
      data%order = order
    end if
  end subroutine isr_data_set_order

```

Handle error conditions. Should always be done after initialization, unless we are sure everything is ok.

```

<SF isr: isr data: TBP>+≡
  procedure :: check => isr_data_check

```

```

<SF isr: procedures>+=
subroutine isr_data_check (data)
  class(isr_data_t), intent(in) :: data
  select case (data%error)
  case (ZERO_MASS)
    call msg_fatal ("ISR: Particle mass is zero")
  case (Q_MAX_TOO_SMALL)
    call msg_fatal ("ISR: Particle mass exceeds Qmax")
  case (EPS_TOO_LARGE)
    call msg_fatal ("ISR: Expansion parameter too large, " // &
      "perturbative expansion breaks down")
  case (INVALID_ORDER)
    call msg_error ("ISR: LLA order invalid (valid values are 0,1,2,3)")
  case (MASS_MIX)
    call msg_fatal ("ISR: Incoming particle masses must be uniform")
  case (CHARGE_MIX)
    call msg_fatal ("ISR: Incoming particle charges must be uniform")
  case (CHARGE_ZERO)
    call msg_fatal ("ISR: Incoming particle must be charged")
  end select
end subroutine isr_data_check

```

Output

```

<SF isr: isr data: TBP>+=
  procedure :: write => isr_data_write

<SF isr: procedures>+=
subroutine isr_data_write (data, unit, verbose)
  class(isr_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)") "ISR data:"
  if (allocated (data%flv_in)) then
    write (u, "(3x,A)", advance="no") " flavor = "
    do i = 1, size (data%flv_in)
      if (i > 1) write (u, "(',',1x)", advance="no")
      call data%flv_in(i)%write (u)
    end do
    write (u, *)
    write (u, "(3x,A," // FMT_19 // ")") " alpha    = ", data%alpha
    write (u, "(3x,A," // FMT_19 // ")") " q_max    = ", data%q_max
    write (u, "(3x,A," // FMT_19 // ")") " mass     = ", data%mass
    write (u, "(3x,A," // FMT_19 // ")") " eps      = ", data%eps
    write (u, "(3x,A," // FMT_19 // ")") " log      = ", data%log
    write (u, "(3x,A,I2)") " order    = ", data%order
    write (u, "(3x,A,L2)") " recoil   = ", data%recoil
    write (u, "(3x,A,L2)") " keep en. = ", data%keep_energy
  else
    write (u, "(3x,A)") "[undefined]"
  end if
end subroutine isr_data_write

```

For ISR, there is the option to generate transverse momentum is generated. Hence, there can be up to three parameters, x , and two angles.

```

<SF isr: isr data: TBP>+≡
  procedure :: get_n_par => isr_data_get_n_par

<SF isr: procedures>+≡
  function isr_data_get_n_par (data) result (n)
    class(isr_data_t), intent(in) :: data
    integer :: n
    if (data%recoil) then
      n = 3
    else
      n = 1
    end if
  end function isr_data_get_n_par

```

Return the outgoing particles PDG codes. For ISR, these are identical to the incoming particles.

```

<SF isr: isr data: TBP>+≡
  procedure :: get_pdg_out => isr_data_get_pdg_out

<SF isr: procedures>+≡
  subroutine isr_data_get_pdg_out (data, pdg_out)
    class(isr_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    pdg_out(1) = data%flv_in%get_pdg ()
  end subroutine isr_data_get_pdg_out

```

Return the `eps` value. We need it for an appropriate mapping of structure-function parameters.

```

<SF isr: isr data: TBP>+≡
  procedure :: get_eps => isr_data_get_eps

<SF isr: procedures>+≡
  function isr_data_get_eps (data) result (eps)
    class(isr_data_t), intent(in) :: data
    real(default) :: eps
    eps = data%eps
  end function isr_data_get_eps

```

Allocate the interaction record.

```

<SF isr: isr data: TBP>+≡
  procedure :: allocate_sf_int => isr_data_allocate_sf_int

<SF isr: procedures>+≡
  subroutine isr_data_allocate_sf_int (data, sf_int)
    class(isr_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (isr_t :: sf_int)
  end subroutine isr_data_allocate_sf_int

```


16.6.4 The ISR object

The `isr_t` data type is a $1 \rightarrow 2$ interaction, i.e., we allow for single-photon emission only (but use the multi-photon resummed radiator function). The particles are ordered as (incoming, photon, outgoing).

There is no need to handle several flavors (and data blocks) in parallel, since ISR is always applied immediately after beam collision. (ISR for partons is accounted for by the PDFs themselves.) Polarization is carried through, i.e., we retain the polarization of the incoming particle and treat the emitted photon as unpolarized. Color is trivially carried through. This implies that particles 1 and 3 should be locked together. For ISR we don't need the `q` variable.

```
<SF isr: public>+≡
  public :: isr_t
<SF isr: types>+≡
  type, extends (sf_int_t) :: isr_t
    private
      type(isr_data_t), pointer :: data => null ()
      real(default) :: x = 0
      real(default) :: xb= 0
    contains
      <SF isr: isr: TBP>
    end type isr_t
```

Type string: has to be here, but there is no string variable on which ISR depends. Hence, a dummy routine.

```
<SF isr: isr: TBP>≡
  procedure :: type_string => isr_type_string
<SF isr: procedures>+≡
  function isr_type_string (object) result (string)
    class(isr_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "ISR: e+ e- ISR spectrum"
    else
      string = "ISR: [undefined]"
    end if
  end function isr_type_string
```

Output. Call the interaction routine after displaying the configuration.

```
<SF isr: isr: TBP>+≡
  procedure :: write => isr_write
<SF isr: procedures>+≡
  subroutine isr_write (object, unit, testflag)
    class(isr_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      if (object%status >= SF_DONE_KINEMATICS) then
```

```

        write (u, "(1x,A)") "SF parameters:"
        write (u, "(3x,A," // FMT_15 // ")") "x =", object%x
        write (u, "(3x,A," // FMT_15 // ")") "xb=", object%xb
    end if
    call object%base_write (u, testflag)
else
    write (u, "(1x,A)") "ISR data: [undefined]"
end if
end subroutine isr_write

```

Explicitly set ISR order (for unit test).

```

⟨SF isr: isr: TBP⟩+≡
    procedure :: set_order => isr_set_order

⟨SF isr: procedures⟩+≡
    subroutine isr_set_order (object, order)
        class(isr_t), intent(inout) :: object
        integer, intent(in) :: order
        call object%data%set_order (order)
        call object%data%pdf%set_order (order)
    end subroutine isr_set_order

```

16.6.5 Kinematics

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ were trivial. The ISR structure function allows for a straightforward mapping of the unit interval. So, to leading order, the structure function value is unity, but the x value is transformed. Higher orders affect the function value.

The structure function implementation applies the above mapping to the input (random) number r to generate the momentum fraction x and the function value f . For numerical stability reasons, we also output xb , which is $\bar{x} = 1 - x$.

For the ISR structure function, the mapping Jacobian cancels the structure function (to order zero). We apply the cancellation explicitly, therefore both the Jacobian f and the zeroth-order value (see the `apply` method) are unity if mapping is turned on. If mapping is turned off, the Jacobian f includes the value of the (zeroth-order) structure function, and strongly peaked.

```

⟨SF isr: isr: TBP⟩+≡
    procedure :: complete_kinematics => isr_complete_kinematics

⟨SF isr: procedures⟩+≡
    subroutine isr_complete_kinematics (sf_int, x, xb, f, r, rb, map)
        class(isr_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
        real(default) :: eps
        eps = sf_int%data%eps
        if (map) then
            call map_power_1 (sf_int%xb, f, rb(1), eps)

```

```

else
  sf_int%xb = rb(1)
  if (rb(1) > 0) then
    f = 1
  else
    f = 0
  end if
end if
sf_int%x = 1 - sf_int%xb
x(1) = sf_int%x
xb(1) = sf_int%xb
if (size (x) == 3) then
  x(2:3) = r(2:3)
  xb(2:3) = rb(2:3)
end if
call sf_int%split_momentum (x, xb)
select case (sf_int%status)
case (SF_FAILED_KINEMATICS)
  sf_int%x = 0
  sf_int%xb = 0
  f = 0
end select
end subroutine isr_complete_kinematics

```

Overriding the default method: we compute the x array from the momentum configuration. In the specific case of ISR, we also set the internally stored x and \bar{x} values, so they can be used in the following routine.

```

<SF isr: isr: TBP>+≡
  procedure :: recover_x => sf_isr_recover_x

<SF isr: procedures>+≡
  subroutine sf_isr_recover_x (sf_int, x, xb, x_free)
    class(isr_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb, x_free)
    sf_int%x = x(1)
    sf_int%xb = xb(1)
  end subroutine sf_isr_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

For extracting x , we rely on the stored \bar{x} value, since the x value in the argument is likely imprecise. This means that either `complete_kinematics` or `recover_x` must be called first, for the current sampling point (but maybe another channel).

```

<SF isr: isr: TBP>+≡
  procedure :: inverse_kinematics => isr_inverse_kinematics

<SF isr: procedures>+≡
  subroutine isr_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)

```

```

class(isr_t), intent(inout) :: sf_int
real(default), dimension(:), intent(in) :: x
real(default), dimension(:), intent(in) :: xb
real(default), intent(out) :: f
real(default), dimension(:), intent(out) :: r
real(default), dimension(:), intent(out) :: rb
logical, intent(in) :: map
logical, intent(in), optional :: set_momenta
real(default) :: eps
logical :: set_mom
set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
eps = sf_int%data%eps
if (map) then
    call map_power_inverse_1 (xb(1), f, rb(1), eps)
else
    rb(1) = xb(1)
    if (rb(1) > 0) then
        f = 1
    else
        f = 0
    end if
end if
r(1) = 1 - rb(1)
if (size(r) == 3) then
    r(2:3) = x(2:3)
    rb(2:3) = xb(2:3)
end if
if (set_mom) then
    call sf_int%split_momentum (x, xb)
    select case (sf_int%status)
    case (SF_FAILED_KINEMATICS)
        r = 0
        rb = 0
        f = 0
    end select
end if
end subroutine isr_inverse_kinematics

```

$\langle SF \text{ isr: isr: TBP} \rangle + \equiv$

```

procedure :: init => isr_init

```

$\langle SF \text{ isr: procedures} \rangle + \equiv$

```

subroutine isr_init (sf_int, data)
class(isr_t), intent(out) :: sf_int
class(sf_data_t), intent(in), target :: data
type(quantum_numbers_mask_t), dimension(3) :: mask
integer, dimension(3) :: hel_lock
type(polarization_t), target :: pol
type(quantum_numbers_t), dimension(1) :: qn_fc
type(flavor_t) :: flv_photon
type(color_t) :: col_photon
type(quantum_numbers_t) :: qn_hel, qn_photon, qn
type(polarization_iterator_t) :: it_hel
real(default) :: m2

```

```

integer :: i
mask = quantum_numbers_mask (.false., .false., &
    mask_h = [.false., .true., .false.])
hel_lock = [3, 0, 1]
select type (data)
type is (isr_data_t)
    m2 = data%mass**2
    call sf_int%base_init (mask, [m2], [0._default], [m2], &
        hel_lock = hel_lock)
    sf_int%data => data
    call flv_photon%init (PHOTON, data%model)
    call col_photon%init ()
    call qn_photon%init (flv_photon, col_photon)
    call qn_photon%tag_radiated ()
    do i = 1, size (data%flv_in)
        call pol%init_generic (data%flv_in(i))
        call qn_fc(1)%init (&
            flv = data%flv_in(i), &
            col = color_from_flavor (data%flv_in(i), 1))
        call it_hel%init (pol)
        do while (it_hel%is_valid ())
            qn_hel = it_hel%get_quantum_numbers ()
            qn = qn_hel .merge. qn_fc(1)
            call sf_int%add_state ([qn, qn_photon, qn])
            call it_hel%advance ()
        end do
        ! call pol%final () !!! Obsolete
    end do
    call sf_int%freeze ()
    if (data%keep_energy) then
        sf_int%on_shell_mode = KEEP_ENERGY
    else
        sf_int%on_shell_mode = KEEP_MOMENTUM
    end if
    call sf_int%set_incoming ([1])
    call sf_int%set_radiated ([2])
    call sf_int%set_outgoing ([3])
    sf_int%status = SF_INITIAL
end select
end subroutine isr_init

```

16.6.6 ISR application

For ISR, we could in principle compute kinematics and function value in a single step. In order to be able to reweight matrix elements including structure functions we split kinematics and structure function calculation. The structure function works on a single beam, assuming that the input momentum has been set.

For the structure-function evaluation, we rely on the fact that the power mapping, which we apply in the kinematics method (if the `map` flag is set), has a Jacobian which is just the inverse lowest-order structure function. With mapping active, the two should cancel exactly.

After splitting momenta, we set the outgoing momenta on-shell. We choose to conserve momentum, so energy conservation may be violated.

```

⟨SF isr: isr: TBP⟩+≡
  procedure :: apply => isr_apply

⟨SF isr: procedures⟩+≡
  subroutine isr_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(isr_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: f, finv, x, xb, eps, rb
    real(default) :: log_x, log_xb, x_2
    associate (data => sf_int%data)
      eps = sf_int%data%eps
      x = sf_int%x
      xb = sf_int%xb
      call map_power_inverse_1 (xb, finv, rb, eps)
      if (finv > 0) then
        f = 1 / finv
      else
        f = 0
      end if
      call data%pdf%evolve_qed_pdf (x, xb, rb, f)
    end associate
    call sf_int%set_matrix_element (cmplx (f, kind=default))
    sf_int%status = SF_EVALUATED
  end subroutine isr_apply

```

16.6.7 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨sf_isr_ut.f90⟩≡
  ⟨File header⟩

  module sf_isr_ut
    use unit_tests
    use sf_isr_ut1

    ⟨Standard module head⟩

    ⟨SF isr: public test⟩

    contains

    ⟨SF isr: test driver⟩

  end module sf_isr_ut

⟨sf_isr_uti.f90⟩≡
  ⟨File header⟩

```

```

module sf_isr_uti

  <Use kinds>
  <Use strings>
  use io_units
  use format_defs, only: FMT_12
  use physics_defs, only: ELECTRON
  use lorentz
  use pdg_arrays
  use flavors
  use interactions, only: reset_interaction_counter
  use interactions, only: interaction_pacify_momenta
  use model_data
  use sf_aux, only: KEEP_ENERGY
  use sf_mappings
  use sf_base

  use sf_isr

  <Standard module head>

  <SF isr: test declarations>

  contains

  <SF isr: tests>

  end module sf_isr_uti
API: driver for the unit tests below.
<SF isr: public test>≡
  public :: sf_isr_test
<SF isr: test driver>≡
  subroutine sf_isr_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <SF isr: execute tests>
  end subroutine sf_isr_test

```

Test structure function data

Construct and display a test structure function data object.

```

<SF isr: execute tests>≡
  call test (sf_isr_1, "sf_isr_1", &
    "structure function configuration", &
    u, results)
<SF isr: test declarations>≡
  public :: sf_isr_1
<SF isr: tests>≡
  subroutine sf_isr_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model

```

```

type(pdg_array_t) :: pdg_in
type(pdg_array_t), dimension(1) :: pdg_out
integer, dimension(:), allocatable :: pdg1
class(sf_data_t), allocatable :: data

write (u, "(A)")  "* Test output: sf_isr_1"
write (u, "(A)")  "* Purpose: initialize and display &
                    &test structure function data"
write (u, "(A)")

write (u, "(A)")  "* Create empty data object"
write (u, "(A)")

call model%init_qed_test ()
pdg_in = ELECTRON

allocate (isr_data_t :: data)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

select type (data)
type is (isr_data_t)
    call data%init (model, pdg_in, 1./137._default, 10._default, &
                    0.000511_default, order = 3, recoil = .false.)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_1"

end subroutine sf_isr_1

```

Structure function without mapping

Direct ISR evaluation. This is the use case for a double-beam structure function. The parameter pair is mapped in the calling program.

```

<SF isr: execute tests>+≡
    call test (sf_isr_2, "sf_isr_2", &
               "no ISR mapping", &

```



```

        u, results)
<SF isr: test declarations>+=
    public :: sf_isr_2
<SF isr: tests>+=
    subroutine sf_isr_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(pdg_array_t) :: pdg_in
        type(flavor_t) :: flv
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        type(vector4_t) :: k
        real(default) :: E
        real(default), dimension(:), allocatable :: r, rb, x, xb
        real(default) :: f, f_isr

        write (u, "(A)")  "* Test output: sf_isr_2"
        write (u, "(A)")  "*   Purpose: initialize and fill &
            &test structure function object"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize configuration data"
        write (u, "(A)")

        call model%init_qed_test ()
        pdg_in = ELECTRON
        call flv%init (ELECTRON, model)

        call reset_interaction_counter ()

        allocate (isr_data_t :: data)
        select type (data)
        type is (isr_data_t)
            call data%init (model, pdg_in, 1./137._default, 500._default, &
                0.000511_default, order = 3, recoil = .false.)
        end select

        write (u, "(A)")  "* Initialize structure-function object"
        write (u, "(A)")

        call data%allocate_sf_int (sf_int)
        call sf_int%init (data)
        call sf_int%set_beam_index ([1])

        write (u, "(A)")  "* Initialize incoming momentum with E=500"
        write (u, "(A)")
        E = 500
        k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
        call pacify (k, 1e-10_default)
        call vector4_write (k, u)
        call sf_int%seed_kinematics ([k])

        write (u, "(A)")

```

```

write (u, "(A)")  "* Set kinematics for r=0.9, no ISR mapping, &
                  &collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.9_default
rb = 1 - r
write (u, "(A,9(1x," // FMT_12 // "))") "r =", r
write (u, "(A,9(1x," // FMT_12 // "))") "rb=", rb

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A)")
write (u, "(A,9(1x," // FMT_12 // "))") "x =", x
write (u, "(A,9(1x," // FMT_12 // "))") "xb=", xb
write (u, "(A,9(1x," // FMT_12 // "))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Invert kinematics"
write (u, "(A)")

call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)
write (u, "(A,9(1x," // FMT_12 // "))") "r =", r
write (u, "(A,9(1x," // FMT_12 // "))") "rb=", rb
write (u, "(A,9(1x," // FMT_12 // "))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate ISR structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Structure-function value, default order"
write (u, "(A)")

f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // "))") "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))") "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Re-evaluate structure function, leading order"
write (u, "(A)")

select type (sf_int)
type is (isr_t)
    call sf_int%set_order (0)
end select

```

```

call sf_int%apply (scale = 100._default)
f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // "))" ) "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))" ) "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_2"

end subroutine sf_isr_2

```

Structure function with mapping

Apply the optimal ISR mapping. This is the use case for a single-beam structure function.

```

<SF isr: execute tests>+≡
  call test (sf_isr_3, "sf_isr_3", &
    "ISR mapping", &
    u, results)

<SF isr: test declarations>+≡
  public :: sf_isr_3

<SF isr: tests>+≡
  subroutine sf_isr_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, f_isr

    write (u, "(A)")  "* Test output: sf_isr_3"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv%init (ELECTRON, model)
    pdg_in = ELECTRON

```

```

call reset_interaction_counter ()

allocate (isr_data_t :: data)
select type (data)
type is (isr_data_t)
    call data%init (model, pdg_in, 1./137._default, 500._default, &
        0.000511_default, order = 3, recoil = .false.)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.7, with ISR mapping, &
    &collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.7_default
rb = 1 - r
write (u, "(A,9(1x," // FMT_12 // "))")  "r =", r
write (u, "(A,9(1x," // FMT_12 // "))")  "rb=", rb

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)

write (u, "(A)")
write (u, "(A,9(1x," // FMT_12 // "))")  "x =", x
write (u, "(A,9(1x," // FMT_12 // "))")  "xb=", xb
write (u, "(A,9(1x," // FMT_12 // "))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Invert kinematics"
write (u, "(A)")

call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true.)
write (u, "(A,9(1x," // FMT_12 // "))")  "r =", r
write (u, "(A,9(1x," // FMT_12 // "))")  "rb=", rb

```

```

write (u, "(A,9(1x," // FMT_12 // "))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate ISR structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Structure-function value, default order"
write (u, "(A)")

f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // "))") "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))") "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Re-evaluate structure function, leading order"
write (u, "(A)")

select type (sf_int)
type is (isr_t)
  call sf_int%set_order (0)
end select
call sf_int%apply (scale = 100._default)
f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // "))") "f_isr          =", f_isr
write (u, "(A,9(1x," // FMT_12 // "))") "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_3"

end subroutine sf_isr_3

```

Non-collinear ISR splitting

Construct and display a structure function object based on the ISR structure function. We blank out numerical fluctuations for 32bit.

```

<SF isr: execute tests>+≡
  call test (sf_isr_4, "sf_isr_4", &
    "ISR non-collinear", &
    u, results)

```

```

<SF isr: test declarations>+=
  public :: sf_isr_4

<SF isr: tests>+=
  subroutine sf_isr_4 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, f_isr
    character(len=80) :: buffer
    integer :: u_scratch, iostat

    write (u, "(A)")  "* Test output: sf_isr_4"
    write (u, "(A)")  "*   Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv%init (ELECTRON, model)
    pdg_in = ELECTRON

    call reset_interaction_counter ()

    write (u, "(A)")
    write (u, "(A)")  "* Initialize structure-function object"
    write (u, "(A)")

    allocate (isr_data_t :: data)
    select type (data)
    type is (isr_data_t)
      call data%init (model, pdg_in, 1./137._default, 500._default, &
        0.000511_default, order = 3, recoil = .true.)
    end select

    call data%allocate_sf_int (sf_int)
    call sf_int%init (data)
    call sf_int%set_beam_index ([1])

    write (u, "(A)")
    write (u, "(A)")  "* Initialize incoming momentum with E=500"
    write (u, "(A)")
    E = 500
    k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
    call pacify (k, 1e-10_default)
    call vector4_write (k, u)

```

```

call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5/0.5/0.25, with ISR mapping, "
write (u, "(A)")  "          non-coll., keeping energy"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.5_default, 0.5_default, 0.25_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call interaction_pacify_momenta (sf_int%interaction_t, 1e-10_default)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x and r from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true.)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "r =", r

write (u, "(A)")
write (u, "(A)")  "* Evaluate ISR structure function"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call interaction_pacify_momenta (sf_int%interaction_t, 1e-10_default)
call sf_int%apply (scale = 10._default)
u_scratch = free_unit ()
open (u_scratch, status="scratch", action = "readwrite")
call sf_int%write (u_scratch, testflag = .true.)
rewind (u_scratch)

```

```

do
  read (u_scratch, "(A)", iostat=iostat) buffer
  if (iostat /= 0) exit
  if (buffer(1:25) == " P = 0.000000E+00 9.57") then
    buffer = replace (buffer, 26, "XXXX")
  end if
  if (buffer(1:25) == " P = 0.000000E+00 -9.57") then
    buffer = replace (buffer, 26, "XXXX")
  end if
  write (u, "(A)") buffer
end do
close (u_scratch)

write (u, "(A)")
write (u, "(A)")  "* Structure-function value"
write (u, "(A)")

f_isr = sf_int%get_matrix_element (1)

write (u, "(A,9(1x," // FMT_12 // ")") "f_isr      =", f_isr
write (u, "(A,9(1x," // FMT_12 // ")") "f_isr * f_map =", f_isr * f

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_4"

end subroutine sf_isr_4

```

Structure function pair with mapping

Apply the ISR mapping for a ISR pair. structure function.

```

<SF isr: execute tests>+≡
  call test (sf_isr_5, "sf_isr_5", &
    "ISR pair mapping", &
    u, results)

<SF isr: test declarations>+≡
  public :: sf_isr_5

<SF isr: tests>+≡
  subroutine sf_isr_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_mapping_t), allocatable :: mapping
    class(sf_int_t), dimension(:), allocatable :: sf_int
    type(vector4_t), dimension(2) :: k

```



```

real(default) :: E, f_map
real(default), dimension(:), allocatable :: p, pb, r, rb, x, xb
real(default), dimension(2) :: f, f_isr
integer :: i

write (u, "(A)")  "* Test output: sf_isr_5"
write (u, "(A)")  "* Purpose: initialize and fill &
                  &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_qed_test ()
call flv%init (ELECTRON, model)
pdg_in = ELECTRON

call reset_interaction_counter ()

allocate (isr_data_t :: data)
select type (data)
type is (isr_data_t)
    call data%init (model, pdg_in, 1./137._default, 500._default, &
                   0.000511_default, order = 3, recoil = .false.)
end select

allocate (sf_ip_mapping_t :: mapping)
select type (mapping)
type is (sf_ip_mapping_t)
    select type (data)
    type is (isr_data_t)
        call mapping%init (eps = data%get_eps ())
    end select
    call mapping%set_index (1, 1)
    call mapping%set_index (2, 2)
end select

call mapping%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

allocate (isr_t :: sf_int (2))

do i = 1, 2
    call sf_int(i)%init (data)
    call sf_int(i)%set_beam_index ([i])
end do

write (u, "(A)")  "* Initialize incoming momenta with E=500"
write (u, "(A)")
E = 500
k(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)

```

```

k(2) = vector4_moving (E, - sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
do i = 1, 2
    call vector4_write (k(i), u)
    call sf_int(i)%seed_kinematics (k(i:i))
end do

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for p=[0.7,0.4], collinear"
write (u, "(A)")

allocate (p (2 * data%get_n_par ()))
allocate (pb(size (p)))
allocate (r (size (p)))
allocate (rb(size (p)))
allocate (x (size (p)))
allocate (xb(size (p)))

p = [0.7_default, 0.4_default]
pb= 1 - p
call mapping%compute (r, rb, f_map, p, pb)

write (u, "(A,9(1x," // FMT_12 // "))")  "p =", p
write (u, "(A,9(1x," // FMT_12 // "))")  "pb=", pb
write (u, "(A,9(1x," // FMT_12 // "))")  "r =", r
write (u, "(A,9(1x," // FMT_12 // "))")  "rb=", rb
write (u, "(A,9(1x," // FMT_12 // "))")  "fm=", f_map

do i = 1, 2
    call sf_int(i)%complete_kinematics (x(i:i), xb(i:i), f(i), r(i:i), rb(i:i), &
        map=.false.)
end do

write (u, "(A)")
write (u, "(A,9(1x," // FMT_12 // "))")  "x =", x
write (u, "(A,9(1x," // FMT_12 // "))")  "xb=", xb
write (u, "(A,9(1x," // FMT_12 // "))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Invert kinematics"
write (u, "(A)")

do i = 1, 2
    call sf_int(i)%inverse_kinematics (x(i:i), xb(i:i), f(i), r(i:i), rb(i:i), &
        map=.false.)
end do
call mapping%inverse (r, rb, f_map, p, pb)

write (u, "(A,9(1x," // FMT_12 // "))")  "p =", p
write (u, "(A,9(1x," // FMT_12 // "))")  "pb=", pb
write (u, "(A,9(1x," // FMT_12 // "))")  "r =", r
write (u, "(A,9(1x," // FMT_12 // "))")  "rb=", rb
write (u, "(A,9(1x," // FMT_12 // "))")  "fm=", f_map

```

```

write (u, "(A)")
write (u, "(A)")  "* Evaluate ISR structure function"

call sf_int(1)%apply (scale = 100._default)
call sf_int(2)%apply (scale = 100._default)

write (u, "(A)")
write (u, "(A)")  "* Structure function #1"
write (u, "(A)")
call sf_int(1)%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Structure function #2"
write (u, "(A)")
call sf_int(2)%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Structure-function value, default order"
write (u, "(A)")

do i = 1, 2
  f_isr(i) = sf_int(i)%get_matrix_element (1)
end do

write (u, "(A,9(1x," // FMT_12 // "))")  "f_isr          =", &
  product (f_isr)
write (u, "(A,9(1x," // FMT_12 // "))")  "f_isr * f_map =", &
  product (f_isr * f) * f_map

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

do i = 1, 2
  call sf_int(i)%final ()
end do
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_isr_5"

end subroutine sf_isr_5

```

16.7 EPA

```

⟨sf_epa.f90⟩≡
  ⟨File header⟩

  module sf_epa

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use io_units
    use constants, only: pi
    use format_defs, only: FMT_17, FMT_19
    use numeric_utils
    use diagnostics
    use physics_defs, only: PHOTON
    use lorentz
    use pdg_arrays
    use model_data
    use flavors
    use colors
    use quantum_numbers
    use state_matrices
    use polarizations
    use interactions
    use sf_aux
    use sf_base

    ⟨Standard module head⟩

    ⟨SF epa: public⟩

    ⟨SF epa: parameters⟩

    ⟨SF epa: types⟩

    contains

    ⟨SF epa: procedures⟩

  end module sf_epa

```

16.7.1 Physics

The EPA structure function for a photon inside an (elementary) particle p with energy E , mass m and charge q_p (e.g., electron) is given by ($\bar{x} \equiv 1 - x$)

There are several variants of the EPA, which are steered by the `\$epa_mode` switch. The formula (6.17b) from the report by Budnev et al. is given by

$$\begin{aligned}
 f(x) = \frac{\alpha}{\pi} q_p^2 \frac{1}{x} & \left[\left(\bar{x} + \frac{x^2}{2} \right) \ln \frac{Q_{\max}^2}{Q_{\min}^2} \right. \\
 & \left. - \left(1 - \frac{x}{2} \right)^2 \ln \frac{x^2 + \frac{Q_{\max}^2}{E^2}}{x^2 + \frac{Q_{\min}^2}{E^2}} - x^2 \frac{m^2}{Q_{\min}^2} \left(1 - \frac{Q_{\min}^2}{Q_{\max}^2} \right) \right]. \quad (16.39)
 \end{aligned}$$

If no explicit Q bounds are provided, the kinematical bounds are

$$-Q_{\max}^2 = t_0 = -2\bar{x}(E^2 + p\bar{p}) + 2m^2 \approx -4\bar{x}E^2, \quad (16.40)$$

$$-Q_{\min}^2 = t_1 = -2\bar{x}(E^2 - p\bar{p}) + 2m^2 \approx -\frac{x^2}{\bar{x}}m^2. \quad (16.41)$$

The second and third terms in (16.39) are negative definite (and subleading). Noting that $\bar{x} + x^2/2$ is bounded between $1/2$ and 1 , we derive that $f(x)$ is always smaller than

$$\bar{f}(x) = \frac{\alpha}{\pi} q_p^2 \frac{L - 2 \ln x}{x} \quad \text{where} \quad L = \ln \frac{\min(4E_{\max}^2, Q_{\max}^2)}{\max(m^2, Q_{\min}^2)}, \quad (16.42)$$

where we allow for explicit Q bounds that narrow the kinematical range. Therefore, we generate this distribution:

$$\int_{x_0}^{x_1} dx \bar{f}(x) = C(x_0, x_1) \int_0^1 dx' \quad (16.43)$$

We set

$$\ln x = \frac{1}{2} \left\{ L - \sqrt{L^2 - 4 [x' \ln x_1 (L - \ln x_1) + \bar{x}' \ln x_0 (L - \ln x_0)]} \right\} \quad (16.44)$$

such that $x(0) = x_0$ and $x(1) = x_1$ and

$$\frac{dx}{dx'} = \left(\frac{\alpha}{\pi} q_p^2 \right)^{-1} x \frac{C(x_0, x_1)}{L - 2 \ln x} \quad (16.45)$$

with

$$C(x_0, x_1) = \frac{\alpha}{\pi} q_p^2 [\ln x_1 (L - \ln x_1) - \ln x_0 (L - \ln x_0)] \quad (16.46)$$

such that (16.43) is satisfied. Finally, we have

$$\int_{x_0}^{x_1} dx f(x) = C(x_0, x_1) \int_0^1 dx' \frac{f(x(x'))}{\bar{f}(x(x'))} \quad (16.47)$$

where x' is calculated from x via (16.44).

The structure of the mapping is most obvious from:

$$x'(x) = \frac{\log x (L - \log x) - \log x_0 (L - \log x_0)}{\log x_1 (L - \log x_1) - \log x_0 (L - \log x_0)}. \quad (16.48)$$

Taking the Eq. (6.16e) from the Budnev et al. report, and integrating it over q^2 yields the modified result

$$f(x) = \frac{\alpha}{\pi} q_p^2 \frac{1}{x} \left[\left(\bar{x} + \frac{x^2}{2} \right) \ln \frac{Q_{\max}^2}{Q_{\min}^2} - x^2 \frac{m^2}{Q_{\min}^2} \left(1 - \frac{Q_{\min}^2}{Q_{\max}^2} \right) \right]. \quad (16.49)$$

This is closer to many standard papers from LEP times, and to textbook formulae like e.g. in Peskin/Schroeder. For historical reasons, we keep Eq. (16.39) as the default in WHIZARD.

16.7.2 The EPA data block

The EPA parameters are: α , E_{\max} , m , Q_{\min} , and x_{\min} . Instead of m we can use the incoming particle PDG code as input; from this we can deduce the mass and charge.

Internally we store in addition $C_{0/1} = \frac{\alpha}{\pi} q_e^2 \ln x_{0/1} (L - \ln x_{0/1})$, the c.m. energy squared and the incoming particle mass.

```

<SF epa: public>≡
  public :: EPA_MODE_DEFAULT
  public :: EPA_MODE_BUDNEV_617
  public :: EPA_MODE_BUDNEV_616E
  public :: EPA_MODE_LOG_POWER
  public :: EPA_MODE_LOG_SIMPLE
  public :: EPA_MODE_LOG

<SF epa: parameters>≡
  integer, parameter :: EPA_MODE_DEFAULT = 0
  integer, parameter :: EPA_MODE_BUDNEV_617 = 0
  integer, parameter :: EPA_MODE_BUDNEV_616E = 1
  integer, parameter :: EPA_MODE_LOG_POWER = 2
  integer, parameter :: EPA_MODE_LOG_SIMPLE = 3
  integer, parameter :: EPA_MODE_LOG = 4

<SF epa: public>+≡
  public :: epa_data_t

<SF epa: types>≡
  type, extends(sf_data_t) :: epa_data_t
    private
    class(model_data_t), pointer :: model => null ()
    type(flavor_t), dimension(:), allocatable :: flv_in
    real(default) :: alpha
    real(default) :: x_min
    real(default) :: x_max
    real(default) :: q_min
    real(default) :: q_max
    real(default) :: E_max
    real(default) :: mass
    real(default) :: log
    real(default) :: a
    real(default) :: c0
    real(default) :: c1
    real(default) :: dc
    integer :: mode = EPA_MODE_DEFAULT
    integer :: error = NONE
    logical :: recoil = .false.
    logical :: keep_energy = .true.
  contains
    <SF epa: epa data: TBP>
  end type epa_data_t

```

Error codes

```

<SF epa: parameters>+≡
  integer, parameter :: NONE = 0

```

```

integer, parameter :: ZERO_QMIN = 1
integer, parameter :: Q_MAX_TOO_SMALL = 2
integer, parameter :: ZERO_XMIN = 3
integer, parameter :: MASS_MIX = 4
integer, parameter :: NO_EPA = 5

<SF epa: epa data: TBP>≡
  procedure :: init => epa_data_init

<SF epa: procedures>≡
  subroutine epa_data_init (data, model, mode, pdg_in, alpha, &
    x_min, q_min, q_max, mass, recoil, keep_energy)
    class(epa_data_t), intent(inout) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    integer, intent(in) :: mode
    real(default), intent(in) :: alpha, x_min, q_min, q_max
    real(default), intent(in), optional :: mass
    logical, intent(in), optional :: recoil
    logical, intent(in), optional :: keep_energy
    integer :: n_flv, i
    data%model => model
    data%mode = mode
    n_flv = pdg_array_get_length (pdg_in)
    allocate (data%flv_in (n_flv))
    do i = 1, n_flv
      call data%flv_in(i)%init (pdg_array_get (pdg_in, i), model)
    end do
    data%alpha = alpha
    data%E_max = q_max / 2
    data%x_min = x_min
    data%x_max = 1
    if (vanishes (data%x_min)) then
      data%error = ZERO_XMIN; return
    end if
    data%q_min = q_min
    data%q_max = q_max
    select case (char (data%model%get_name ()))
    case ("QCD", "Test")
      data%error = NO_EPA; return
    end select
    if (present (recoil)) then
      data%recoil = recoil
    end if
    if (present (keep_energy)) then
      data%keep_energy = keep_energy
    end if
    if (present (mass)) then
      data%mass = mass
    else
      data%mass = data%flv_in(1)%get_mass ()
      if (any (data%flv_in%get_mass () /= data%mass)) then
        data%error = MASS_MIX; return
      end if
    end if
  end if
end if

```

```

if (max (data%mass, data%q_min) == 0) then
  data%error = ZERO_QMIN; return
else if (max (data%mass, data%q_min) >= data%E_max) then
  data%error = Q_MAX_TOO_SMALL; return
end if
data%log = log ((data%q_max / max (data%mass, data%q_min)) ** 2 )
data%a = data%alpha / pi
data%c0 = log (data%x_min) * (data%log - log (data%x_min))
data%c1 = log (data%x_max) * (data%log - log (data%x_max))
data%dc = data%c1 - data%c0
end subroutine epa_data_init

```

Handle error conditions. Should always be done after initialization, unless we are sure everything is ok.

```

<SF epa: epa data: TBP>+≡
  procedure :: check => epa_data_check

<SF epa: procedures>+≡
  subroutine epa_data_check (data)
    class(epa_data_t), intent(in) :: data
    select case (data%error)
      case (NO_EPA)
        call msg_fatal ("EPA structure function not available for model " &
          // char (data%model%get_name ()) // ".")
      case (ZERO_QMIN)
        call msg_fatal ("EPA: Particle mass is zero")
      case (Q_MAX_TOO_SMALL)
        call msg_fatal ("EPA: Particle mass exceeds Qmax")
      case (ZERO_XMIN)
        call msg_fatal ("EPA: x_min must be larger than zero")
      case (MASS_MIX)
        call msg_fatal ("EPA: incoming particle masses must be uniform")
    end select
  end subroutine epa_data_check

```

Output

```

<SF epa: epa data: TBP>+≡
  procedure :: write => epa_data_write

<SF epa: procedures>+≡
  subroutine epa_data_write (data, unit, verbose)
    class(epa_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "EPA data:"
    if (allocated (data%flv_in)) then
      write (u, "(3x,A)", advance="no") " flavor = "
      do i = 1, size (data%flv_in)
        if (i > 1) write (u, "(',',1x)", advance="no")
        call data%flv_in(i)%write (u)
      end do
      write (u, *)
    end if
  end subroutine epa_data_write

```



```

write (u, "(3x,A," // FMT_19 // ")") " alpha = ", data%alpha
write (u, "(3x,A," // FMT_19 // ")") " x_min = ", data%x_min
write (u, "(3x,A," // FMT_19 // ")") " x_max = ", data%x_max
write (u, "(3x,A," // FMT_19 // ")") " q_min = ", data%q_min
write (u, "(3x,A," // FMT_19 // ")") " q_max = ", data%q_max
write (u, "(3x,A," // FMT_19 // ")") " E_max = ", data%e_max
write (u, "(3x,A," // FMT_19 // ")") " mass = ", data%mass
write (u, "(3x,A," // FMT_19 // ")") " a = ", data%a
write (u, "(3x,A," // FMT_19 // ")") " c0 = ", data%c0
write (u, "(3x,A," // FMT_19 // ")") " c1 = ", data%c1
write (u, "(3x,A," // FMT_19 // ")") " log = ", data%log
write (u, "(3x,A,L2)") " recoil = ", data%recoil
write (u, "(3x,A,L2)") " keep en. = ", data%keep_energy
else
  write (u, "(3x,A)") "[undefined]"
end if
end subroutine epa_data_write

```

The number of kinematic parameters.

```

<SF epa: epa data: TBP>+≡
  procedure :: get_n_par => epa_data_get_n_par

<SF epa: procedures>+≡
  function epa_data_get_n_par (data) result (n)
    class(epa_data_t), intent(in) :: data
    integer :: n
    if (data%recoil) then
      n = 3
    else
      n = 1
    end if
  end function epa_data_get_n_par

```

Return the outgoing particles PDG codes. The outgoing particle is always the photon while the radiated particle is identical to the incoming one.

```

<SF epa: epa data: TBP>+≡
  procedure :: get_pdg_out => epa_data_get_pdg_out

<SF epa: procedures>+≡
  subroutine epa_data_get_pdg_out (data, pdg_out)
    class(epa_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    pdg_out(1) = PHOTON
  end subroutine epa_data_get_pdg_out

```

Allocate the interaction record.

```

<SF epa: epa data: TBP>+≡
  procedure :: allocate_sf_int => epa_data_allocate_sf_int

<SF epa: procedures>+≡
  subroutine epa_data_allocate_sf_int (data, sf_int)
    class(epa_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int

```

```

allocate (epa_t :: sf_int)
end subroutine epa_data_allocate_sf_int

```

16.7.3 The EPA object

The `epa_t` data type is a $1 \rightarrow 2$ interaction. We should be able to handle several flavors in parallel, since EPA is not necessarily applied immediately after beam collision: Photons may be radiated from quarks. In that case, the partons are massless and q_{\min} applies instead, so we do not need to generate several kinematical configurations in parallel.

The squared charge values multiply the matrix elements, depending on the flavour. We scan the interaction after building it, so we have the correct assignments.

The particles are ordered as (incoming, radiated, photon), where the photon initiates the hard interaction.

We generate an unpolarized photon and transfer initial polarization to the radiated parton. Color is transferred in the same way.

```

<SF epa: types>+≡
type, extends (sf_int_t) :: epa_t
  type(epa_data_t), pointer :: data => null ()
  real(default) :: x = 0
  real(default) :: xb = 0
  real(default) :: E = 0
  real(default), dimension(:), allocatable :: charge2
contains
  <SF epa: epa: TBP>
end type epa_t

```

Type string: has to be here, but there is no string variable on which EPA depends. Hence, a dummy routine.

```

<SF epa: epa: TBP>≡
  procedure :: type_string => epa_type_string

<SF epa: procedures>+≡
function epa_type_string (object) result (string)
  class(epa_t), intent(in) :: object
  type(string_t) :: string
  if (associated (object%data)) then
    string = "EPA: equivalent photon approx."
  else
    string = "EPA: [undefined]"
  end if
end function epa_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF epa: epa: TBP>+≡
  procedure :: write => epa_write

```

<SF epa: procedures>+≡

```

subroutine epa_write (object, unit, testflag)
  class(epa_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u
  u = given_output_unit (unit)
  if (associated (object%data)) then
    call object%data%write (u)
    if (object%status >= SF_DONE_KINEMATICS) then
      write (u, "(1x,A)") "SF parameters:"
      write (u, "(3x,A," // FMT_17 // ")") "x =", object%x
      if (object%status >= SF_FAILED_EVALUATION) then
        write (u, "(3x,A," // FMT_17 // ")") "E =", object%E
      end if
    end if
    call object%base_write (u, testflag)
  else
    write (u, "(1x,A)") "EPA data: [undefined]"
  end if
end subroutine epa_write

```

Prepare the interaction object. We have to construct transition matrix elements for all flavor and helicity combinations.

<SF epa: epa: TBP>+≡

```

procedure :: init => epa_init

```

<SF epa: procedures>+≡

```

subroutine epa_init (sf_int, data)
  class(epa_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
  type(quantum_numbers_mask_t), dimension(3) :: mask
  integer, dimension(3) :: hel_lock
  type(polarization_t), target :: pol
  type(quantum_numbers_t), dimension(1) :: qn_fc
  type(flavor_t) :: flv_photon
  type(color_t) :: col_photon
  type(quantum_numbers_t) :: qn_hel, qn_photon, qn, qn_rad
  type(polarization_iterator_t) :: it_hel
  integer :: i
  mask = quantum_numbers_mask (.false., .false., &
    mask_h = [.false., .false., .true.])
  hel_lock = [2, 1, 0]
  select type (data)
  type is (epa_data_t)
    call sf_int%base_init (mask, [data%mass**2], &
      [data%mass**2], [0._default], hel_lock = hel_lock)
    sf_int%data => data
    call flv_photon%init (PHOTON, data%model)
    call col_photon%init ()
    call qn_photon%init (flv_photon, col_photon)
    do i = 1, size (data%flv_in)
      call pol%init_generic (data%flv_in(i))
      call qn_fc(1)%init ( &

```

```

        flv = data%flv_in(i), &
        col = color_from_flavor (data%flv_in(i), 1))
    call it_hel%init (pol)
    do while (it_hel%is_valid ())
        qn_hel = it_hel%get_quantum_numbers ()
        qn = qn_hel .merge. qn_fc(1)
        qn_rad = qn
        call qn_rad%tag_radiated ()
        call sf_int%add_state ([qn, qn_rad, qn_photon])
        call it_hel%advance ()
    end do
    ! call pol%final ()
end do
call sf_int%freeze ()
if (data%keep_energy) then
    sf_int%on_shell_mode = KEEP_ENERGY
else
    sf_int%on_shell_mode = KEEP_MOMENTUM
end if
call sf_int%set_incoming ([1])
call sf_int%set_radiated ([2])
call sf_int%set_outgoing ([3])
end select
end subroutine epa_init

```

Prepare the charge array. This is separate from the previous routine since the state matrix may be helicity-contracted.

```

<SF epa: epa: TBP>+≡
    procedure :: setup_constants => epa_setup_constants

<SF epa: procedures>+≡
    subroutine epa_setup_constants (sf_int)
        class(epa_t), intent(inout), target :: sf_int
        type(state_iterator_t) :: it
        type(flavor_t) :: flv
        integer :: i, n_me
        n_me = sf_int%get_n_matrix_elements ()
        allocate (sf_int%charge2 (n_me))
        call it%init (sf_int%interaction_t%get_state_matrix_ptr ())
        do while (it%is_valid ())
            i = it%get_me_index ()
            flv = it%get_flavor (1)
            sf_int%charge2(i) = flv%get_charge () ** 2
            call it%advance ()
        end do
        sf_int%status = SF_INITIAL
    end subroutine epa_setup_constants

```

16.7.4 Kinematics

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

The EPA structure function allows for a straightforward mapping of the unit interval. The x value is transformed, and the mapped structure function becomes unity at its upper boundary.

The structure function implementation applies the above mapping to the input (random) number r to generate the momentum fraction x and the function value f . For numerical stability reasons, we also output xb , which is $\bar{x} = 1 - x$.

```

<SF epa: epa: TBP>+≡
  procedure :: complete_kinematics => epa_complete_kinematics

<SF epa: procedures>+≡
  subroutine epa_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(epa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    real(default) :: delta, sqrt_delta, lx
    if (map) then
      associate (data => sf_int%data)
        delta = data%log ** 2 - 4 * (r(1) * data%c1 + rb(1) * data%c0)
        if (delta > 0) then
          sqrt_delta = sqrt (delta)
          lx = (data%log - sqrt_delta) / 2
        else
          sf_int%status = SF_FAILED_KINEMATICS
          f = 0
          return
        end if
        x(1) = exp (lx)
        f = x(1) * data%dc / sqrt_delta
      end associate
    else
      x(1) = r(1)
      if (sf_int%data%x_min < x(1) .and. x(1) < sf_int%data%x_max) then
        f = 1
      else
        sf_int%status = SF_FAILED_KINEMATICS
        f = 0
        return
      end if
    end if
    xb(1) = 1 - x(1)
    if (size(x) == 3) then
      x(2:3) = r(2:3)
      xb(2:3) = rb(2:3)
    end if
    call sf_int%split_momentum (x, xb)
    select case (sf_int%status)
    case (SF_DONE_KINEMATICS)
      sf_int%x = x(1)
      sf_int%xb= xb(1)
      sf_int%E = energy (sf_int%get_momentum (1))

```

```

case (SF_FAILED_KINEMATICS)
  sf_int%x = 0
  sf_int%xb= 0
  f = 0
end select
end subroutine epa_complete_kinematics

```

Overriding the default method: we compute the x array from the momentum configuration. In the specific case of EPA, we also set the internally stored x and \bar{x} values, so they can be used in the following routine.

Note: the extraction of \bar{x} is not numerically safe, but it cannot be as long as the base `recover_x` is not.

```

<SF epa: epa: TBP>+≡
  procedure :: recover_x => sf_epa_recover_x

<SF epa: procedures>+≡
  subroutine sf_epa_recover_x (sf_int, x, xb, x_free)
    class(epa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb, x_free)
    sf_int%x = x(1)
    sf_int%xb = xb(1)
  end subroutine sf_epa_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF epa: epa: TBP>+≡
  procedure :: inverse_kinematics => epa_inverse_kinematics

<SF epa: procedures>+≡
  subroutine epa_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(epa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    real(default) :: lx, delta, sqrt_delta, c
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    if (map) then
      associate (data => sf_int%data)
        lx = log (x(1))
        sqrt_delta = data%log - 2 * lx
        delta = sqrt_delta ** 2
        c = (data%log ** 2 - delta) / 4
        r (1) = (c - data%c0) / data%dc
        rb(1) = (data%c1 - c) / data%dc
      end associate
    end if
  end subroutine epa_inverse_kinematics

```

```

        f = x(1) * data%dc / sqrt_delta
    end associate
else
    r (1) = x(1)
    rb(1) = xb(1)
    if (sf_int%data%x_min < x(1) .and. x(1) < sf_int%data%x_max) then
        f = 1
    else
        f = 0
    end if
end if
if (size(r) == 3) then
    r (2:3) = x(2:3)
    rb(2:3) = xb(2:3)
end if
if (set_mom) then
    call sf_int%split_momentum (x, xb)
    select case (sf_int%status)
    case (SF_FAILED_KINEMATICS); f = 0
    end select
end if
sf_int%E = energy (sf_int%get_momentum (1))
end subroutine epa_inverse_kinematics

```

16.7.5 EPA application

For EPA, we can in principle compute kinematics and function value in a single step. In order to be able to reweight events, kinematics and structure function application are separated. This function works on a single beam, assuming that the input momentum has been set. We need three random numbers as input: one for x , and two for the polar and azimuthal angles. Alternatively, for the no-recoil case, we can skip p_T generation; in this case, we only need one.

For obtaining splitting kinematics, we rely on the assumption that all in-particles are mass-degenerate (or there is only one), so the generated x values are identical.

Fix 2020-03-10: Divide by two if there is polarization. In the polarized case, the outgoing electron/positron retains the incoming polarization. The latter is summed over when convoluting with the beam, but there are still two states with different outgoing polarization but identical structure-function value. This leads to double-counting for the overall cross section.

```

<SF epa: epa: TBP>+≡
    procedure :: apply => epa_apply

<SF epa: procedures>+≡
    subroutine epa_apply (sf_int, scale, negative_sf, rescale, i_sub)
        class(epa_t), intent(inout) :: sf_int
        real(default), intent(in) :: scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(in), optional :: rescale
        integer, intent(in), optional :: i_sub
        real(default) :: x, xb, qminsq, qmaxsq, f, E, m2
        associate (data => sf_int%data)

```

```

x = sf_int%x
xb= sf_int%xb
E = sf_int%E
m2 = data%mass ** 2
qminsq = max (x ** 2 / xb * data%mass ** 2, data%q_min ** 2)
select case (data%mode)
case (0)
  qmaxsq = min (4 * xb * E ** 2, data%q_max ** 2)
  if (qminsq < qmaxsq) then
    f = data%a / x &
      * ((xb + x ** 2 / 2) * log (qmaxsq / qminsq) &
        - (1 - x / 2) ** 2 &
        * log ((x**2 + qmaxsq / E ** 2) / (x**2 + qminsq / E ** 2)) &
        - x ** 2 * data%mass ** 2 / qminsq * (1 - qminsq / qmaxsq))
  else
    f = 0
  end if
case (1)
  qmaxsq = min (4 * xb * E ** 2, data%q_max ** 2)
  if (qminsq < qmaxsq) then
    f = data%a / x &
      * ((xb + x ** 2 / 2) * log (qmaxsq / qminsq) &
        - x ** 2 * data%mass ** 2 / qminsq * (1 - qminsq / qmaxsq))
  else
    f = 0
  end if
case (2)
  qmaxsq = data%q_max ** 2
  if (data%mass ** 2 < qmaxsq) then
    f = data%a / x &
      * ((xb + x ** 2 / 2) * log (qmaxsq / m2) &
        - x ** 2 * data%mass ** 2 / qminsq * (1 - qminsq / qmaxsq))
  else
    f = 0
  end if
case (3)
  qmaxsq = data%q_max ** 2
  if (data%mass ** 2 < qmaxsq) then
    f = data%a / x &
      * ((xb + x ** 2 / 2) * log (qmaxsq / m2) &
        - x ** 2 * (1 - m2 / qmaxsq))
  else
    f = 0
  end if
case (4)
  qmaxsq = data%q_max ** 2
  if (data%mass ** 2 < qmaxsq) then
    f = data%a / x &
      * ((xb + x ** 2 / 2) * log (qmaxsq / m2))
  else
    f = 0
  end if
end select
f = f / sf_int%get_n_matrix_elements ()

```



```

        call sf_int%set_matrix_element &
            (cplx (f, kind=default) * sf_int%charge2)
    end associate
    sf_int%status = SF_EVALUATED
end subroutine epa_apply

```

16.7.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_epa_ut.f90>≡
  <File header>

  module sf_epa_ut
    use unit_tests
    use sf_epa_util

    <Standard module head>

    <SF epa: public test>

    contains

    <SF epa: test driver>

  end module sf_epa_ut

<sf_epa_util.f90>≡
  <File header>

  module sf_epa_util

    <Use kinds>
    use physics_defs, only: ELECTRON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use interactions, only: interaction_pacify_momenta
    use model_data
    use sf_aux
    use sf_base

    use sf_epa

    <Standard module head>

    <SF epa: test declarations>

    contains

    <SF epa: tests>

  end module sf_epa_util

```

API: driver for the unit tests below.

```
<SF epa: public test>≡
  public :: sf_epa_test

<SF epa: test driver>≡
  subroutine sf_epa_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <SF epa: execute tests>
  end subroutine sf_epa_test
```

Test structure function data

Construct and display a test structure function data object.

```
<SF epa: execute tests>≡
  call test (sf_epa_1, "sf_epa_1", &
    "structure function configuration", &
    u, results)

<SF epa: test declarations>≡
  public :: sf_epa_1

<SF epa: tests>≡
  subroutine sf_epa_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(pdg_array_t), dimension(1) :: pdg_out
    integer, dimension(:), allocatable :: pdg1
    class(sf_data_t), allocatable :: data

    write (u, "(A)")  "* Test output: sf_epa_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &test structure function data"
    write (u, "(A)")

    write (u, "(A)")  "* Create empty data object"
    write (u, "(A)")

    call model%init_qed_test ()
    pdg_in = ELECTRON

    allocate (epa_data_t :: data)
    call data%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize"
    write (u, "(A)")

    select type (data)
    type is (epa_data_t)
      call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
        10._default, 100._default, 0.000511_default, recoil = .false.)
    end select
```

```

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_1"

end subroutine sf_epa_1

```

Test and probe structure function

Construct and display a structure function object based on the EPA structure function.

```

<SF epa: execute tests>+≡
  call test (sf_epa_2, "sf_epa_2", &
    "structure function instance", &
    u, results)

<SF epa: test declarations>+≡
  public :: sf_epa_2

<SF epa: tests>+≡
  subroutine sf_epa_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_epa_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv%init (ELECTRON, model)

```

```

pdg_in = ELECTRON

call reset_interaction_counter ()

allocate (epa_data_t :: data)
select type (data)
type is (epa_data_t)
    call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
        10._default, 100._default, 0.000511_default, recoil = .false.)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, no EPA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

```

```

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false., &
    set_momenta=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EPA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_2"

end subroutine sf_epa_2

```

Standard mapping

Construct and display a structure function object based on the EPA structure function, applying the standard single-particle mapping.

```

<SF epa: execute tests>+≡
    call test (sf_epa_3, "sf_epa_3", &
        "apply mapping", &
        u, results)

<SF epa: test declarations>+≡
    public :: sf_epa_3

<SF epa: tests>+≡
    subroutine sf_epa_3 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(pdg_array_t) :: pdg_in

```

```

class(sf_data_t), allocatable, target :: data
class(sf_int_t), allocatable :: sf_int
type(vector4_t) :: k
type(vector4_t), dimension(2) :: q
real(default) :: E
real(default), dimension(:), allocatable :: r, rb, x, xb
real(default) :: f

write (u, "(A)")  "* Test output: sf_epa_3"
write (u, "(A)")  "* Purpose: initialize and fill &
                  &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_qed_test ()
call flv%init (ELECTRON, model)
pdg_in = ELECTRON

call reset_interaction_counter ()

allocate (epa_data_t :: data)
select type (data)
type is (epa_data_t)
    call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
        10._default, 100._default, 0.000511_default, recoil = .false.)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, with EPA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

```

```

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true., &
    set_momenta=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EPA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_3"

end subroutine sf_epa_3

```

Non-collinear case

Construct and display a structure function object based on the EPA structure function.

```
<SF epa: execute tests>+≡
    call test (sf_epa_4, "sf_epa_4", &
               "non-collinear", &
               u, results)

<SF epa: test declarations>+≡
    public :: sf_epa_4

<SF epa: tests>+≡
    subroutine sf_epa_4 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        type(vector4_t) :: k
        type(vector4_t), dimension(2) :: q
        real(default) :: E, m
        real(default), dimension(:), allocatable :: r, rb, x, xb
        real(default) :: f

        write (u, "(A)")  "* Test output: sf_epa_4"
        write (u, "(A)")  "*   Purpose: initialize and fill &
                           &test structure function object"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize configuration data"
        write (u, "(A)")

        call model%init_qed_test ()
        call flv%init (ELECTRON, model)
        pdg_in = ELECTRON

        call reset_interaction_counter ()

        allocate (epa_data_t :: data)
        select type (data)
        type is (epa_data_t)
            call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
                           10._default, 100._default, 5.0_default, recoil = .true.)
        end select

        write (u, "(A)")  "* Initialize structure-function object"
        write (u, "(A)")

        call data%allocate_sf_int (sf_int)
        call sf_int%init (data)
        call sf_int%set_beam_index ([1])
        call sf_int%setup_constants ()
```



```

write (u, "(A)")  "* Initialize incoming momentum with E=500, me = 5 GeV"
write (u, "(A)")
E = 500
m = 5
k = vector4_moving (E, sqrt (E**2 - m**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.5/0.5/0.25, with EPA mapping, "
write (u, "(A)")  "          non-coll., keeping energy, me = 5 GeV"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.5_default, 0.5_default, 0.25_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call interaction_pacify_momenta (sf_int%interaction_t, 1e-10_default)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x and r from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true., &
    set_momenta=.true.)
call interaction_pacify_momenta (sf_int%interaction_t, 1e-10_default)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x

```

```

write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EPA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_4"

end subroutine sf_epa_4

```

Structure function for multiple flavors

Construct and display a structure function object based on the EPA structure function. The incoming state has multiple particles with non-uniform charge.

```

<SF epa: execute tests>+≡
  call test (sf_epa_5, "sf_epa_5", &
    "multiple flavors", &
    u, results)

<SF epa: test declarations>+≡
  public :: sf_epa_5

<SF epa: tests>+≡
  subroutine sf_epa_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_epa_5"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

```

```

call model%init_sm_test ()
call flv%init (1, model)
pdg_in = [1, 2, -1, -2]

call reset_interaction_counter ()

allocate (epa_data_t :: data)
select type (data)
type is (epa_data_t)
    call data%init (model, 0, pdg_in, 1./137._default, 0.01_default, &
        10._default, 100._default, 0.000511_default, recoil = .false.)
    call data%check ()
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, no EPA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EPA structure function"
write (u, "(A)")

```

```

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_epa_5"

end subroutine sf_epa_5

```

16.8 EWA

```
<sf_ewa.f90>≡  
<File header>  
  
module sf_ewa  
  
  <Use kinds>  
  <Use strings>  
  use io_units  
  use constants, only: pi  
  use format_defs, only: FMT_17, FMT_19  
  use numeric_utils  
  use diagnostics  
  use physics_defs, only: W_BOSON, Z_BOSON  
  use lorentz  
  use pdg_arrays  
  use model_data  
  use flavors  
  use colors  
  use quantum_numbers  
  use state_matrices  
  use polarizations  
  use interactions  
  use sf_aux  
  use sf_base  
  
  <Standard module head>  
  
  <SF ewa: public>  
  
  <SF ewa: parameters>  
  
  <SF ewa: types>  
  
contains  
  
  <SF ewa: procedures>  
  
end module sf_ewa
```

16.8.1 Physics

The EWA structure function for a Z or W inside a fermion (lepton or quark) depends on the vector-boson polarization. We distinguish transversal (\pm) and

longitudinal (0) polarization.

$$F_+(x) = \frac{1}{16\pi^2} \frac{(v-a)^2 + (v+a)^2 \bar{x}^2}{x} \left[\ln \left(\frac{p_{\perp,\max}^2 + \bar{x}M^2}{\bar{x}M^2} \right) - \frac{p_{\perp,\max}^2}{p_{\perp,\max}^2 + \bar{x}M^2} \right] \quad (16.50)$$

$$F_-(x) = \frac{1}{16\pi^2} \frac{(v+a)^2 + (v-a)^2 \bar{x}^2}{x} \left[\ln \left(\frac{p_{\perp,\max}^2 + \bar{x}M^2}{\bar{x}M^2} \right) - \frac{p_{\perp,\max}^2}{p_{\perp,\max}^2 + \bar{x}M^2} \right] \quad (16.51)$$

$$F_0(x) = \frac{v^2 + a^2}{8\pi^2} \frac{2\bar{x}}{x} \frac{p_{\perp,\max}^2}{p_{\perp,\max}^2 + \bar{x}M^2} \quad (16.52)$$

where $p_{\perp,\max}$ is the cutoff in transversal momentum, M is the vector-boson mass, v and a are the vector and axial-vector couplings, and $\bar{x} \equiv 1-x$. Note that the longitudinal structure function is finite for large cutoff, while the transversal structure function is logarithmically divergent.

The maximal transverse momentum is given by the kinematical limit, it is

$$p_{\perp,\max} = \bar{x}\sqrt{s}/2. \quad (16.53)$$

The vector and axial couplings for a fermion branching into a W are

$$v_W = \frac{g}{2\sqrt{2}}, \quad a_W = \frac{g}{2\sqrt{2}}. \quad (16.54)$$

For Z emission, this is replaced by

$$v_Z = \frac{g}{2\cos\theta_w} (t_3 - 2q\sin^2\theta_w), \quad a_Z = \frac{g}{2\cos\theta_w} t_3, \quad (16.55)$$

where $t_3 = \pm\frac{1}{2}$ is the fermion isospin, and q its charge.

For an initial antifermion, the signs of the axial couplings are inverted. Note that a common sign change of v and a is irrelevant.

The EWA depends on the parameters g , $\sin^2\theta_w$, M_W , and M_Z . These can all be taken from the SM input, and the prefactors are calculated from those and the incoming particle type.

Since these structure functions have a $1/x$ singularity (which is not really relevant in practice, however, since the vector boson mass is finite), we map this singularity allowing for nontrivial x bounds:

$$x = \exp(\bar{r} \ln x_0 + r \ln x_1) \quad (16.56)$$

such that

$$\int_{x_0}^{x_1} \frac{dx}{x} = (\ln x_1 - \ln x_0) \int_0^1 dr. \quad (16.57)$$

As a user parameter, we have the cutoff $p_{\perp,\max}$. The divergence $1/x$ also requires a x_0 cutoff; and for completeness we introduce a corresponding x_1 . Physically, the minimal sensible value of x is M^2/s , although the approximation loses its value already at higher x values.

16.8.2 The EWA data block

The EWA parameters are: $p_{T,\max}$, c_V , c_A , and m . Instead of m we can use the incoming particle PDG code as input; from this we can deduce the mass and charges. In the initialization phase it is not yet determined whether a W or a Z is radiated, hence we set the vector and axial-vector couplings equal to the common prefactors $g/2 = e/2/\sin\theta_W$.

In principle, for EWA it would make sense to allow the user to also set the upper bound for x , x_{\max} , but we fix it to one here.

```

<SF ewa: public>≡
    public :: ewa_data_t

<SF ewa: types>≡
    type, extends(sf_data_t) :: ewa_data_t
        private
            class(model_data_t), pointer :: model => null ()
            type(flavor_t), dimension(:), allocatable :: flv_in
            type(flavor_t), dimension(:), allocatable :: flv_out
            real(default) :: pt_max
            real(default) :: sqrts
            real(default) :: x_min
            real(default) :: x_max
            real(default) :: mass
            real(default) :: m_out
            real(default) :: q_min
            real(default) :: cv
            real(default) :: ca
            real(default) :: costhw
            real(default) :: sinthw
            real(default) :: mW
            real(default) :: mZ
            real(default) :: coeff
            logical :: mass_set = .false.
            logical :: recoil = .false.
            logical :: keep_energy = .false.
            integer :: id = 0
            integer :: error = NONE
        contains
            <SF ewa: ewa data: TBP>
        end type ewa_data_t

```

Error codes

```

<SF ewa: parameters>≡
    integer, parameter :: NONE = 0
    integer, parameter :: ZERO_QMIN = 1
    integer, parameter :: Q_MAX_TOO_SMALL = 2
    integer, parameter :: ZERO_XMIN = 3
    integer, parameter :: MASS_MIX = 4
    integer, parameter :: ZERO_SW = 5
    integer, parameter :: ISOSPIN_MIX = 6
    integer, parameter :: WRONG_PRT = 7
    integer, parameter :: MASS_MIX_OUT = 8
    integer, parameter :: NO_EWA = 9

```

```

<SF ewa: ewa data: TBP>≡
  procedure :: init => ewa_data_init

<SF ewa: procedures>≡
  subroutine ewa_data_init (data, model, pdg_in, x_min, pt_max, &
    sqrts, recoil, keep_energy, mass)
    class(ewa_data_t), intent(inout) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    real(default), intent(in) :: x_min, pt_max, sqrts
    logical, intent(in) :: recoil, keep_energy
    real(default), intent(in), optional :: mass
    real(default) :: g, ee
    integer :: n_flv, i
    data%model => model
    if (.not. any (pdg_in .match. &
      [1,2,3,4,5,6,11,13,15,-1,-2,-3,-4,-5,-6,-11,-13,-15])) then
      data%error = WRONG_PRT; return
    end if
    n_flv = pdg_array_get_length (pdg_in)
    allocate (data%flv_in (n_flv))
    allocate (data%flv_out(n_flv))
    do i = 1, n_flv
      call data%flv_in(i)%init (pdg_array_get (pdg_in, i), model)
    end do
    data%pt_max = pt_max
    data%sqrts = sqrts
    data%x_min = x_min
    data%x_max = 1
    if (vanishes (data%x_min)) then
      data%error = ZERO_XMIN; return
    end if
    select case (char (data%model%get_name ()))
    case ("QCD","QED","Test")
      data%error = NO_EWA; return
    end select
    ee = data%model%get_real (var_str ("ee"))
    data%sinhw = data%model%get_real (var_str ("sw"))
    data%costhw = data%model%get_real (var_str ("cw"))
    data%mZ = data%model%get_real (var_str ("mZ"))
    data%mW = data%model%get_real (var_str ("mW"))
    if (data%sinhw /= 0) then
      g = ee / data%sinhw
    else
      data%error = ZERO_SW; return
    end if
    data%cv = g / 2._default
    data%ca = g / 2._default
    data%coeff = 1._default / (8._default * PI**2)
    data%recoil = recoil
    data%keep_energy = keep_energy
    if (present (mass)) then
      data%mass = mass
      data%m_out = mass
      data%mass_set = .true.

```



```

else
  data%mass = data%flv_in(1)%get_mass ()
  if (any (data%flv_in%get_mass () /= data%mass)) then
    data%error = MASS_MIX; return
  end if
end if
end subroutine ewa_data_init

```

Set the vector boson ID for distinguishing W and Z bosons.

```

<SF ewa: ewa data: TBP>+=
  procedure :: set_id => ewa_set_id

<SF ewa: procedures>+=
  subroutine ewa_set_id (data, id)
    class(ewa_data_t), intent(inout) :: data
    integer, intent(in) :: id
    integer :: i, isospin, pdg
    if (.not. allocated (data%flv_in)) &
      call msg_bug ("EWA: incoming particles not set")
    data%id = id
    select case (data%id)
    case (23)
      data%m_out = data%mass
      data%flv_out = data%flv_in
    case (24)
      do i = 1, size (data%flv_in)
        pdg = data%flv_in(i)%get_pdg ()
        isospin = data%flv_in(i)%get_isospin_type ()
        if (isospin > 0) then
          !!! up-type quark or neutrinos
          if (data%flv_in(i)%is_antiparticle ()) then
            call data%flv_out(i)%init (pdg + 1, data%model)
          else
            call data%flv_out(i)%init (pdg - 1, data%model)
          end if
        else
          !!! down-type quark or lepton
          if (data%flv_in(i)%is_antiparticle ()) then
            call data%flv_out(i)%init (pdg - 1, data%model)
          else
            call data%flv_out(i)%init (pdg + 1, data%model)
          end if
        end if
      end do
      if (.not. data%mass_set) then
        data%m_out = data%flv_out(1)%get_mass ()
        if (any (data%flv_out%get_mass () /= data%m_out)) then
          data%error = MASS_MIX_OUT; return
        end if
      end if
    end select
  end subroutine ewa_set_id

```

Handle error conditions. Should always be done after initialization, unless we are sure everything is ok.

```

<SF ewa: ewa data: TBP>+≡
  procedure :: check => ewa_data_check

<SF ewa: procedures>+≡
  subroutine ewa_data_check (data)
    class(ewa_data_t), intent(in) :: data
    select case (data%error)
    case (WRONG_PRT)
      call msg_fatal ("EWA structure function only accessible for " &
        // "SM quarks and leptons.")
    case (NO_EWA)
      call msg_fatal ("EWA structure function not available for model " &
        // char (data%model%get_name ()))
    case (ZERO_SW)
      call msg_fatal ("EWA: Vanishing value of sin(theta_w)")
    case (ZERO_QMIN)
      call msg_fatal ("EWA: Particle mass is zero")
    case (Q_MAX_TOO_SMALL)
      call msg_fatal ("EWA: Particle mass exceeds Qmax")
    case (ZERO_XMIN)
      call msg_fatal ("EWA: x_min must be larger than zero")
    case (MASS_MIX)
      call msg_fatal ("EWA: incoming particle masses must be uniform")
    case (MASS_MIX_OUT)
      call msg_fatal ("EWA: outgoing particle masses must be uniform")
    case (ISOSPIN_MIX)
      call msg_fatal ("EWA: incoming particle isospins must be uniform")
    end select
  end subroutine ewa_data_check

```

Output

```

<SF ewa: ewa data: TBP>+≡
  procedure :: write => ewa_data_write

<SF ewa: procedures>+≡
  subroutine ewa_data_write (data, unit, verbose)
    class(ewa_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "EWA data:"
    if (allocated (data%flv_in) .and. allocated (data%flv_out)) then
      write (u, "(3x,A)", advance="no") " flavor(in) = "
      do i = 1, size (data%flv_in)
        if (i > 1) write (u, "(',',1x)", advance="no")
        call data%flv_in(i)%write (u)
      end do
    end
    write (u, *)
    write (u, "(3x,A)", advance="no") " flavor(out) = "
    do i = 1, size (data%flv_out)
      if (i > 1) write (u, "(',',1x)", advance="no")
    end do
  end subroutine ewa_data_write

```

```

        call data%flv_out(i)%write (u)
    end do
    write (u, *)
    write (u, "(3x,A," // FMT_19 // ")") " x_min      = ", data%x_min
    write (u, "(3x,A," // FMT_19 // ")") " x_max      = ", data%x_max
    write (u, "(3x,A," // FMT_19 // ")") " pt_max     = ", data%pt_max
    write (u, "(3x,A," // FMT_19 // ")") " sqrts      = ", data%sqrts
    write (u, "(3x,A," // FMT_19 // ")") " mass       = ", data%mass
    write (u, "(3x,A," // FMT_19 // ")") " cv         = ", data%cv
    write (u, "(3x,A," // FMT_19 // ")") " ca         = ", data%ca
    write (u, "(3x,A," // FMT_19 // ")") " coeff      = ", data%coeff
    write (u, "(3x,A," // FMT_19 // ")") " costhw     = ", data%costhw
    write (u, "(3x,A," // FMT_19 // ")") " sinthw     = ", data%sinthw
    write (u, "(3x,A," // FMT_19 // ")") " mZ         = ", data%mZ
    write (u, "(3x,A," // FMT_19 // ")") " mW         = ", data%mW
    write (u, "(3x,A,L2)") " recoil    = ", data%recoil
    write (u, "(3x,A,L2)") " keep en.  = ", data%keep_energy
    write (u, "(3x,A,I2)") " PDG (VB) = ", data%id
else
    write (u, "(3x,A)") "[undefined]"
end if
end subroutine ewa_data_write

```

The number of parameters is one for collinear splitting, in case the recoil option is set, we take the recoil into account.

```

<SF ewa: ewa data: TBP>+=
    procedure :: get_n_par => ewa_data_get_n_par

<SF ewa: procedures>+=
    function ewa_data_get_n_par (data) result (n)
        class(ewa_data_t), intent(in) :: data
        integer :: n
        if (data%recoil) then
            n = 3
        else
            n = 1
        end if
    end function ewa_data_get_n_par

```

Return the outgoing particles PDG codes. This depends, whether this is a charged-current or neutral-current interaction.

```

<SF ewa: ewa data: TBP>+=
    procedure :: get_pdg_out => ewa_data_get_pdg_out

<SF ewa: procedures>+=
    subroutine ewa_data_get_pdg_out (data, pdg_out)
        class(ewa_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        integer, dimension(:), allocatable :: pdg1
        integer :: i, n_flv
        if (allocated (data%flv_out)) then
            n_flv = size (data%flv_out)
        else
            n_flv = 0
        end if
    end subroutine ewa_data_get_pdg_out

```

```

end if
allocate (pdg1 (n_flv))
do i = 1, n_flv
    pdg1(i) = data%flv_out(i)%get_pdg ()
end do
pdg_out(1) = pdg1
end subroutine ewa_data_get_pdg_out

```

Allocate the interaction record.

```

<SF ewa: ewa data: TBP>+≡
    procedure :: allocate_sf_int => ewa_data_allocate_sf_int

<SF ewa: procedures>+≡
    subroutine ewa_data_allocate_sf_int (data, sf_int)
        class(ewa_data_t), intent(in) :: data
        class(sf_int_t), intent(inout), allocatable :: sf_int
        allocate (ewa_t :: sf_int)
    end subroutine ewa_data_allocate_sf_int

```

16.8.3 The EWA object

The `ewa_t` data type is a $1 \rightarrow 2$ interaction. We should be able to handle several flavors in parallel, since EWA is not necessarily applied immediately after beam collision: W/Z bosons may be radiated from quarks. In that case, the partons are massless and q_{\min} applies instead, so we do not need to generate several kinematical configurations in parallel.

The particles are ordered as (incoming, radiated, W/Z), where the W/Z initiates the hard interaction.

In the case of EPA, we generated an unpolarized photon and transferred initial polarization to the radiated parton. Color is transferred in the same way. I do not know whether the same can/should be done for EWA, as the structure functions depend on the W/Z polarization. If we are having Z bosons, both up- and down-type fermions can participate. Otherwise, with a W^+ an up-type fermion is transferred to a down-type fermion, and the other way round.

```

<SF ewa: types>+≡
    type, extends (sf_int_t) :: ewa_t
        type(ewa_data_t), pointer :: data => null ()
        real(default) :: x = 0
        real(default) :: xb = 0
        integer :: n_me = 0
        real(default), dimension(:), allocatable :: cv
        real(default), dimension(:), allocatable :: ca
    contains
        <SF ewa: ewa: TBP>
    end type ewa_t

```

Type string: has to be here, but there is no string variable on which EWA depends. Hence, a dummy routine.

```

<SF ewa: ewa: TBP>≡
    procedure :: type_string => ewa_type_string

```

```

<SF ewa: procedures>+≡
function ewa_type_string (object) result (string)
  class(ewa_t), intent(in) :: object
  type(string_t) :: string
  if (associated (object%data)) then
    string = "EWA: equivalent W/Z approx."
  else
    string = "EWA: [undefined]"
  end if
end function ewa_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF ewa: ewa: TBP>+≡
  procedure :: write => ewa_write

<SF ewa: procedures>+≡
  subroutine ewa_write (object, unit, testflag)
    class(ewa_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      if (object%status >= SF_DONE_KINEMATICS) then
        write (u, "(1x,A)") "SF parameters:"
        write (u, "(3x,A," // FMT_17 // ")") "x =", object%x
        write (u, "(3x,A," // FMT_17 // ")") "xb=", object%xb
      end if
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "EWA data: [undefined]"
    end if
  end subroutine ewa_write

```

The current implementation requires uniform isospin for all incoming particles, therefore we need to probe only the first one.

```

<SF ewa: ewa: TBP>+≡
  procedure :: init => ewa_init

<SF ewa: procedures>+≡
  subroutine ewa_init (sf_int, data)
    class(ewa_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(3) :: mask
    integer, dimension(3) :: hel_lock
    type(polarization_t), target :: pol
    type(quantum_numbers_t), dimension(1) :: qn_fc, qn_fc_fin
    type(flavor_t) :: flv_z, flv_wp, flv_wm
    type(color_t) :: col0
    type(quantum_numbers_t) :: qn_hel, qn_z, qn_wp, qn_wm, qn, qn_rad, qn_w
    type(polarization_iterator_t) :: it_hel
    integer :: i, isospin
    select type (data)

```

```

type is (ewa_data_t)
mask = quantum_numbers_mask (.false., .false., &
    mask_h = [.false., .false., .true.])
hel_lock = [2, 1, 0]
call col0%init ()
select case (data%id)
case (23)
    !!! Z boson, flavor is not changing
    call sf_int%base_init (mask, [data%mass**2], [data%mass**2], &
        [data%mZ**2], hel_lock = hel_lock)
    sf_int%data => data
    call flv_z%init (Z_BOSON, data%model)
    call qn_z%init (flv_z, col0)
    do i = 1, size (data%flv_in)
        call pol%init_generic (data%flv_in(i))
        call qn_fc(1)%init ( &
            flv = data%flv_in(i), &
            col = color_from_flavor (data%flv_in(i), 1))
        call it_hel%init (pol)
        do while (it_hel%is_valid ())
            qn_hel = it_hel%get_quantum_numbers ()
            qn = qn_hel .merge. qn_fc(1)
            qn_rad = qn
            call qn_rad%tag_radiated ()
            call sf_int%add_state ([qn, qn_rad, qn_z])
            call it_hel%advance ()
        end do
        ! call pol%final ()
    end do
case (24)
    call sf_int%base_init (mask, [data%mass**2], [data%m_out**2], &
        [data%mW**2], hel_lock = hel_lock)
    sf_int%data => data
    call flv_wp%init (W_BOSON, data%model)
    call flv_wm%init (- W_BOSON, data%model)
    call qn_wp%init (flv_wp, col0)
    call qn_wm%init (flv_wm, col0)
    do i = 1, size (data%flv_in)
        isospin = data%flv_in(i)%get_isospin_type ()
        if (isospin > 0) then
            !!! up-type quark or neutrinos
            if (data%flv_in(i)%is_antiparticle ()) then
                qn_w = qn_wm
            else
                qn_w = qn_wp
            end if
        else
            !!! down-type quark or lepton
            if (data%flv_in(i)%is_antiparticle ()) then
                qn_w = qn_wp
            else
                qn_w = qn_wm
            end if
        end if
    end if
end if

```

```

        call pol%init_generic (data%flv_in(i))
        call qn_fc(1)%init ( &
            flv = data%flv_in(i), &
            col = color_from_flavor (data%flv_in(i), 1))
        call qn_fc_fin(1)%init ( &
            flv = data%flv_out(i), &
            col = color_from_flavor (data%flv_out(i), 1))
        call it_hel%init (pol)
        do while (it_hel%is_valid ())
            qn_hel = it_hel%get_quantum_numbers ()
            qn = qn_hel .merge. qn_fc(1)
            qn_rad = qn_hel .merge. qn_fc_fin(1)
            call qn_rad%tag_radiated ()
            call sf_int%add_state ([qn, qn_rad, qn_w])
            call it_hel%advance ()
        end do
        ! call pol%final ()
    end do
case default
    call msg_fatal ("EWA initialization failed: wrong particle type.")
end select
call sf_int%freeze ()
if (data%keep_energy) then
    sf_int%on_shell_mode = KEEP_ENERGY
else
    sf_int%on_shell_mode = KEEP_MOMENTUM
end if
call sf_int%set_incoming ([1])
call sf_int%set_radiated ([2])
call sf_int%set_outgoing ([3])
end select
end subroutine ewa_init

```

Prepare the coupling arrays. This is separate from the previous routine since the state matrix may be helicity-contracted.

```

<SF ewa: ewa: TBP>+≡
    procedure :: setup_constants => ewa_setup_constants

<SF ewa: procedures>+≡
    subroutine ewa_setup_constants (sf_int)
        class(ewa_t), intent(inout), target :: sf_int
        type(state_iterator_t) :: it
        type(flavor_t) :: flv
        real(default) :: q, t3
        integer :: i
        sf_int%n_me = sf_int%get_n_matrix_elements ()
        allocate (sf_int%cv (sf_int%n_me))
        allocate (sf_int%ca (sf_int%n_me))
        associate (data => sf_int%data)
            select case (data%id)
            case (23)
                call it%init (sf_int%interaction_t%get_state_matrix_ptr ())
                do while (it%is_valid ())
                    i = it%get_me_index ()

```

```

        flv = it%get_flavor (1)
        q = flv%get_charge ()
        t3 = flv%get_isospin ()
        if (flv%is_antiparticle ()) then
            sf_int%cv(i) = - data%cv &
                * (t3 - 2._default * q * data%sinthw**2) / data%costhw
            sf_int%ca(i) = data%ca * t3 / data%costhw
        else
            sf_int%cv(i) = data%cv &
                * (t3 - 2._default * q * data%sinthw**2) / data%costhw
            sf_int%ca(i) = data%ca * t3 / data%costhw
        end if
        call it%advance ()
    end do
case (24)
    call it%init (sf_int%interaction_t%get_state_matrix_ptr ())
    do while (it%is_valid ())
        i = it%get_me_index ()
        flv = it%get_flavor (1)
        if (flv%is_antiparticle ()) then
            sf_int%cv(i) = data%cv / sqrt(2._default)
            sf_int%ca(i) = - data%ca / sqrt(2._default)
        else
            sf_int%cv(i) = data%cv / sqrt(2._default)
            sf_int%ca(i) = data%ca / sqrt(2._default)
        end if
        call it%advance ()
    end do
end select
end associate
sf_int%status = SF_INITIAL
end subroutine ewa_setup_constants

```

16.8.4 Kinematics

Set kinematics. The EWA structure function allows for a straightforward mapping of the unit interval. So, to leading order, the structure function value is unity, but the x value is transformed. Higher orders affect the function value. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, the exponential mapping for the $1/x$ singularity discussed above is applied.

```

<SF ewa: ewa: TBP>+≡
    procedure :: complete_kinematics => ewa_complete_kinematics

<SF ewa: procedures>+≡
    subroutine ewa_complete_kinematics (sf_int, x, xb, f, r, rb, map)
        class(ewa_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
    end subroutine

```



```

logical, intent(in) :: map
real(default) :: e_1
real(default) :: x0, x1, lx0, lx1, lx
e_1 = energy (sf_int%get_momentum (1))
if (sf_int%data%recoil) then
  select case (sf_int%data%id)
    case (23)
      x0 = max (sf_int%data%x_min, sf_int%data%mz / e_1)
    case (24)
      x0 = max (sf_int%data%x_min, sf_int%data%mw / e_1)
  end select
else
  x0 = sf_int%data%x_min
end if
x1 = sf_int%data%x_max
if ( x0 >= x1) then
  f = 0
  sf_int%status = SF_FAILED_KINEMATICS
  return
end if
if (map) then
  lx0 = log (x0)
  lx1 = log (x1)
  lx = lx1 * r(1) + lx0 * rb(1)
  x(1) = exp(lx)
  f = x(1) * (lx1 - lx0)
else
  x(1) = r(1)
  if (x0 < x(1) .and. x(1) < x1) then
    f = 1
  else
    sf_int%status = SF_FAILED_KINEMATICS
    f = 0
    return
  end if
end if
xb(1) = 1 - x(1)
if (size(x) == 3) then
  x(2:3) = r(2:3)
  xb(2:3) = rb(2:3)
end if
call sf_int%split_momentum (x, xb)
select case (sf_int%status)
case (SF_DONE_KINEMATICS)
  sf_int%x = x(1)
  sf_int%xb = xb(1)
case (SF_FAILED_KINEMATICS)
  sf_int%x = 0
  sf_int%xb = 0
  f = 0
end select
end subroutine ewa_complete_kinematics

```

Overriding the default method: we compute the x array from the momentum

configuration. In the specific case of EWA, we also set the internally stored x and \bar{x} values, so they can be used in the following routine.

```

<SF ewa: ewa: TBP>+≡
  procedure :: recover_x => sf_ewa_recover_x

<SF ewa: procedures>+≡
  subroutine sf_ewa_recover_x (sf_int, x, xb, x_free)
    class(ewa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb, x_free)
    sf_int%x = x(1)
    sf_int%xb = xb(1)
  end subroutine sf_ewa_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF ewa: ewa: TBP>+≡
  procedure :: inverse_kinematics => ewa_inverse_kinematics

<SF ewa: procedures>+≡
  subroutine ewa_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(ewa_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    real(default) :: x0, x1, lx0, lx1, lx, e_1
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    e_1 = energy (sf_int%get_momentum (1))
    if (sf_int%data%recoil) then
      select case (sf_int%data%id)
        case (23)
          x0 = max (sf_int%data%x_min, sf_int%data%mz / e_1)
        case (24)
          x0 = max (sf_int%data%x_min, sf_int%data%mw / e_1)
        end select
    else
      x0 = sf_int%data%x_min
    end if
    x1 = sf_int%data%x_max
    if (map) then
      lx0 = log (x0)
      lx1 = log (x1)
      lx = log (x(1))
      r(1) = (lx - lx0) / (lx1 - lx0)
      rb(1) = (lx1 - lx) / (lx1 - lx0)
      f = x(1) * (lx1 - lx0)
    end if
  end subroutine ewa_inverse_kinematics

```

```

else
  r (1) = x(1)
  rb(1) = 1 - x(1)
  if (x0 < x(1) .and. x(1) < x1) then
    f = 1
  else
    f = 0
  end if
end if
if (size(r) == 3) then
  r (2:3) = x(2:3)
  rb(2:3) = xb(2:3)
end if
if (set_mom) then
  call sf_int%split_momentum (x, xb)
  select case (sf_int%status)
  case (SF_FAILED_KINEMATICS); f = 0
  end select
end if
end subroutine ewa_inverse_kinematics

```

16.8.5 EWA application

For EWA, we can compute kinematics and function value in a single step. This function works on a single beam, assuming that the input momentum has been set. We need four random numbers as input: one for x , one for Q^2 , and two for the polar and azimuthal angles. Alternatively, we can skip p_T generation; in this case, we only need one.

For obtaining splitting kinematics, we rely on the assumption that all in-particles are mass-degenerate (or there is only one), so the generated x values are identical.

```

<SF ewa: ewa: TBP>+=
  procedure :: apply => ewa_apply

<SF ewa: procedures>+=
  subroutine ewa_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(ewa_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: x, xb, pt2, c1, c2
    real(default) :: cv, ca
    real(default) :: f, fm, fp, fL
    integer :: i
    associate (data => sf_int%data)
      x = sf_int%x
      xb = sf_int%xb
      pt2 = min ((data%pt_max)**2, (xb * data%sqrts / 2)**2)
      select case (data%id)
      case (23)
        !!! Z boson structure function

```

```

        c1 = log (1 + pt2 / (xb * (data%mZ)**2))
        c2 = 1 / (1 + (xb * (data%mZ)**2) / pt2)
    case (24)
        !!! W boson structure function
        c1 = log (1 + pt2 / (xb * (data%mW)**2))
        c2 = 1 / (1 + (xb * (data%mW)**2) / pt2)
    end select
    do i = 1, sf_int%n_me
        cv = sf_int%cv(i)
        ca = sf_int%ca(i)
        fm = data%coeff * &
            ((cv + ca)**2 + ((cv - ca) * xb)**2) * (c1 - c2) / (2 * x)
        fp = data%coeff * &
            ((cv - ca)**2 + ((cv + ca) * xb)**2) * (c1 - c2) / (2 * x)
        fL = data%coeff * &
            (cv**2 + ca**2) * (2 * xb / x) * c2
        f = fp + fm + fL
        if (.not. vanishes (f)) then
            fp = fp / f
            fm = fm / f
            fL = fL / f
        end if
        call sf_int%set_matrix_element (i, cmplx (f, kind=default))
    end do
end associate
sf_int%status = SF_EVALUATED
end subroutine ewa_apply

```

16.8.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_ewa_ut.f90>≡
  <File header>

  module sf_ewa_ut
    use unit_tests
    use sf_ewa_util

    <Standard module head>

    <SF ewa: public test>

    contains

    <SF ewa: test driver>

  end module sf_ewa_ut
<sf_ewa_util.f90>≡
  <File header>

  module sf_ewa_util

```

```

    <Use kinds>
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use interactions, only: interaction_pacify_momenta
    use model_data
    use sf_aux
    use sf_base

    use sf_ewa

    <Standard module head>

    <SF ewa: test declarations>

    contains

    <SF ewa: tests>

    end module sf_ewa_util

API: driver for the unit tests below.
    <SF ewa: public test>≡
    public :: sf_ewa_test

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

```

Test structure function data

Construct and display a test structure function data object.

```

    <SF ewa: execute tests>≡
    call test (sf_ewa_1, "sf_ewa_1", &
        "structure function configuration", &
        u, results)

    <SF ewa: test declarations>≡
    public :: sf_ewa_1

    <SF ewa: tests>≡
    subroutine sf_ewa_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(pdg_array_t) :: pdg_in
        type(pdg_array_t), dimension(1) :: pdg_out
        integer, dimension(:), allocatable :: pdg1
        class(sf_data_t), allocatable :: data

        write (u, "(A)")  "* Test output: sf_ewa_1"
        write (u, "(A)")  "* Purpose: initialize and display &

```

```

        &test structure function data"
write (u, "(A)")

write (u, "(A)")  "* Create empty data object"
write (u, "(A)")

call model%init_sm_test ()
pdg_in = 2

allocate (ewa_data_t :: data)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize for Z boson"
write (u, "(A)")

select type (data)
type is (ewa_data_t)
    call data%init (model, pdg_in, 0.01_default, &
        500._default, 5000._default, .false., .false.)
    call data%set_id (23)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)")  "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))")  pdg1

write (u, "(A)")
write (u, "(A)")  "* Initialize for W boson"
write (u, "(A)")

deallocate (data)
allocate (ewa_data_t :: data)
select type (data)
type is (ewa_data_t)
    call data%init (model, pdg_in, 0.01_default, &
        500._default, 5000._default, .false., .false.)
    call data%set_id (24)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)")  "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))")  pdg1

```

```

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_1"

end subroutine sf_ewa_1

```

Test and probe structure function

Construct and display a structure function object based on the EWA structure function.

```

<SF ewa: execute tests>+≡
  call test (sf_ewa_2, "sf_ewa_2", &
    "structure function instance", &
    u, results)

<SF ewa: test declarations>+≡
  public :: sf_ewa_2

<SF ewa: tests>+≡
  subroutine sf_ewa_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_ewa_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_sm_test ()
    call flv%init (2, model)
    pdg_in = 2

    call reset_interaction_counter ()

    allocate (ewa_data_t :: data)
    select type (data)
    type is (ewa_data_t)
      call data%init (model, pdg_in, 0.01_default, &
        500._default, 3000._default, .false., .true.)
      call data%set_id (24)

```

```

end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=1500"
write (u, "(A)")
E = 1500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, no EWA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])

```



```

call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false., &
    set_momenta=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EWA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_2"

end subroutine sf_ewa_2

```

Standard mapping

Construct and display a structure function object based on the EWA structure function, applying the standard single-particle mapping.

```

<SF ewa: execute tests>+=
    call test (sf_ewa_3, "sf_ewa_3", &
        "apply mapping", &
        u, results)

<SF ewa: test declarations>+=
    public :: sf_ewa_3

<SF ewa: tests>+=
    subroutine sf_ewa_3 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        type(vector4_t) :: k
        type(vector4_t), dimension(2) :: q
        real(default) :: E
        real(default), dimension(:), allocatable :: r, rb, x, xb

```

```

real(default) :: f

write (u, "(A)")  "* Test output: sf_ewa_3"
write (u, "(A)")  "* Purpose: initialize and fill &
                  &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_sm_test ()
call flv%init (2, model)
pdg_in = 2

call reset_interaction_counter ()

allocate (ewa_data_t :: data)
select type (data)
type is (ewa_data_t)
    call data%init (model, pdg_in, 0.01_default, &
                  500._default, 3000._default, .false., .true.)
    call data%set_id (24)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=1500"
write (u, "(A)")
E = 1500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write(k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, with EWA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r

```

```

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true., &
    set_momenta=.true.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EWA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_3"

end subroutine sf_ewa_3

```

Non-collinear case

Construct and display a structure function object based on the EPA structure function.

```
<SF ewa: execute tests>+≡
    call test (sf_ewa_4, "sf_ewa_4", &
               "non-collinear", &
               u, results)

<SF ewa: test declarations>+≡
    public :: sf_ewa_4

<SF ewa: tests>+≡
    subroutine sf_ewa_4 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        type(vector4_t) :: k
        type(vector4_t), dimension(2) :: q
        real(default) :: E
        real(default), dimension(:), allocatable :: r, rb, x, xb
        real(default) :: f

        write (u, "(A)")  "* Test output: sf_ewa_4"
        write (u, "(A)")  "*   Purpose: initialize and fill &
                           &test structure function object"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize configuration data"
        write (u, "(A)")

        call model%init_sm_test ()
        call flv%init (2, model)
        pdg_in = 2

        call reset_interaction_counter ()

        allocate (ewa_data_t :: data)
        select type (data)
        type is (ewa_data_t)
            call data%init (model, pdg_in, 0.01_default, &
                           500._default, 3000.0_default, .true., .true.)
            call data%set_id (24)
        end select

        write (u, "(A)")  "* Initialize structure-function object"
        write (u, "(A)")

        call data%allocate_sf_int (sf_int)
        call sf_int%init (data)
        call sf_int%set_beam_index ([1])
        call sf_int%setup_constants ()
```

```

write (u, "(A)")  "* Initialize incoming momentum with E=1500"
write (u, "(A)")
E = 1500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.5/0.5/0.25, with EWA mapping, "
write (u, "(A)")  "          non-coll., keeping energy"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.5_default, 0.5_default, 0.25_default]
rb = 1 - r
sf_int%on_shell_mode = KEEP_ENERGY
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.true.)
call interaction_pacify_momenta (sf_int%interaction_t, 1e-10_default)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x and r from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.true., &
    set_momenta=.true.)
call interaction_pacify_momenta (sf_int%interaction_t, 1e-10_default)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x

```

```

write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Evaluate EWA structure function"
write (u, "(A)")

call sf_int%apply (scale = 1500._default)
call sf_int%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_4"

end subroutine sf_ewa_4

```

Structure function for multiple flavors

Construct and display a structure function object based on the EWA structure function. The incoming state has multiple particles with non-uniform quantum numbers.

```

<SF ewa: execute tests>+≡
  call test (sf_ewa_5, "sf_ewa_5", &
    "structure function instance", &
    u, results)

<SF ewa: test declarations>+≡
  public :: sf_ewa_5

<SF ewa: tests>+≡
  subroutine sf_ewa_5 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_ewa_5"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &test structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"

```

```

write (u, "(A)")

call model%init_sm_test ()
call flv%init (2, model)
pdg_in = [1, 2, -1, -2]

call reset_interaction_counter ()

allocate (ewa_data_t :: data)
select type (data)
type is (ewa_data_t)
    call data%init (model, pdg_in, 0.01_default, &
        500._default, 3000._default, .false., .true.)
    call data%set_id (24)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])
call sf_int%setup_constants ()

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=1500"
write (u, "(A)")
E = 1500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call pacify (k, 1e-10_default)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for r=0.4, no EWA mapping, collinear"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.4_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

```

```

write (u, "(A)")
write (u, "(A)")  "* Evaluate EWA structure function"
write (u, "(A)")

call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_ewa_5"

end subroutine sf_ewa_5

```


16.9 Energy-scan spectrum

This spectrum is actually a trick that allows us to plot the c.m. energy dependence of a cross section without scanning the input energy. We start with the observation that a spectrum $f(x)$, applied to one of the incoming beams only, results in a cross section

$$\sigma = \int dx f(x) \hat{\sigma}(xs). \quad (16.58)$$

We want to compute the distribution of $E = \sqrt{\hat{s}} = \sqrt{xs}$, i.e.,

$$\frac{d\sigma}{dE} = \frac{2\sqrt{x}}{\sqrt{s}} \frac{d\sigma}{dx} = \frac{2\sqrt{x}}{\sqrt{s}} f(x) \hat{\sigma}(xs), \quad (16.59)$$

so if we set

$$f(x) = \frac{\sqrt{s}}{2\sqrt{x}}, \quad (16.60)$$

we get the distribution

$$\frac{d\sigma}{dE} = \hat{\sigma}(\hat{s} = E^2). \quad (16.61)$$

We implement this as a spectrum with a single parameter x . The parameters for the individual beams are computed as $x_i = \sqrt{x}$, so they are equal and the kinematics is always symmetric.

`<sf_escan.f90>`≡
<File header>

`module sf_escan`

<Use kinds>

<Use strings>

`use io_units`

`use format_defs, only: FMT_12`

`use numeric_utils`

`use diagnostics`

`use lorentz`

`use pdg_arrays`

`use model_data`

`use flavors`

`use quantum_numbers`

`use state_matrices`

`use polarizations`

`use sf_base`

<Standard module head>

<SF_escan: public>

<SF_escan: types>

`contains`

<SF_escan: procedures>

`end module sf_escan`

16.9.1 Data type

The `norm` is unity if the total cross section should be normalized to one, and \sqrt{s} if it should be normalized to the total energy. In the latter case, the differential distribution $d\sigma/d\sqrt{\hat{s}}$ coincides with the partonic cross section $\hat{\sigma}$ as a function of $\sqrt{\hat{s}}$.

```

<SF escan: public>≡
  public :: escan_data_t

<SF escan: types>≡
  type, extends(sf_data_t) :: escan_data_t
  private
    type(flavor_t), dimension(:, :), allocatable :: flv_in
    integer, dimension(2) :: n_flv = 0
    real(default) :: norm = 1
  contains
    <SF escan: escan data: TBP>
  end type escan_data_t

<SF escan: escan data: TBP>≡
  procedure :: init => escan_data_init

<SF escan: procedures>≡
  subroutine escan_data_init (data, model, pdg_in, norm)
    class(escan_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), dimension(2), intent(in) :: pdg_in
    real(default), intent(in), optional :: norm
    real(default), dimension(2) :: m2
    integer :: i, j
    data%n_flv = pdg_array_get_length (pdg_in)
    allocate (data%flv_in (maxval (data%n_flv), 2))
    do i = 1, 2
      do j = 1, data%n_flv(i)
        call data%flv_in(j, i)%init (pdg_array_get (pdg_in(i), j), model)
      end do
    end do
    m2 = data%flv_in(1, :)%get_mass ()
    do i = 1, 2
      if (.not. any (nearly_equal (data%flv_in(1:data%n_flv(i), i)%get_mass (), m2(i)))) then
        call msg_fatal ("Energy scan: incoming particle mass must be uniform")
      end if
    end do
    if (present (norm)) data%norm = norm
  end subroutine escan_data_init

Output

<SF escan: escan data: TBP>+≡
  procedure :: write => escan_data_write

<SF escan: procedures>+≡
  subroutine escan_data_write (data, unit, verbose)
    class(escan_data_t), intent(in) :: data
    integer, intent(in), optional :: unit

```

```

logical, intent(in), optional :: verbose
integer :: u, i, j
u = given_output_unit (unit); if (u < 0) return
write (u, "(1x,A)") "Energy-scan data:"
write (u, "(3x,A)", advance="no") "prt_in = "
do i = 1, 2
  if (i > 1) write (u, "(',',1x)", advance="no")
  do j = 1, data%n_flv(i)
    if (j > 1) write (u, "(::)", advance="no")
    write (u, "(A)", advance="no") char (data%flv_in(j,i)%get_name ())
  end do
end do
write (u, *)
write (u, "(3x,A," // FMT_12 // ")") "norm   =", data%norm
end subroutine escan_data_write

```

Kinematics is completely collinear, hence there is only one parameter for a pair spectrum.

```

<SF escan: escan data: TBP>+≡
  procedure :: get_n_par => escan_data_get_n_par

<SF escan: procedures>+≡
  function escan_data_get_n_par (data) result (n)
    class(escan_data_t), intent(in) :: data
    integer :: n
    n = 1
  end function escan_data_get_n_par

```

Return the outgoing particles PDG codes. This is always the same as the incoming particle, where we use two indices for the two beams.

```

<SF escan: escan data: TBP>+≡
  procedure :: get_pdg_out => escan_data_get_pdg_out

<SF escan: procedures>+≡
  subroutine escan_data_get_pdg_out (data, pdg_out)
    class(escan_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    integer :: i, n
    n = 2
    do i = 1, n
      pdg_out(i) = data%flv_in(1:data%n_flv(i),i)%get_pdg ()
    end do
  end subroutine escan_data_get_pdg_out

```

Allocate the interaction record.

```

<SF escan: escan data: TBP>+≡
  procedure :: allocate_sf_int => escan_data_allocate_sf_int

<SF escan: procedures>+≡
  subroutine escan_data_allocate_sf_int (data, sf_int)
    class(escan_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (escan_t :: sf_int)

```

```
end subroutine escan_data_allocate_sf_int
```

16.9.2 The Energy-scan object

This is a spectrum, not a radiation. We create an interaction with two incoming and two outgoing particles, flavor, color, and helicity being carried through. x nevertheless is only one-dimensional, as we are always using only one beam parameter.

```
<SF escan: types>+≡
  type, extends (sf_int_t) :: escan_t
    type(escan_data_t), pointer :: data => null ()
    contains
    <SF escan: escan: TBP>
  end type escan_t
```

Type string: for the energy scan this is just a dummy function.

```
<SF escan: escan: TBP>≡
  procedure :: type_string => escan_type_string

<SF escan: procedures>+≡
  function escan_type_string (object) result (string)
    class(escan_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "Escan: energy scan"
    else
      string = "Escan: [undefined]"
    end if
  end function escan_type_string
```

Output. Call the interaction routine after displaying the configuration.

```
<SF escan: escan: TBP>+≡
  procedure :: write => escan_write

<SF escan: procedures>+≡
  subroutine escan_write (object, unit, testflag)
    class(escan_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "Energy scan data: [undefined]"
    end if
  end subroutine escan_write

<SF escan: escan: TBP>+≡
  procedure :: init => escan_init
```

(SF escan: procedures) +=

```

subroutine escan_init (sf_int, data)
  class(escan_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
  type(quantum_numbers_mask_t), dimension(4) :: mask
  integer, dimension(4) :: hel_lock
  real(default), dimension(2) :: m2
  real(default), dimension(0) :: mr2
  type(quantum_numbers_t), dimension(4) :: qn_fc, qn_hel, qn
  type(polarization_t), target :: pol1, pol2
  type(polarization_iterator_t) :: it_hel1, it_hel2
  integer :: j1, j2
  select type (data)
  type is (escan_data_t)
    hel_lock = [3, 4, 1, 2]
    m2 = data%flv_in(1,:)%get_mass ()
    call sf_int%base_init (mask, m2, mr2, m2, hel_lock = hel_lock)
    sf_int%data => data
    do j1 = 1, data%n_flv(1)
      call qn_fc(1)%init ( &
        flv = data%flv_in(j1,1), &
        col = color_from_flavor (data%flv_in(j1,1)))
      call qn_fc(3)%init ( &
        flv = data%flv_in(j1,1), &
        col = color_from_flavor (data%flv_in(j1,1)))
      call pol1%init_generic (data%flv_in(j1,1))
    do j2 = 1, data%n_flv(2)
      call qn_fc(2)%init ( &
        flv = data%flv_in(j2,2), &
        col = color_from_flavor (data%flv_in(j2,2)))
      call qn_fc(4)%init ( &
        flv = data%flv_in(j2,2), &
        col = color_from_flavor (data%flv_in(j2,2)))
      call pol2%init_generic (data%flv_in(j2,2))
      call it_hel1%init (pol1)
      do while (it_hel1%is_valid ())
        qn_hel(1) = it_hel1%get_quantum_numbers ()
        qn_hel(3) = it_hel1%get_quantum_numbers ()
        call it_hel2%init (pol2)
        do while (it_hel2%is_valid ())
          qn_hel(2) = it_hel2%get_quantum_numbers ()
          qn_hel(4) = it_hel2%get_quantum_numbers ()
          qn = qn_hel .merge. qn_fc
          call sf_int%add_state (qn)
          call it_hel2%advance ()
        end do
        call it_hel1%advance ()
      end do
      ! call pol2%final ()
    end do
    ! call pol1%final ()
  end do
  call sf_int%set_incoming ([1,2])
  call sf_int%set_outgoing ([3,4])

```

```

        call sf_int%freeze ()
        sf_int%status = SF_INITIAL
    end select
end subroutine escan_init

```

16.9.3 Kinematics

Set kinematics. We have a single parameter, but reduce both beams. The map flag is ignored.

```

<SF escan: escan: TBP>+=
    procedure :: complete_kinematics => escan_complete_kinematics
<SF escan: procedures>+=
    subroutine escan_complete_kinematics (sf_int, x, xb, f, r, rb, map)
        class(escan_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(out) :: f
        real(default) :: sqrt_x
        real(default), dimension(:), intent(in) :: r
        real(default), dimension(:), intent(in) :: rb
        logical, intent(in) :: map
        x = r
        xb= rb
        sqrt_x = sqrt (x(1))
        if (sqrt_x > 0) then
            f = 1 / (2 * sqrt_x)
        else
            f = 0
            sf_int%status = SF_FAILED_KINEMATICS
            return
        end if
        call sf_int%reduce_momenta ([sqrt_x, sqrt_x])
    end subroutine escan_complete_kinematics

```

Recover x . The base procedure should return two momentum fractions for the two beams, while we have only one parameter. This is the product of the extracted momentum fractions.

```

<SF escan: escan: TBP>+=
    procedure :: recover_x => escan_recover_x
<SF escan: procedures>+=
    subroutine escan_recover_x (sf_int, x, xb, x_free)
        class(escan_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: x
        real(default), dimension(:), intent(out) :: xb
        real(default), intent(inout), optional :: x_free
        real(default), dimension(2) :: xi, xib
        call sf_int%base_recover_x (xi, xib, x_free)
        x = product (xi)
        xb= 1 - x
    end subroutine escan_recover_x

```

Compute inverse kinematics.

```

<SF escan: escan: TBP>+=
  procedure :: inverse_kinematics => escan_inverse_kinematics
<SF escan: procedures>+=
  subroutine escan_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(escan_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    real(default) :: sqrt_x
    logical :: set_mom

    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    sqrt_x = sqrt (x(1))
    if (sqrt_x > 0) then
      f = 1 / (2 * sqrt_x)
    else
      f = 0
      sf_int%status = SF_FAILED_KINEMATICS
      return
    end if
    r = x
    rb = xb
    if (set_mom) then
      call sf_int%reduce_momenta ([sqrt_x, sqrt_x])
    end if
  end subroutine escan_inverse_kinematics

```

16.9.4 Energy scan application

Here, we insert the predefined norm.

```

<SF escan: escan: TBP>+=
  procedure :: apply => escan_apply
<SF escan: procedures>+=
  subroutine escan_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(escan_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: f
    associate (data => sf_int%data)
      f = data%norm
    end associate
    call sf_int%set_matrix_element (cmplx (f, kind=default))
    sf_int%status = SF_EVALUATED
  end subroutine escan_apply

```

16.9.5 Unit tests

Test module, followed by the corresponding implementation module.

<sf_escan.ut.f90>≡
<File header>

```
module sf_escan_ut
  use unit_tests
  use sf_escan_uti
```

<Standard module head>

<SF escan: public test>

contains

<SF escan: test driver>

```
end module sf_escan_ut
```

<sf_escan.uti.f90>≡
<File header>

```
module sf_escan_uti
```

<Use kinds>

```
  use physics_defs, only: ELECTRON
  use lorentz
  use pdg_arrays
  use flavors
  use interactions, only: reset_interaction_counter
  use model_data
  use sf_aux
  use sf_base
```

```
  use sf_escan
```

<Standard module head>

<SF escan: test declarations>

contains

<SF escan: tests>

```
end module sf_escan_uti
```

API: driver for the unit tests below.

<SF escan: public test>≡

```
  public :: sf_escan_test
```

<SF escan: test driver>≡

```
  subroutine sf_escan_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
<SF escan: execute tests>
```



```
end subroutine sf_escan_test
```

Test structure function data

Construct and display a test structure function data object.

```
<SF escan: execute tests>≡
  call test (sf_escan_1, "sf_escan_1", &
    "structure function configuration", &
    u, results)

<SF escan: test declarations>≡
  public :: sf_escan_1

<SF escan: tests>≡
  subroutine sf_escan_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(pdg_array_t), dimension(2) :: pdg_in
    type(pdg_array_t), dimension(2) :: pdg_out
    integer, dimension(:), allocatable :: pdg1, pdg2
    class(sf_data_t), allocatable :: data

    write (u, "(A)")  "* Test output: sf_escan_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &energy-scan structure function data"
    write (u, "(A)")

    call model%init_qed_test ()
    pdg_in(1) = ELECTRON
    pdg_in(2) = -ELECTRON

    allocate (escan_data_t :: data)
    select type (data)
    type is (escan_data_t)
      call data%init (model, pdg_in, norm = 2._default)
    end select

    call data%write (u)

    write (u, "(A)")

    write (u, "(1x,A)") "Outgoing particle codes:"
    call data%get_pdg_out (pdg_out)
    pdg1 = pdg_out(1)
    pdg2 = pdg_out(2)
    write (u, "(2x,99(1x,I0))")  pdg1, pdg2

    call model%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: sf_escan_1"

  end subroutine sf_escan_1
```

g@

Probe the structure-function object

Active the beam event reader, generate an event.

```
(SF escan: execute tests)+≡
  call test (sf_escan_2, "sf_escan_2", &
    "generate event", &
    u, results)

(SF escan: test declarations)+≡
  public :: sf_escan_2

(SF escan: tests)+≡
  subroutine sf_escan_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: x_free, f

    write (u, "(A)")  "* Test output: sf_escan_2"
    write (u, "(A)")  "* Purpose: initialize and display &
      &beam-events structure function data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv(1)%init (ELECTRON, model)
    call flv(2)%init (-ELECTRON, model)
    pdg_in(1) = ELECTRON
    pdg_in(2) = -ELECTRON

    call reset_interaction_counter ()

    allocate (escan_data_t :: data)
    select type (data)
    type is (escan_data_t)
      call data%init (model, pdg_in)
    end select

    write (u, "(A)")  "* Initialize structure-function object"
    write (u, "(A)")

    call data%allocate_sf_int (sf_int)
    call sf_int%init (data)
    call sf_int%set_beam_index ([1,2])

    write (u, "(A)")  "* Initialize incoming momentum with E=500"
    write (u, "(A)")
    E = 250
```

```

k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E,-sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Set dummy parameters and generate x"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.8
rb = 1 - r
x_free = 1

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f
write (u, "(A,9(1x,F10.7))") "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call sf_int%recover_x (x, xb, x_free)
call sf_int%inverse_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f
write (u, "(A,9(1x,F10.7))") "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "** Test output end: sf_escan_2"

end subroutine sf_escan_2

```

16.10 Gaussian beam spread

Instead of an analytic beam description, beam data may be provided in form of an event file. In its most simple form, the event file contains pairs of x values, relative to nominal beam energies. More advanced formats may include polarization, etc. The current implementation carries beam polarization through, if specified.

The code is very similar to the energy scan described above.

However, we must include a file-handle manager for the beam-event files. Two different processes may access a given beam-event file at the same time (i.e., serially but alternating). Accessing an open file from two different units is non-standard and not supported by all compilers. Therefore, we keep a global registry of open files, associated units, and reference counts. The `gaussian_t` objects act as proxies to this registry.

```

⟨sf_gaussian.f90⟩≡
  ⟨File header⟩

  module sf_gaussian

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use io_units
    use format_defs, only: FMT_12
    use file_registries
    use diagnostics
    use lorentz
    use rng_base
    use pdg_arrays
    use model_data
    use flavors
    use quantum_numbers
    use state_matrices
    use polarizations
    use sf_base

    ⟨Standard module head⟩

    ⟨SF gaussian: public⟩

    ⟨SF gaussian: types⟩

    contains

    ⟨SF gaussian: procedures⟩

```

```
end module sf_gaussian
```

16.10.1 The beam-data file registry

We manage data files via the `file_registries` module. To this end, we keep the registry as a private module variable here.

```
<CCC SF gaussian: variables>≡
  type(file_registry_t), save :: beam_file_registry
```

16.10.2 Data type

We store the spread for each beam, as a relative number related to the beam energy. For the actual generation, we include an (abstract) random-number generator factory.

```
<SF gaussian: public>≡
  public :: gaussian_data_t

<SF gaussian: types>≡
  type, extends(sf_data_t) :: gaussian_data_t
    private
      type(flavor_t), dimension(2) :: flv_in
      real(default), dimension(2) :: spread
      class(rng_factory_t), allocatable :: rng_factory
    contains
      <SF gaussian: gaussian data: TBP>
    end type gaussian_data_t

<SF gaussian: gaussian data: TBP>≡
  procedure :: init => gaussian_data_init

<SF gaussian: procedures>≡
  subroutine gaussian_data_init (data, model, pdg_in, spread, rng_factory)
    class(gaussian_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), dimension(2), intent(in) :: pdg_in
    real(default), dimension(2), intent(in) :: spread
    class(rng_factory_t), intent(inout), allocatable :: rng_factory
    if (any (spread < 0)) then
      call msg_fatal ("Gaussian beam spread: must not be negative")
    end if
    call data%flv_in(1)%init (pdg_array_get (pdg_in(1), 1), model)
    call data%flv_in(2)%init (pdg_array_get (pdg_in(2), 1), model)
    data%spread = spread
    call move_alloc (from = rng_factory, to = data%rng_factory)
  end subroutine gaussian_data_init
```

Return true since this spectrum is always in generator mode.

```
<SF gaussian: gaussian data: TBP>+≡
  procedure :: is_generator => gaussian_data_is_generator
```

```

<SF gaussian: procedures>+≡
function gaussian_data_is_generator (data) result (flag)
  class(gaussian_data_t), intent(in) :: data
  logical :: flag
  flag = .true.
end function gaussian_data_is_generator

```

The number of parameters is two. They are free parameters.

```

<SF gaussian: gaussian data: TBP>+≡
procedure :: get_n_par => gaussian_data_get_n_par

```

```

<SF gaussian: procedures>+≡
function gaussian_data_get_n_par (data) result (n)
  class(gaussian_data_t), intent(in) :: data
  integer :: n
  n = 2
end function gaussian_data_get_n_par

```

```

<SF gaussian: gaussian data: TBP>+≡
procedure :: get_pdg_out => gaussian_data_get_pdg_out

```

```

<SF gaussian: procedures>+≡
subroutine gaussian_data_get_pdg_out (data, pdg_out)
  class(gaussian_data_t), intent(in) :: data
  type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
  integer :: i, n
  n = 2
  do i = 1, n
    pdg_out(i) = data%flv_in(i)%get_pdg ()
  end do
end subroutine gaussian_data_get_pdg_out

```

Allocate the interaction record.

```

<SF gaussian: gaussian data: TBP>+≡
procedure :: allocate_sf_int => gaussian_data_allocate_sf_int

```

```

<SF gaussian: procedures>+≡
subroutine gaussian_data_allocate_sf_int (data, sf_int)
  class(gaussian_data_t), intent(in) :: data
  class(sf_int_t), intent(inout), allocatable :: sf_int
  allocate (gaussian_t :: sf_int)
end subroutine gaussian_data_allocate_sf_int

```

Output

```

<SF gaussian: gaussian data: TBP>+≡
procedure :: write => gaussian_data_write

```

```

<SF gaussian: procedures>+≡
subroutine gaussian_data_write (data, unit, verbose)
  class(gaussian_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  integer :: u
  u = given_output_unit (unit); if (u < 0) return

```

```

write (u, "(1x,A)") "Gaussian beam spread data:"
write (u, "(3x,A,A,A,A)") "prt_in = ", &
    char (data%flv_in(1)%get_name ()), &
    ", ", char (data%flv_in(2)%get_name ())
write (u, "(3x,A,2(1x," // FMT_12 // ")") "spread =", data%spread
call data%rng_factory%write (u)
end subroutine gaussian_data_write

```

16.10.3 The gaussian object

Flavor and polarization carried through, no radiated particles. The generator needs a random-number generator, obviously.

```

<SF gaussian: public>+≡
    public :: gaussian_t

<SF gaussian: types>+≡
    type, extends (sf_int_t) :: gaussian_t
        type(gaussian_data_t), pointer :: data => null ()
        class(rng_t), allocatable :: rng
    contains
        <SF gaussian: gaussian: TBP>
    end type gaussian_t

```

Type string: show gaussian file.

```

<SF gaussian: gaussian: TBP>≡
    procedure :: type_string => gaussian_type_string

<SF gaussian: procedures>+≡
    function gaussian_type_string (object) result (string)
        class(gaussian_t), intent(in) :: object
        type(string_t) :: string
        if (associated (object%data)) then
            string = "Gaussian: gaussian beam-energy spread"
        else
            string = "Gaussian: [undefined]"
        end if
    end function gaussian_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: write => gaussian_write

<SF gaussian: procedures>+≡
    subroutine gaussian_write (object, unit, testflag)
        class(gaussian_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%data)) then
            call object%data%write (u)
            call object%rng%write (u)

```

```

        call object%base_write (u, testflag)
    else
        write (u, "(1x,A)") "gaussian data: [undefined]"
    end if
end subroutine gaussian_write

```

(SF gaussian: gaussian: TBP)+≡

```

procedure :: init => gaussian_init

```

(SF gaussian: procedures)+≡

```

subroutine gaussian_init (sf_int, data)
    class(gaussian_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    real(default), dimension(2) :: m2
    real(default), dimension(0) :: mr2
    type(quantum_numbers_mask_t), dimension(4) :: mask
    integer, dimension(4) :: hel_lock
    type(quantum_numbers_t), dimension(4) :: qn_fc, qn_hel, qn
    type(polarization_t), target :: pol1, pol2
    type(polarization_iterator_t) :: it_hel1, it_hel2
    integer :: i
    select type (data)
    type is (gaussian_data_t)
        m2 = data%flv_in%get_mass () ** 2
        hel_lock = [3, 4, 1, 2]
        mask = quantum_numbers_mask (.false., .false., .false.)
        call sf_int%base_init (mask, m2, mr2, m2, hel_lock = hel_lock)
        sf_int%data => data
        do i = 1, 2
            call qn_fc(i)%init ( &
                flv = data%flv_in(i), &
                col = color_from_flavor (data%flv_in(i)))
            call qn_fc(i+2)%init ( &
                flv = data%flv_in(i), &
                col = color_from_flavor (data%flv_in(i)))
        end do
        call pol1%init_generic (data%flv_in(1))
        call it_hel1%init (pol1)
        do while (it_hel1%is_valid ())
            qn_hel(1) = it_hel1%get_quantum_numbers ()
            qn_hel(3) = it_hel1%get_quantum_numbers ()
            call pol2%init_generic (data%flv_in(2))
            call it_hel2%init (pol2)
            do while (it_hel2%is_valid ())
                qn_hel(2) = it_hel2%get_quantum_numbers ()
                qn_hel(4) = it_hel2%get_quantum_numbers ()
                qn = qn_hel .merge. qn_fc
                call sf_int%add_state (qn)
                call it_hel2%advance ()
            end do
            ! call pol2%final ()
            call it_hel1%advance ()
        end do
        ! call pol1%final ()
    end select
end subroutine gaussian_init

```



```

        call sf_int%freeze ()
        call sf_int%set_incoming ([1,2])
        call sf_int%set_outgoing ([3,4])
        sf_int%status = SF_INITIAL
    end select
    call sf_int%data%rng_factory%make (sf_int%rng)
end subroutine gaussian_init

```

This spectrum type needs a finalizer, which closes the data file.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: final => sf_gaussian_final

<SF gaussian: procedures>+≡
    subroutine sf_gaussian_final (object)
        class(gaussian_t), intent(inout) :: object
        call object%interaction_t%final ()
    end subroutine sf_gaussian_final

```

16.10.4 Kinematics

Refer to the data component.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: is_generator => gaussian_is_generator

<SF gaussian: procedures>+≡
    function gaussian_is_generator (sf_int) result (flag)
        class(gaussian_t), intent(in) :: sf_int
        logical :: flag
        flag = sf_int%data%is_generator ()
    end function gaussian_is_generator

```

Generate free parameters. The x value should be distributed with mean 1 and σ given by the spread. We reject negative x values. (This cut slightly biases the distribution, but for reasonable (small) spreads negative r should not occur.

```

<SF gaussian: gaussian: TBP>+≡
    procedure :: generate_free => gaussian_generate_free

<SF gaussian: procedures>+≡
    subroutine gaussian_generate_free (sf_int, r, rb, x_free)
        class(gaussian_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
        real(default), dimension(size(r)) :: z
        associate (data => sf_int%data)
            do
                call sf_int%rng%generate_gaussian (z)
                rb = z * data%spread
                r = 1 - rb
                x_free = x_free * product (r)
                if (all (r > 0)) exit
            end do
        end associate
    end subroutine gaussian_generate_free

```

```
end subroutine gaussian_generate_free
```

Set kinematics. Trivial transfer since this is a pure generator. The map flag doesn't apply.

```
<SF gaussian: gaussian: TBP>+≡
```

```
procedure :: complete_kinematics => gaussian_complete_kinematics
```

```
<SF gaussian: procedures>+≡
```

```
subroutine gaussian_complete_kinematics (sf_int, x, xb, f, r, rb, map)
  class(gaussian_t), intent(inout) :: sf_int
  real(default), dimension(:), intent(out) :: x
  real(default), dimension(:), intent(out) :: xb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(in) :: r
  real(default), dimension(:), intent(in) :: rb
  logical, intent(in) :: map
  if (map) then
    call msg_fatal ("gaussian: map flag not supported")
  else
    x = r
    xb= rb
    f = 1
  end if
  call sf_int%reduce_momenta (x)
end subroutine gaussian_complete_kinematics
```

Compute inverse kinematics. Trivial in this case.

```
<SF gaussian: gaussian: TBP>+≡
```

```
procedure :: inverse_kinematics => gaussian_inverse_kinematics
```

```
<SF gaussian: procedures>+≡
```

```
subroutine gaussian_inverse_kinematics &
  (sf_int, x, xb, f, r, rb, map, set_momenta)
  class(gaussian_t), intent(inout) :: sf_int
  real(default), dimension(:), intent(in) :: x
  real(default), dimension(:), intent(in) :: xb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: r
  real(default), dimension(:), intent(out) :: rb
  logical, intent(in) :: map
  logical, intent(in), optional :: set_momenta
  logical :: set_mom
  set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
  if (map) then
    call msg_fatal ("gaussian: map flag not supported")
  else
    r = x
    rb= xb
    f = 1
  end if
  if (set_mom) then
    call sf_int%reduce_momenta (x)
  end if
end subroutine gaussian_inverse_kinematics
```

16.10.5 gaussian application

Trivial, just set the unit weight.

```
<SF gaussian: gaussian: TBP>+≡
  procedure :: apply => gaussian_apply

<SF gaussian: procedures>+≡
  subroutine gaussian_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(gaussian_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: f
    f = 1
    call sf_int%set_matrix_element (cmplx (f, kind=default))
    sf_int%status = SF_EVALUATED
  end subroutine gaussian_apply
```

16.10.6 Unit tests

Test module, followed by the corresponding implementation module.

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

  module sf_gaussian_ut
    use unit_tests
    use sf_gaussian_uti

    <Standard module head>

    <SF gaussian: public test>

    contains

    <SF gaussian: test driver>

  end module sf_gaussian_ut

<sf_gaussian_uti.f90>≡
  <File header>

  module sf_gaussian_uti

    <Use kinds>
    use physics_defs, only: ELECTRON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
```

```

    use model_data
    use rng_base
    use sf_aux
    use sf_base

    use sf_gaussian

    use rng_base_ut, only: rng_test_factory_t

    <Standard module head>

    <SF gaussian: test declarations>

contains

    <SF gaussian: tests>

end module sf_gaussian_ut
API: driver for the unit tests below.
<SF gaussian: public test>≡
    public :: sf_gaussian_test
<SF gaussian: test driver>≡
    subroutine sf_gaussian_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <SF gaussian: execute tests>
    end subroutine sf_gaussian_test

```

Test structure function data

Construct and display a test structure function data object.

```

<SF gaussian: execute tests>≡
    call test (sf_gaussian_1, "sf_gaussian_1", &
        "structure function configuration", &
        u, results)
<SF gaussian: test declarations>≡
    public :: sf_gaussian_1
<SF gaussian: tests>≡
    subroutine sf_gaussian_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(pdg_array_t), dimension(2) :: pdg_in
        type(pdg_array_t), dimension(2) :: pdg_out
        integer, dimension(:), allocatable :: pdg1, pdg2
        class(sf_data_t), allocatable :: data
        class(rng_factory_t), allocatable :: rng_factory

        write (u, "(A)")  "* Test output: sf_gaussian_1"
        write (u, "(A)")  "* Purpose: initialize and display &
            &gaussian-spread structure function data"
        write (u, "(A)")
    end subroutine sf_gaussian_1

```

```

call model%init_qed_test ()
pdg_in(1) = ELECTRON
pdg_in(2) = -ELECTRON

allocate (gaussian_data_t :: data)
allocate (rng_test_factory_t :: rng_factory)
select type (data)
type is (gaussian_data_t)
    call data%init (model, pdg_in, [1e-2_default, 2e-2_default], rng_factory)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
pdg2 = pdg_out(2)
write (u, "(2x,99(1x,I0))") pdg1, pdg2

call model%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_gaussian_1"

end subroutine sf_gaussian_1

```

Probe the structure-function object

Active the beam event reader, generate an event.

```

<SF gaussian: execute tests>+≡
    call test (sf_gaussian_2, "sf_gaussian_2", &
        "generate event", &
        u, results)

<SF gaussian: test declarations>+≡
    public :: sf_gaussian_2

<SF gaussian: tests>+≡
    subroutine sf_gaussian_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t), dimension(2) :: flv
        type(pdg_array_t), dimension(2) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(rng_factory_t), allocatable :: rng_factory
        class(sf_int_t), allocatable :: sf_int
        type(vector4_t) :: k1, k2
        real(default) :: E
        real(default), dimension(:), allocatable :: r, rb, x, xb
        real(default) :: x_free, f
        integer :: i

```

```

write (u, "(A)")  "* Test output: sf_gaussian_2"
write (u, "(A)")  "* Purpose: initialize and display &
                    &gaussian-spread structure function data"
write (u, "(A)")

call model%init_qed_test ()
call flv(1)%init (ELECTRON, model)
call flv(2)%init (-ELECTRON, model)
pdg_in(1) = ELECTRON
pdg_in(2) = -ELECTRON

call reset_interaction_counter ()

allocate (gaussian_data_t :: data)
allocate (rng_test_factory_t :: rng_factory)
select type (data)
type is (gaussian_data_t)
    call data%init (model, pdg_in, [1e-2_default, 2e-2_default], rng_factory)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Set dummy parameters and generate x."
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call pacify (rb, 1.e-8_default)
call pacify (xb, 1.e-8_default)

```

```

write (u, "(A,9(1x,F10.7))") "r =", r
write (u, "(A,9(1x,F10.7))") "rb=", rb
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f
write (u, "(A,9(1x,F10.7))") "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate more events"
write (u, "(A)")

select type (sf_int)
type is (gaussian_t)
  do i = 1, 3
    call sf_int%generate_free (r, rb, x_free)
    write (u, "(A,9(1x,F10.7))") "r =", r
  end do
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_gaussian_2"

end subroutine sf_gaussian_2

```

16.11 Using beam event data

Instead of an analytic beam description, beam data may be provided in form of an event file. In its most simple form, the event file contains pairs of x values, relative to nominal beam energies. More advanced formats may include polarization, etc. The current implementation carries beam polarization through, if specified.

The code is very similar to the energy scan described above.

However, we must include a file-handle manager for the beam-event files. Two different processes may access a given beam-event file at the same time (i.e., serially but alternating). Accessing an open file from two different units is non-standard and not supported by all compilers. Therefore, we keep a global registry of open files, associated units, and reference counts. The `beam_events_t` objects act as proxies to this registry.

```
(sf_beam_events.f90)≡
  <File header>

  module sf_beam_events

    <Use kinds>
    <Use strings>
    use io_units
    use file_registries
    use diagnostics
    use lorentz
    use pdg_arrays
    use model_data
    use flavors
    use quantum_numbers
    use state_matrices
    use polarizations
    use sf_base

    <Standard module head>

    <SF beam events: public>

    <SF beam events: types>

    <SF beam events: variables>

    contains

    <SF beam events: procedures>

  end module sf_beam_events
```

16.11.1 The beam-data file registry

We manage data files via the `file_registries` module. To this end, we keep the registry as a private module variable here.

This is public only for the unit tests.

```

<SF beam events: public>≡
    public :: beam_file_registry

<SF beam events: variables>≡
    type(file_registry_t), save :: beam_file_registry

```

16.11.2 Data type

```

<SF beam events: public>+≡
    public :: beam_events_data_t

<SF beam events: types>≡
    type, extends(sf_data_t) :: beam_events_data_t
        private
            type(flavor_t), dimension(2) :: flv_in
            type(string_t) :: dir
            type(string_t) :: file
            type(string_t) :: fqn
            integer :: unit = 0
            logical :: warn_eof = .true.
        contains
            <SF beam events: beam events data: TBP>
        end type beam_events_data_t

<SF beam events: beam events data: TBP>≡
    procedure :: init => beam_events_data_init

<SF beam events: procedures>≡
    subroutine beam_events_data_init (data, model, pdg_in, dir, file, warn_eof)
        class(beam_events_data_t), intent(out) :: data
        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), dimension(2), intent(in) :: pdg_in
        type(string_t), intent(in) :: dir
        type(string_t), intent(in) :: file
        logical, intent(in), optional :: warn_eof
        if (any (pdg_array_get_length (pdg_in) /= 1)) then
            call msg_fatal ("Beam events: incoming beam particles must be unique")
        end if
        call data%flv_in(1)%init (pdg_array_get (pdg_in(1), 1), model)
        call data%flv_in(2)%init (pdg_array_get (pdg_in(2), 1), model)
        data%dir = dir
        data%file = file
        if (present (warn_eof)) data%warn_eof = warn_eof
    end subroutine beam_events_data_init

```

Return true since this spectrum is always in generator mode.

```

<SF beam events: beam events data: TBP>+≡
    procedure :: is_generator => beam_events_data_is_generator

```

```

<SF beam events: procedures>+≡
  function beam_events_data_is_generator (data) result (flag)
    class(beam_events_data_t), intent(in) :: data
    logical :: flag
    flag = .true.
  end function beam_events_data_is_generator

```

The number of parameters is two. They are free parameters.

```

<SF beam events: beam events data: TBP>+≡
  procedure :: get_n_par => beam_events_data_get_n_par

```

```

<SF beam events: procedures>+≡
  function beam_events_data_get_n_par (data) result (n)
    class(beam_events_data_t), intent(in) :: data
    integer :: n
    n = 2
  end function beam_events_data_get_n_par

```

```

<SF beam events: beam events data: TBP>+≡
  procedure :: get_pdg_out => beam_events_data_get_pdg_out

```

```

<SF beam events: procedures>+≡
  subroutine beam_events_data_get_pdg_out (data, pdg_out)
    class(beam_events_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    integer :: i, n
    n = 2
    do i = 1, n
      pdg_out(i) = data%flv_in(i)%get_pdg ()
    end do
  end subroutine beam_events_data_get_pdg_out

```

Allocate the interaction record.

```

<SF beam events: beam events data: TBP>+≡
  procedure :: allocate_sf_int => beam_events_data_allocate_sf_int

```

```

<SF beam events: procedures>+≡
  subroutine beam_events_data_allocate_sf_int (data, sf_int)
    class(beam_events_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (beam_events_t :: sf_int)
  end subroutine beam_events_data_allocate_sf_int

```

Output

```

<SF beam events: beam events data: TBP>+≡
  procedure :: write => beam_events_data_write

```

```

<SF beam events: procedures>+≡
  subroutine beam_events_data_write (data, unit, verbose)
    class(beam_events_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit); if (u < 0) return

```

```

write (u, "(1x,A)") "Beam-event file data:"
write (u, "(3x,A,A,A,A)") "prt_in = ", &
    char (data%flv_in(1)%get_name ()), &
    ", ", char (data%flv_in(2)%get_name ())
write (u, "(3x,A,A,A)") "file   = '", char (data%file), "'"
write (u, "(3x,A,I0)")  "unit   = ", data%unit
write (u, "(3x,A,L1)")  "warn   = ", data%warn_eof
end subroutine beam_events_data_write

```

The data file needs to be opened and closed explicitly. The open/close message is communicated to the file handle registry, which does the actual work.

We determine first whether to look in the local directory or in the given system directory.

```

<SF beam events: beam events data: TBP>+≡
  procedure :: open => beam_events_data_open
  procedure :: close => beam_events_data_close

<SF beam events: procedures>+≡
  subroutine beam_events_data_open (data)
    class(beam_events_data_t), intent(inout) :: data
    logical :: exist
    if (data%unit == 0) then
      data%fqn = data%file
      if (data%fqn == "") &
        call msg_fatal ("Beam events: $beam_events_file is not set")
      inquire (file = char (data%fqn), exist = exist)
      if (.not. exist) then
        data%fqn = data%dir // "/" // data%file
        inquire (file = char (data%fqn), exist = exist)
        if (.not. exist) then
          data%fqn = ""
          call msg_fatal ("Beam events: file '" &
            // char (data%file) // "' not found")
          return
        end if
      end if
      call msg_message ("Beam events: reading from file '" &
        // char (data%file) // "'")
      call beam_file_registry%open (data%fqn, data%unit)
    else
      call msg_bug ("Beam events: file '" &
        // char (data%file) // "' is already open")
    end if
  end subroutine beam_events_data_open

  subroutine beam_events_data_close (data)
    class(beam_events_data_t), intent(inout) :: data
    if (data%unit /= 0) then
      call beam_file_registry%close (data%fqn)
      call msg_message ("Beam events: closed file '" &
        // char (data%file) // "'")
      data%unit = 0
    end if
  end subroutine beam_events_data_close

```

Return the beam event file.

```

<SF beam events: beam events data: TBP>+≡
  procedure :: get_beam_file => beam_events_data_get_beam_file

<SF beam events: procedures>+≡
  function beam_events_data_get_beam_file (data) result (file)
    class(beam_events_data_t), intent(in) :: data
    type(string_t) :: file
    file = "Beam events: " // data%file
  end function beam_events_data_get_beam_file

```

16.11.3 The beam events object

Flavor and polarization carried through, no radiated particles.

```

<SF beam events: public>+≡
  public :: beam_events_t

<SF beam events: types>+≡
  type, extends (sf_int_t) :: beam_events_t
    type(beam_events_data_t), pointer :: data => null ()
    integer :: count = 0
  contains
    <SF beam events: beam events: TBP>
  end type beam_events_t

```

Type string: show beam events file.

```

<SF beam events: beam events: TBP>≡
  procedure :: type_string => beam_events_type_string

<SF beam events: procedures>+≡
  function beam_events_type_string (object) result (string)
    class(beam_events_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "Beam events: " // object%data%file
    else
      string = "Beam events: [undefined]"
    end if
  end function beam_events_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF beam events: beam events: TBP>+≡
  procedure :: write => beam_events_write

<SF beam events: procedures>+≡
  subroutine beam_events_write (object, unit, testflag)
    class(beam_events_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)

```

```

    if (associated (object%data)) then
        call object%data%write (u)
        call object%base_write (u, testflag)
    else
        write (u, "(ix,A)") "Beam events data: [undefined]"
    end if
end subroutine beam_events_write

```

<SF beam events: beam events: TBP>+≡

```

    procedure :: init => beam_events_init

```

<SF beam events: procedures>+≡

```

subroutine beam_events_init (sf_int, data)
    class(beam_events_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    real(default), dimension(2) :: m2
    real(default), dimension(0) :: mr2
    type(quantum_numbers_mask_t), dimension(4) :: mask
    integer, dimension(4) :: hel_lock
    type(quantum_numbers_t), dimension(4) :: qn_fc, qn_hel, qn
    type(polarization_t), target :: pol1, pol2
    type(polarization_iterator_t) :: it_hel1, it_hel2
    integer :: i
    select type (data)
    type is (beam_events_data_t)
        m2 = data%flv_in%get_mass () ** 2
        hel_lock = [3, 4, 1, 2]
        mask = quantum_numbers_mask (.false., .false., .false.)
        call sf_int%base_init (mask, m2, mr2, m2, hel_lock = hel_lock)
        sf_int%data => data
        do i = 1, 2
            call qn_fc(i)%init ( &
                flv = data%flv_in(i), &
                col = color_from_flavor (data%flv_in(i)))
            call qn_fc(i+2)%init ( &
                flv = data%flv_in(i), &
                col = color_from_flavor (data%flv_in(i)))
        end do
        call pol1%init_generic (data%flv_in(1))
        call it_hel1%init (pol1)
        do while (it_hel1%is_valid ())
            qn_hel(1) = it_hel1%get_quantum_numbers ()
            qn_hel(3) = it_hel1%get_quantum_numbers ()
            call pol2%init_generic (data%flv_in(2))
            call it_hel2%init (pol2)
            do while (it_hel2%is_valid ())
                qn_hel(2) = it_hel2%get_quantum_numbers ()
                qn_hel(4) = it_hel2%get_quantum_numbers ()
                qn = qn_hel .merge. qn_fc
                call sf_int%add_state (qn)
                call it_hel2%advance ()
            end do
            ! call pol2%final ()
            call it_hel1%advance ()
        end do
    end select
end subroutine beam_events_init

```

```

        end do
        ! call poll%final ()
        call sf_int%freeze ()
        call sf_int%set_incoming ([1,2])
        call sf_int%set_outgoing ([3,4])
        call sf_int%data%open ()
        sf_int%status = SF_INITIAL
    end select
end subroutine beam_events_init

```

This spectrum type needs a finalizer, which closes the data file.

```

<SF beam events: beam events: TBP>+≡
    procedure :: final => sf_beam_events_final

<SF beam events: procedures>+≡
    subroutine sf_beam_events_final (object)
        class(beam_events_t), intent(inout) :: object
        call object%data%close ()
        call object%interaction_t%final ()
    end subroutine sf_beam_events_final

```

16.11.4 Kinematics

Refer to the data component.

```

<SF beam events: beam events: TBP>+≡
    procedure :: is_generator => beam_events_is_generator

<SF beam events: procedures>+≡
    function beam_events_is_generator (sf_int) result (flag)
        class(beam_events_t), intent(in) :: sf_int
        logical :: flag
        flag = sf_int%data%is_generator ()
    end function beam_events_is_generator

```

Generate free parameters. We read them from file.

```

<SF beam events: beam events: TBP>+≡
    procedure :: generate_free => beam_events_generate_free

<SF beam events: procedures>+≡
    recursive subroutine beam_events_generate_free (sf_int, r, rb, x_free)
        class(beam_events_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free
        integer :: iostat
        associate (data => sf_int%data)
            if (data%unit /= 0) then
                read (data%unit, fmt=*, iostat=iostat) r
                if (iostat > 0) then
                    write (msg_buffer, "(A,I0,A)") &
                        "Beam events: I/O error after reading ", sf_int%count, &
                        " events"
                    call msg_fatal ()
                end if
            end if
        end associate
    end subroutine beam_events_generate_free

```

```

else if (iostat < 0) then
  if (sf_int%count == 0) then
    call msg_fatal ("Beam events: file is empty")
  else if (sf_int%data%warn_eof) then
    write (msg_buffer, "(A,I0,A)") &
      "Beam events: End of file after reading ", sf_int%count, &
      " events, rewinding"
    call msg_warning ()
  end if
  rewind (data%unit)
  sf_int%count = 0
  call sf_int%generate_free (r, rb, x_free)
else
  sf_int%count = sf_int%count + 1
  rb = 1 - r
  x_free = x_free * product (r)
end if
else
  call msg_bug ("Beam events: file is not open for reading")
end if
end associate
end subroutine beam_events_generate_free

```

Set kinematics. Trivial transfer since this is a pure generator. The map flag doesn't apply.

```

<SF beam events: beam events: TBP>+≡
  procedure :: complete_kinematics => beam_events_complete_kinematics

<SF beam events: procedures>+≡
  subroutine beam_events_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(beam_events_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    if (map) then
      call msg_fatal ("Beam events: map flag not supported")
    else
      x = r
      xb = rb
      f = 1
    end if
    call sf_int%reduce_momenta (x)
  end subroutine beam_events_complete_kinematics

```

Compute inverse kinematics. Trivial in this case.

```

<SF beam events: beam events: TBP>+≡
  procedure :: inverse_kinematics => beam_events_inverse_kinematics

<SF beam events: procedures>+≡
  subroutine beam_events_inverse_kinematics &
    (sf_int, x, xb, f, r, rb, map, set_momenta)

```

```

class(beam_events_t), intent(inout) :: sf_int
real(default), dimension(:), intent(in) :: x
real(default), dimension(:), intent(in) :: xb
real(default), intent(out) :: f
real(default), dimension(:), intent(out) :: r
real(default), dimension(:), intent(out) :: rb
logical, intent(in) :: map
logical, intent(in), optional :: set_momenta
logical :: set_mom
set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
if (map) then
    call msg_fatal ("Beam events: map flag not supported")
else
    r = x
    rb= xb
    f = 1
end if
if (set_mom) then
    call sf_int%reduce_momenta (x)
end if
end subroutine beam_events_inverse_kinematics

```

16.11.5 Beam events application

Trivial, just set the unit weight.

```

<SF beam events: beam events: TBP>+≡
    procedure :: apply => beam_events_apply

<SF beam events: procedures>+≡
    subroutine beam_events_apply (sf_int, scale, negative_sf, rescale, i_sub)
        class(beam_events_t), intent(inout) :: sf_int
        real(default), intent(in) :: scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(in), optional :: rescale
        integer, intent(in), optional :: i_sub
        real(default) :: f
        f = 1
        call sf_int%set_matrix_element (cmplx (f, kind=default))
        sf_int%status = SF_EVALUATED
    end subroutine beam_events_apply

```

16.11.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_beam_events_ut.f90>≡
    <File header>

    module sf_beam_events_ut
        use unit_tests
        use sf_beam_events_ut

```



```

    <Standard module head>

    <SF beam events: public test>

    contains

    <SF beam events: test driver>

    end module sf_beam_events_ut

    <sf_beam_events_uti.f90>≡
    <File header>

    module sf_beam_events_uti

    <Use kinds>
    <Use strings>
    use io_units
    use physics_defs, only: ELECTRON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use sf_aux
    use sf_base

    use sf_beam_events

    <Standard module head>

    <SF beam events: test declarations>

    contains

    <SF beam events: tests>

    end module sf_beam_events_uti
API: driver for the unit tests below.
    <SF beam events: public test>≡
        public :: sf_beam_events_test
    <SF beam events: test driver>≡
        subroutine sf_beam_events_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <SF beam events: execute tests>
        end subroutine sf_beam_events_test

```

Test structure function data

Construct and display a test structure function data object.

```

    <SF beam events: execute tests>≡

```

```

        call test (sf_beam_events_1, "sf_beam_events_1", &
            "structure function configuration", &
            u, results)
<SF beam events: test declarations>≡
    public :: sf_beam_events_1
<SF beam events: tests>≡
    subroutine sf_beam_events_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(pdg_array_t), dimension(2) :: pdg_in
        type(pdg_array_t), dimension(2) :: pdg_out
        integer, dimension(:), allocatable :: pdg1, pdg2
        class(sf_data_t), allocatable :: data

        write (u, "(A)")  "* Test output: sf_beam_events_1"
        write (u, "(A)")  "*   Purpose: initialize and display &
            &beam-events structure function data"
        write (u, "(A)")

        call model%init_qed_test ()
        pdg_in(1) = ELECTRON
        pdg_in(2) = -ELECTRON

        allocate (beam_events_data_t :: data)
        select type (data)
        type is (beam_events_data_t)
            call data%init (model, pdg_in, var_str (""), var_str ("beam_events.dat"))
        end select

        call data%write (u)

        write (u, "(A)")

        write (u, "(1x,A)") "Outgoing particle codes:"
        call data%get_pdg_out (pdg_out)
        pdg1 = pdg_out(1)
        pdg2 = pdg_out(2)
        write (u, "(2x,99(1x,I0))")  pdg1, pdg2

        call model%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: sf_beam_events_1"

    end subroutine sf_beam_events_1

```

Probe the structure-function object

Active the beam event reader, generate an event.

```

<SF beam events: execute tests>+≡
    call test (sf_beam_events_2, "sf_beam_events_2", &
        "generate event", &

```

```

        u, results)
<SF beam events: test declarations>+≡
    public :: sf_beam_events_2
<SF beam events: tests>+≡
    subroutine sf_beam_events_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t), dimension(2) :: flv
        type(pdg_array_t), dimension(2) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        class(sf_int_t), allocatable :: sf_int
        type(vector4_t) :: k1, k2
        real(default) :: E
        real(default), dimension(:), allocatable :: r, rb, x, xb
        real(default) :: x_free, f
        integer :: i

        write (u, "(A)")  "* Test output: sf_beam_events_2"
        write (u, "(A)")  "*   Purpose: initialize and display &
            &beam-events structure function data"
        write (u, "(A)")

        call model%init_qed_test ()
        call flv(1)%init (ELECTRON, model)
        call flv(2)%init (-ELECTRON, model)
        pdg_in(1) = ELECTRON
        pdg_in(2) = -ELECTRON

        call reset_interaction_counter ()

        allocate (beam_events_data_t :: data)
        select type (data)
        type is (beam_events_data_t)
            call data%init (model, pdg_in, &
                var_str (""), var_str ("test_beam_events.dat"))
        end select

        write (u, "(A)")  "* Initialize structure-function object"
        write (u, "(A)")

        call data%allocate_sf_int (sf_int)
        call sf_int%init (data)
        call sf_int%set_beam_index ([1,2])

        write (u, "(A)")  "* Initialize incoming momentum with E=500"
        write (u, "(A)")
        E = 250
        k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
        k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
        call vector4_write (k1, u)
        call vector4_write (k2, u)
        call sf_int%seed_kinematics ([k1, k2])

```

```

write (u, "(A)")
write (u, "(A)")  "* Set dummy parameters and generate x."
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "r =", r
write (u, "(A,9(1x,F10.7))")  "rb=", rb
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free
select type (sf_int)
type is (beam_events_t)
    write (u, "(A,1x,I0)")  "count =", sf_int%count
end select

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate more events, rewind"
write (u, "(A)")

select type (sf_int)
type is (beam_events_t)
    do i = 1, 3
        call sf_int%generate_free (r, rb, x_free)
        write (u, "(A,9(1x,F10.7))")  "r =", r
        write (u, "(A,1x,I0)")  "count =", sf_int%count
    end do
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_beam_events_2"

```

```
end subroutine sf_beam_events_2
```

Check the file handle registry

Open and close some files, checking the registry contents.

```
<SF beam events: execute tests>+≡
  call test (sf_beam_events_3, "sf_beam_events_3", &
    "check registry", &
    u, results)

<SF beam events: test declarations>+≡
  public :: sf_beam_events_3

<SF beam events: tests>+≡
  subroutine sf_beam_events_3 (u)
    integer, intent(in) :: u
    integer :: u1

    write (u, "(A)")  "* Test output: sf_beam_events_2"
    write (u, "(A)")  "* Purpose: check file handle registry"
    write (u, "(A)")

    write (u, "(A)")  "* Create some empty files"
    write (u, "(A)")

    u1 = free_unit ()
    open (u1, file = "sf_beam_events_f1.tmp", action="write", status="new")
    close (u1)
    open (u1, file = "sf_beam_events_f2.tmp", action="write", status="new")
    close (u1)
    open (u1, file = "sf_beam_events_f3.tmp", action="write", status="new")
    close (u1)

    write (u, "(A)")  "* Empty registry"
    write (u, "(A)")

    call beam_file_registry%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Insert three entries"
    write (u, "(A)")

    call beam_file_registry%open (var_str ("sf_beam_events_f3.tmp"))
    call beam_file_registry%open (var_str ("sf_beam_events_f2.tmp"))
    call beam_file_registry%open (var_str ("sf_beam_events_f1.tmp"))
    call beam_file_registry%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Open a second channel"
    write (u, "(A)")

    call beam_file_registry%open (var_str ("sf_beam_events_f2.tmp"))
    call beam_file_registry%write (u)
```

```

write (u, "(A)")
write (u, "(A)")  "* Close second entry twice"
write (u, "(A)")

call beam_file_registry%close (var_str ("sf_beam_events_f2.tmp"))
call beam_file_registry%close (var_str ("sf_beam_events_f2.tmp"))
call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Close last entry"
write (u, "(A)")

call beam_file_registry%close (var_str ("sf_beam_events_f3.tmp"))
call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Close remaining entry"
write (u, "(A)")

call beam_file_registry%close (var_str ("sf_beam_events_f1.tmp"))
call beam_file_registry%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

open (u1, file = "sf_beam_events_f1.tmp", action="write")
close (u1, status = "delete")
open (u1, file = "sf_beam_events_f2.tmp", action="write")
close (u1, status = "delete")
open (u1, file = "sf_beam_events_f3.tmp", action="write")
close (u1, status = "delete")

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_beam_events_3"

end subroutine sf_beam_events_3

```

16.12 Lepton collider beamstrahlung: CIRCE1

```
<sf_circe1.f90>≡  
<File header>  
  
module sf_circe1  
  
  <Use kinds>  
  use kinds, only: double  
  <Use strings>  
  use io_units  
  use format_defs, only: FMT_17, FMT_19  
  use diagnostics  
  use physics_defs, only: ELECTRON, PHOTON  
  use lorentz  
  use rng_base  
  use pdg_arrays  
  use model_data  
  use flavors  
  use colors  
  use quantum_numbers  
  use state_matrices  
  use polarizations  
  use sf_mappings  
  use sf_base  
  use circe1, circe1_rng_t => rng_type !NODEP!  
  
  <Standard module head>  
  
  <SF circe1: public>  
  
  <SF circe1: types>  
  
  contains  
  
  <SF circe1: procedures>  
  
end module sf_circe1
```

16.12.1 Physics

Beamstrahlung is applied before ISR. The **CIRCE1** implementation has a single structure function for both beams (which makes sense since it has to be switched on or off for both beams simultaneously). Nevertheless it is factorized:

The functional form in the **CIRCE1** parameterization is defined for electrons or photons

$$f(x) = \alpha x^\beta (1-x)^\gamma \quad (16.62)$$

for $x < 1 - \epsilon$ (resp. $x > \epsilon$ in the photon case). In the remaining interval, the standard form is zero, with a delta singularity at $x = 1$ (resp. $x = 0$). Equivalently, the delta part may be distributed uniformly among this interval. This latter form is implemented in the **kirke** version of the **CIRCE1** subroutines, and is used here.

The parameter `circe1\eps` sets the peak mapping of the CIRCE1 structure function. Its default value is 10^{-5} . The other parameters are the parameterization version and revision number, the accelerator type, and the \sqrt{s} value used by CIRCE1. The chattiness can also be set.

Since the energy is distributed in a narrow region around unity (for electrons) or zero (for photons), it is advantageous to map the interval first. The mapping is controlled by the parameter `circe1\epsilon` which is taken from the CIRCE1 internal data structure.

The \sqrt{s} value, if not explicitly set, is taken from the process data. Note that interpolating \sqrt{s} is not recommended; one should rather choose one of the distinct values known to CIRCE1.

16.12.2 The CIRCE1 data block

The CIRCE1 parameters are: The incoming flavors, the flags whether the photon or the lepton is the parton in the hard interaction, the flags for the generation mode (generator/mapping/no mapping), the mapping parameter ϵ , \sqrt{s} and several steering parameters: `ver`, `rev`, `acc`, `chat`.

In generator mode, the x values are actually discarded and a random number generator is used instead.

```

<SF circe1: public>≡
  public :: circe1_data_t

<SF circe1: types>≡
  type, extends (sf_data_t) :: circe1_data_t
  private
    class(model_data_t), pointer :: model => null ()
    type(flavor_t), dimension(2) :: flv_in
    integer, dimension(2) :: pdg_in
    real(default), dimension(2) :: m_in = 0
    logical, dimension(2) :: photon = .false.
    logical :: generate = .false.
    class(rng_factory_t), allocatable :: rng_factory
    real(default) :: sqrts = 0
    real(default) :: eps = 0
    integer :: ver = 0
    integer :: rev = 0
    character(6) :: acc = "?"
    integer :: chat = 0
    logical :: with_radiation = .false.
  contains
    <SF circe1: circe1 data: TBP>
  end type circe1_data_t

<SF circe1: circe1 data: TBP>≡
  procedure :: init => circe1_data_init

<SF circe1: procedures>≡
  subroutine circe1_data_init &
    (data, model, pdg_in, sqrts, eps, out_photon, &
     ver, rev, acc, chat, with_radiation)
    class(circe1_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model

```



```

type(pdg_array_t), dimension(2), intent(in) :: pdg_in
real(default), intent(in) :: sqrts
real(default), intent(in) :: eps
logical, dimension(2), intent(in) :: out_photon
character(*), intent(in) :: acc
integer, intent(in) :: ver, rev, chat
logical, intent(in) :: with_radiation
data%model => model
if (any (pdg_array_get_length (pdg_in) /= 1)) then
    call msg_fatal ("CIRCE1: incoming beam particles must be unique")
end if
call data%flv_in(1)%init (pdg_array_get (pdg_in(1), 1), model)
call data%flv_in(2)%init (pdg_array_get (pdg_in(2), 1), model)
data%pdg_in = data%flv_in%get_pdg ()
data%m_in = data%flv_in%get_mass ()
data%sqrts = sqrts
data%eps = eps
data%photon = out_photon
data%ver = ver
data%rev = rev
data%acc = acc
data%chat = chat
data%with_radiation = with_radiation
call data%check ()
call circex (0.d0, 0.d0, dble (data%sqrts), &
    data%acc, data%ver, data%rev, data%chat)
end subroutine circe1_data_init

```

Activate the generator mode. We import a RNG factory into the data type, which can then spawn RNG generator objects.

```

<SF circe1: circe1 data: TBP>+≡
    procedure :: set_generator_mode => circe1_data_set_generator_mode

<SF circe1: procedures>+≡
    subroutine circe1_data_set_generator_mode (data, rng_factory)
        class(circe1_data_t), intent(inout) :: data
        class(rng_factory_t), intent(inout), allocatable :: rng_factory
        data%generate = .true.
        call move_alloc (from = rng_factory, to = data%rng_factory)
    end subroutine circe1_data_set_generator_mode

```

Handle error conditions.

```

<SF circe1: circe1 data: TBP>+≡
    procedure :: check => circe1_data_check

<SF circe1: procedures>+≡
    subroutine circe1_data_check (data)
        class(circe1_data_t), intent(in) :: data
        type(flavor_t) :: flv_electron, flv_photon
        call flv_electron%init (ELECTRON, data%model)
        call flv_photon%init (PHOTON, data%model)
        if (.not. flv_electron%is_defined () &
            .or. .not. flv_photon%is_defined ()) then
            call msg_fatal ("CIRCE1: model must contain photon and electron")
        end if
    end subroutine circe1_data_check

```

```

end if
if (any (abs (data%pdg_in) /= ELECTRON) &
    .or. (data%pdg_in(1) /= - data%pdg_in(2))) then
    call msg_fatal ("CIRCE1: applicable only for e+e- or e-e+ collisions")
end if
if (data%eps <= 0) then
    call msg_error ("CIRCE1: circe1_eps = 0: integration will &
        &miss x=1 peak")
end if
end subroutine circe1_data_check

```

Output

```

<SF circe1: circe1 data: TBP>+=
    procedure :: write => circe1_data_write

<SF circe1: procedures>+=
    subroutine circe1_data_write (data, unit, verbose)
        class(circe1_data_t), intent(in) :: data
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u
        logical :: verb
        verb = .false.; if (present (verbose)) verb = verbose
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1x,A)") "CIRCE1 data:"
        write (u, "(3x,A,2(1x,A))") "prt_in   =", &
            char (data%flv_in(1)%get_name ()), &
            char (data%flv_in(2)%get_name ())
        write (u, "(3x,A,2(1x,L1))") "photon   =", data%photon
        write (u, "(3x,A,L1)") "generate =", data%generate
        write (u, "(3x,A,2(1x," // FMT_19 // ")") "m_in     =", data%m_in
        write (u, "(3x,A," // FMT_19 // ")") "sqrts    =", data%sqrts
        write (u, "(3x,A," // FMT_19 // ")") "eps      =", data%eps
        write (u, "(3x,A,I0)") "ver      =", data%ver
        write (u, "(3x,A,I0)") "rev      =", data%rev
        write (u, "(3x,A,A)") "acc      =", data%acc
        write (u, "(3x,A,I0)") "chat     =", data%chat
        write (u, "(3x,A,L1)") "with rad.=", data%with_radiation
        if (data%generate) then
            if (verb) then
                call data%rng_factory%write (u)
            end if
        end if
    end subroutine circe1_data_write

```

Return true if this structure function is in generator mode. In that case, all parameters are free, otherwise bound. (We do not support mixed cases.) Default is: no generator.

```

<SF circe1: circe1 data: TBP>+=
    procedure :: is_generator => circe1_data_is_generator

<SF circe1: procedures>+=
    function circe1_data_is_generator (data) result (flag)
        class(circe1_data_t), intent(in) :: data

```

```

    logical :: flag
    flag = data%generate
end function circe1_data_is_generator

```

The number of parameters is two, collinear splitting for the two beams.

```

<SF circe1: circe1 data: TBP>+≡
  procedure :: get_n_par => circe1_data_get_n_par

<SF circe1: procedures>+≡
  function circe1_data_get_n_par (data) result (n)
    class(circe1_data_t), intent(in) :: data
    integer :: n
    n = 2
  end function circe1_data_get_n_par

```

Return the outgoing particles PDG codes. This is either the incoming particle (if a photon is radiated), or the photon if that is the particle of the hard interaction. The latter is determined via the photon flag. There are two entries for the two beams.

```

<SF circe1: circe1 data: TBP>+≡
  procedure :: get_pdg_out => circe1_data_get_pdg_out

<SF circe1: procedures>+≡
  subroutine circe1_data_get_pdg_out (data, pdg_out)
    class(circe1_data_t), intent(in) :: data
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
    integer :: i, n
    n = 2
    do i = 1, n
      if (data%photon(i)) then
        pdg_out(i) = PHOTON
      else
        pdg_out(i) = data%pdg_in(i)
      end if
    end do
  end subroutine circe1_data_get_pdg_out

```

This variant is not inherited, it returns integers.

```

<SF circe1: circe1 data: TBP>+≡
  procedure :: get_pdg_int => circe1_data_get_pdg_int

<SF circe1: procedures>+≡
  function circe1_data_get_pdg_int (data) result (pdg)
    class(circe1_data_t), intent(in) :: data
    integer, dimension(2) :: pdg
    integer :: i
    do i = 1, 2
      if (data%photon(i)) then
        pdg(i) = PHOTON
      else
        pdg(i) = data%pdg_in(i)
      end if
    end do
  end function

```

```
end function circe1_data_get_pdg_int
```

Allocate the interaction record.

```
<SF circe1: circe1 data: TBP>+≡
  procedure :: allocate_sf_int => circe1_data_allocate_sf_int
<SF circe1: procedures>+≡
  subroutine circe1_data_allocate_sf_int (data, sf_int)
    class(circe1_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (circe1_t :: sf_int)
  end subroutine circe1_data_allocate_sf_int
```

Return the accelerator type.

```
<SF circe1: circe1 data: TBP>+≡
  procedure :: get_beam_file => circe1_data_get_beam_file
<SF circe1: procedures>+≡
  function circe1_data_get_beam_file (data) result (file)
    class(circe1_data_t), intent(in) :: data
    type(string_t) :: file
    file = "CIRCE1: " // data%acc
  end function circe1_data_get_beam_file
```

16.12.3 Random Number Generator for CIRCE

The CIRCE implementation now supports a generic random-number generator object that allows for a local state as a component. To support this, we must extend the abstract type provided by CIRCE and delegate the generator call to the (also abstract) RNG used by WHIZARD.

```
<SF circe1: types>+≡
  type, extends (circe1_rng_t) :: rng_obj_t
    class(rng_t), allocatable :: rng
  contains
    procedure :: generate => rng_obj_generate
  end type rng_obj_t

<SF circe1: procedures>+≡
  subroutine rng_obj_generate (rng_obj, u)
    class(rng_obj_t), intent(inout) :: rng_obj
    real(double), intent(out) :: u
    real(default) :: x
    call rng_obj%rng%generate (x)
    u = x
  end subroutine rng_obj_generate
```

16.12.4 The CIRCE1 object

This is a $2 \rightarrow 4$ interaction, where, depending on the parameters, any two of the four outgoing particles are connected to the hard interactions, the others

are radiated. Knowing that all particles are colorless, we do not have to deal with color.

The flavors are sorted such that the first two particles are the incoming leptons, the next two are the radiated particles, and the last two are the partons initiating the hard interaction.

CIRCE1 does not support polarized beams explicitly. For simplicity, we nevertheless carry beam polarization through to the outgoing electrons and make the photons unpolarized.

In the case that no radiated particle is kept (which actually is the default), polarization is always transferred to the electrons, too. If there is a recoil photon in the event, the radiated particles are 3 and 4, respectively, and 5 and 6 are the outgoing ones (triggering the hard scattering process), while in the case of no radiation, the outgoing particles are 3 and 4, respectively. In the case of the electron being the radiated particle, helicity is not kept.

```

<SF circe1: public>+≡
  public :: circe1_t

<SF circe1: types>+≡
  type, extends (sf_int_t) :: circe1_t
    type(circe1_data_t), pointer :: data => null ()
    real(default), dimension(2) :: x = 0
    real(default), dimension(2) :: xb= 0
    real(default) :: f = 0
    logical, dimension(2) :: continuum = .true.
    logical, dimension(2) :: peak = .true.
    type(rng_obj_t) :: rng_obj
  contains
    <SF circe1: circe1: TBP>
  end type circe1_t

```

Type string: has to be here, but there is no string variable on which CIRCE1 depends. Hence, a dummy routine.

```

<SF circe1: circe1: TBP>≡
  procedure :: type_string => circe1_type_string

<SF circe1: procedures>+≡
  function circe1_type_string (object) result (string)
    class(circe1_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "CIRCE1: beamstrahlung"
    else
      string = "CIRCE1: [undefined]"
    end if
  end function circe1_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF circe1: circe1: TBP>+≡
  procedure :: write => circe1_write

<SF circe1: procedures>+≡
  subroutine circe1_write (object, unit, testflag)
    class(circe1_t), intent(in) :: object

```

```

integer, intent(in), optional :: unit
logical, intent(in), optional :: testflag
integer :: u
u = given_output_unit (unit)
if (associated (object%data)) then
  call object%data%write (u)
  if (object%data%generate) call object%rng_obj%rng%write (u)
  if (object%status >= SF_DONE_KINEMATICS) then
    write (u, "(3x,A,2(1x," // FMT_17 // "))" ) "x =", object%x
    write (u, "(3x,A,2(1x," // FMT_17 // "))" ) "xb=", object%xb
    if (object%status >= SF_FAILED_EVALUATION) then
      write (u, "(3x,A,1x," // FMT_17 // "))" "f =", object%f
    end if
  end if
  call object%base_write (u, testflag)
else
  write (u, "(1x,A)" ) "CIRCE1 data: [undefined]"
end if
end subroutine circe1_write

```

<SF circe1: circe1: TBP>+≡

```

procedure :: init => circe1_init

```

<SF circe1: procedures>+≡

```

subroutine circe1_init (sf_int, data)
  class(circe1_t), intent(out) :: sf_int
  class(sf_data_t), intent(in), target :: data
  logical, dimension(6) :: mask_h
  type(quantum_numbers_mask_t), dimension(6) :: mask
  integer, dimension(6) :: hel_lock
  type(polarization_t), target :: pol1, pol2
  type(quantum_numbers_t), dimension(1) :: qn_fc1, qn_fc2
  type(flavor_t) :: flv_photon
  type(color_t) :: col0
  real(default), dimension(2) :: mi2, mr2, mo2
  type(quantum_numbers_t) :: qn_hel1, qn_hel2, qn_photon, qn1, qn2
  type(quantum_numbers_t), dimension(6) :: qn
  type(polarization_iterator_t) :: it_hel1, it_hel2
  hel_lock = 0
  mask_h = .false.
  select type (data)
  type is (circe1_data_t)
    mi2 = data%m_in**2
    if (data%with_radiation) then
      if (data%photon(1)) then
        hel_lock(1) = 3; hel_lock(3) = 1; mask_h(5) = .true.
        mr2(1) = mi2(1)
        mo2(1) = 0._default
      else
        hel_lock(1) = 5; hel_lock(5) = 1; mask_h(3) = .true.
        mr2(1) = 0._default
        mo2(1) = mi2(1)
      end if
    if (data%photon(2)) then

```

```

        hel_lock(2) = 4; hel_lock(4) = 2; mask_h(6) = .true.
        mr2(2) = mi2(2)
        mo2(2) = 0._default
    else
        hel_lock(2) = 6; hel_lock(6) = 2; mask_h(4) = .true.
        mr2(2) = 0._default
        mo2(2) = mi2(2)
    end if
    mask = quantum_numbers_mask (.false., .false., mask_h)
    call sf_int%base_init (mask, mi2, mr2, mo2, &
        hel_lock = hel_lock)
    sf_int%data => data
    call flv_photon%init (PHOTON, data%model)
    call col0%init ()
    call qn_photon%init (flv_photon, col0)
    call pol1%init_generic (data%flv_in(1))
    call qn_fc1(1)%init (flv = data%flv_in(1), col = col0)
    call pol2%init_generic (data%flv_in(2))
    call qn_fc2(1)%init (flv = data%flv_in(2), col = col0)
    call it_hel1%init (pol1)

    do while (it_hel1%is_valid ())
        qn_hel1 = it_hel1%get_quantum_numbers ()
        qn1 = qn_hel1 .merge. qn_fc1(1)
        qn(1) = qn1
        if (data%photon(1)) then
            qn(3) = qn1; qn(5) = qn_photon
        else
            qn(3) = qn_photon; qn(5) = qn1
        end if
        call it_hel2%init (pol2)
        do while (it_hel2%is_valid ())
            qn_hel2 = it_hel2%get_quantum_numbers ()
            qn2 = qn_hel2 .merge. qn_fc2(1)
            qn(2) = qn2
            if (data%photon(2)) then
                qn(4) = qn2; qn(6) = qn_photon
            else
                qn(4) = qn_photon; qn(6) = qn2
            end if
            call qn(3:4)%tag_radiated ()
            call sf_int%add_state (qn)
            call it_hel2%advance ()
        end do
        call it_hel1%advance ()
    end do
    call pol1%final ()
    call pol2%final ()
    call sf_int%freeze ()
    call sf_int%set_incoming ([1,2])
    call sf_int%set_radiated ([3,4])
    call sf_int%set_outgoing ([5,6])
else
    if (data%photon(1)) then

```

```

        mask_h(3) = .true.
        mo2(1) = 0._default
    else
        hel_lock(1) = 3; hel_lock(3) = 1
        mo2(1) = mi2(1)
    end if
    if (data%photon(2)) then
        mask_h(4) = .true.
        mo2(2) = 0._default
    else
        hel_lock(2) = 4; hel_lock(4) = 2
        mo2(2) = mi2(2)
    end if
    mask = quantum_numbers_mask (.false., .false., mask_h)
    call sf_int%base_init (mask(1:4), mi2, [real(default) :: ], mo2, &
        hel_lock = hel_lock(1:4))
    sf_int%data => data
    call flv_photon%init (PHOTON, data%model)
    call col0%init ()
    call qn_photon%init (flv_photon, col0)
    call pol1%init_generic (data%flv_in(1))
    call qn_fc1(1)%init (flv = data%flv_in(1), col = col0)
    call pol2%init_generic (data%flv_in(2))
    call qn_fc2(1)%init (flv = data%flv_in(2), col = col0)
    call it_hel1%init (pol1)

    do while (it_hel1%is_valid ())
        qn_hel1 = it_hel1%get_quantum_numbers ()
        qn1 = qn_hel1 .merge. qn_fc1(1)
        qn(1) = qn1
        if (data%photon(1)) then
            qn(3) = qn_photon
        else
            qn(3) = qn1
        end if
        call it_hel2%init (pol2)
        do while (it_hel2%is_valid ())
            qn_hel2 = it_hel2%get_quantum_numbers ()
            qn2 = qn_hel2 .merge. qn_fc2(1)
            qn(2) = qn2
            if (data%photon(2)) then
                qn(4) = qn_photon
            else
                qn(4) = qn2
            end if
            call sf_int%add_state (qn(1:4))
            call it_hel2%advance ()
        end do
        call it_hel1%advance ()
    end do
    ! call pol1%final ()
    ! call pol2%final ()
    call sf_int%freeze ()
    call sf_int%set_incoming ([1,2])

```



```

        call sf_int%set_outgoing ([3,4])
    end if
    sf_int%status = SF_INITIAL
end select
if (sf_int%data%generate) then
    call sf_int%data%rng_factory%make (sf_int%rng_obj%rng)
end if
end subroutine circe1_init

```

16.12.5 Kinematics

Refer to the data component.

```

<SF circe1: circe1: TBP>+≡
    procedure :: is_generator => circe1_is_generator

<SF circe1: procedures>+≡
    function circe1_is_generator (sf_int) result (flag)
        class(circe1_t), intent(in) :: sf_int
        logical :: flag
        flag = sf_int%data%is_generator ()
    end function circe1_is_generator

```

Generate free parameters, if generator mode is on. Otherwise, the parameters will be discarded.

```

<SF circe1: circe1: TBP>+≡
    procedure :: generate_free => circe1_generate_free

<SF circe1: procedures>+≡
    subroutine circe1_generate_free (sf_int, r, rb, x_free)
        class(circe1_t), intent(inout) :: sf_int
        real(default), dimension(:), intent(out) :: r, rb
        real(default), intent(inout) :: x_free

        if (sf_int%data%generate) then
            call circe_generate (r, sf_int%data%get_pdg_int (), sf_int%rng_obj)
            rb = 1 - r
            x_free = x_free * product (r)
        else
            r = 0
            rb = 1
        end if
    end subroutine circe1_generate_free

```

Generator mode: depending on the particle codes, call one of the available `girce` generators. Illegal particle code combinations should have been caught during data initialization.

```

<SF circe1: procedures>+≡
    subroutine circe_generate (x, pdg, rng_obj)
        real(default), dimension(2), intent(out) :: x
        integer, dimension(2), intent(in) :: pdg
        class(rng_obj_t), intent(inout) :: rng_obj
        real(double) :: xc1, xc2

```

```

select case (abs (pdg(1)))
case (ELECTRON)
  select case (abs (pdg(2)))
  case (ELECTRON)
    call gircee (xc1, xc2, rng_obj = rng_obj)
  case (PHOTON)
    call girceg (xc1, xc2, rng_obj = rng_obj)
  end select
case (PHOTON)
  select case (abs (pdg(2)))
  case (ELECTRON)
    call girceg (xc2, xc1, rng_obj = rng_obj)
  case (PHOTON)
    call gircgg (xc1, xc2, rng_obj = rng_obj)
  end select
end select
x = [xc1, xc2]
end subroutine circe_generate

```

Set kinematics. The r values (either from integration or from the generator call above) are copied to x unchanged, and f is unity. We store the x values, so we can use them for the evaluation later.

```

<SF circe1: circe1: TBP>+≡
  procedure :: complete_kinematics => circe1_complete_kinematics

<SF circe1: procedures>+≡
  subroutine circe1_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(circe1_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    x = r
    xb = rb
    sf_int%x = x
    sf_int%xb= xb
    f = 1
    if (sf_int%data%with_radiation) then
      call sf_int%split_momenta (x, xb)
    else
      call sf_int%reduce_momenta (x)
    end if
    select case (sf_int%status)
    case (SF_FAILED_KINEMATICS); f = 0
    end select
  end subroutine circe1_complete_kinematics

```

Compute inverse kinematics. In generator mode, the r values are meaningless, but we copy them anyway.

```

<SF circe1: circe1: TBP>+≡
  procedure :: inverse_kinematics => circe1_inverse_kinematics

```

```

<SF circe1: procedures>+≡
subroutine circe1_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
  class(circe1_t), intent(inout) :: sf_int
  real(default), dimension(:), intent(in) :: x
  real(default), dimension(:), intent(in) :: xb
  real(default), intent(out) :: f
  real(default), dimension(:), intent(out) :: r
  real(default), dimension(:), intent(out) :: rb
  logical, intent(in) :: map
  logical, intent(in), optional :: set_momenta
  logical :: set_mom
  set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
  r = x
  rb = xb
  sf_int%x = x
  sf_int%xb= xb
  f = 1
  if (set_mom) then
    call sf_int%split_momenta (x, xb)
    select case (sf_int%status)
      case (SF_FAILED_KINEMATICS); f = 0
    end select
  end if
end subroutine circe1_inverse_kinematics

```

16.12.6 CIRCE1 application

CIRCE is applied for the two beams at once. We can safely assume that no structure functions are applied before this, so the incoming particles are on-shell electrons/positrons.

The scale is ignored.

```

<SF circe1: circe1: TBP>+≡
procedure :: apply => circe1_apply

<SF circe1: procedures>+≡
subroutine circe1_apply (sf_int, scale, negative_sf, rescale, i_sub)
  class(circe1_t), intent(inout) :: sf_int
  real(default), intent(in) :: scale
  logical, intent(in), optional :: negative_sf
  class(sf_rescale_t), intent(in), optional :: rescale
  integer, intent(in), optional :: i_sub
  real(default), dimension(2) :: xb
  real(double), dimension(2) :: xc
  real(double), parameter :: one = 1
  associate (data => sf_int%data)
    xc = sf_int%x
    xb = sf_int%xb
    if (data%generate) then
      sf_int%f = 1
    else
      sf_int%f = 0
      if (all (sf_int%continuum)) then
        sf_int%f = circe (xc(1), xc(2), data%pdg_in(1), data%pdg_in(2))
      end if
    end if
  end associate
end subroutine circe1_apply

```

```

end if
if (sf_int%continuum(2) .and. sf_int%peak(1)) then
  sf_int%f = sf_int%f &
    + circe (one, xc(2), data%pdg_in(1), data%pdg_in(2)) &
    * peak (xb(1), data%eps)
end if
if (sf_int%continuum(1) .and. sf_int%peak(2)) then
  sf_int%f = sf_int%f &
    + circe (xc(1), one, data%pdg_in(1), data%pdg_in(2)) &
    * peak (xb(2), data%eps)
end if
if (all (sf_int%peak)) then
  sf_int%f = sf_int%f &
    + circe (one, one, data%pdg_in(1), data%pdg_in(2)) &
    * peak (xb(1), data%eps) * peak (xb(2), data%eps)
end if
end if
end associate
call sf_int%set_matrix_element (cmplx (sf_int%f, kind=default))
sf_int%status = SF_EVALUATED
end subroutine circe1_apply

```

This is a smeared delta peak at zero, as an endpoint singularity. We choose an exponentially decreasing function, starting at zero, with integral (from 0 to 1) $1 - e^{-1/\epsilon}$. For small ϵ , this reduces to one.

```

<SF circe1: procedures>+=
function peak (x, eps) result (f)
  real(default), intent(in) :: x, eps
  real(default) :: f
  f = exp (-x / eps) / eps
end function peak

```

16.12.7 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_circe1_ut.f90>≡
<File header>

module sf_circe1_ut
  use unit_tests
  use sf_circe1_uti

  <Standard module head>

  <SF circe1: public test>

contains

  <SF circe1: test driver>

end module sf_circe1_ut

```

```

<sf_circe1_util.f90>≡
  <File header>

  module sf_circe1_util

    <Use kinds>
    use physics_defs, only: ELECTRON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use rng_base
    use sf_aux
    use sf_base

    use sf_circe1

    use rng_base_util, only: rng_test_factory_t

    <Standard module head>

    <SF circe1: test declarations>

    contains

    <SF circe1: tests>

  end module sf_circe1_util
API: driver for the unit tests below.
<SF circe1: public test>≡
  public :: sf_circe1_test
<SF circe1: test driver>≡
  subroutine sf_circe1_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <SF circe1: execute tests>
  end subroutine sf_circe1_test

```

Test structure function data

Construct and display a test structure function data object.

```

<SF circe1: execute tests>≡
  call test (sf_circe1_1, "sf_circe1_1", &
    "structure function configuration", &
    u, results)
<SF circe1: test declarations>≡
  public :: sf_circe1_1
<SF circe1: tests>≡
  subroutine sf_circe1_1 (u)
    integer, intent(in) :: u

```

```

type(model_data_t), target :: model
type(pdg_array_t), dimension(2) :: pdg_in
type(pdg_array_t), dimension(2) :: pdg_out
integer, dimension(:), allocatable :: pdg1, pdg2
class(sf_data_t), allocatable :: data

write (u, "(A)")  "* Test output: sf_circe1_1"
write (u, "(A)")  "* Purpose: initialize and display &
                  &CIRCE structure function data"
write (u, "(A)")

write (u, "(A)")  "* Create empty data object"
write (u, "(A)")

call model%init_qed_test ()
pdg_in(1) = ELECTRON
pdg_in(2) = -ELECTRON

allocate (circe1_data_t :: data)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

select type (data)
type is (circe1_data_t)
    call data%init (model, pdg_in, &
        sqrts = 500._default, &
        eps = 1e-6_default, &
        out_photon = [.false., .false.], &
        ver = 0, &
        rev = 0, &
        acc = "SBAND", &
        chat = 0, &
        with_radiation = .true.)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
pdg2 = pdg_out(2)
write (u, "(2x,99(1x,I0))") pdg1, pdg2

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe1_1"

end subroutine sf_circe1_1

```

Test and probe structure function

Construct and display a structure function object based on the PDF builtin structure function.

```
<SF circe1: execute tests>+≡
  call test (sf_circe1_2, "sf_circe1_2", &
    "structure function instance", &
    u, results)

<SF circe1: test declarations>+≡
  public :: sf_circe1_2

<SF circe1: tests>+≡
  subroutine sf_circe1_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    type(vector4_t), dimension(4) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_circe1_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &circe1 structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call model%init_qed_test ()
    call flv(1)%init (ELECTRON, model)
    call flv(2)%init (-ELECTRON, model)
    pdg_in(1) = ELECTRON
    pdg_in(2) = -ELECTRON

    call reset_interaction_counter ()

    allocate (circe1_data_t :: data)
    select type (data)
    type is (circe1_data_t)
      call data%init (model, pdg_in, &
        sqrts = 500._default, &
        eps = 1e-6_default, &
        out_photon = [.false., .false.], &
        ver = 0, &
        rev = 0, &
        acc = "SBAND", &
```

```

        chat = 0, &
        with_radiation = .true.)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.95,0.85."
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = [0.9_default, 0.8_default]
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1, 2])

```



```

call sf_int%seed_kinematics ([k1, k2])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe1_2"

end subroutine sf_circe1_2

```

Generator mode

Construct and evaluate a structure function object in generator mode.

```

<SF circe1: execute tests>+≡
  call test (sf_circe1_3, "sf_circe1_3", &
    "generator mode", &
    u, results)

<SF circe1: test declarations>+≡
  public :: sf_circe1_3

<SF circe1: tests>+≡
  subroutine sf_circe1_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(rng_factory_t), allocatable :: rng_factory
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, x_free

    write (u, "(A)")  "* Test output: sf_circe1_3"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &circe1 structure function object"

```

```

write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call model%init_qed_test ()
call flv(1)%init (ELECTRON, model)
call flv(2)%init (-ELECTRON, model)
pdg_in(1) = ELECTRON
pdg_in(2) = -ELECTRON

call reset_interaction_counter ()

allocate (circe1_data_t :: data)
allocate (rng_test_factory_t :: rng_factory)
select type (data)
type is (circe1_data_t)
    call data%init (model, pdg_in, &
        sqrts = 500._default, &
        eps = 1e-6_default, &
        out_photon = [.false., .false.], &
        ver = 0, &
        rev = 0, &
        acc = "SBAND", &
        chat = 0, &
        with_radiation = .true.)
    call data%set_generator_mode (rng_factory)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])
select type (sf_int)
type is (circe1_t)
    call sf_int%rng_obj%rng%init (3)
end select

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Generate x"
write (u, "(A)")

allocate (r (data%get_n_par ()))

```

```

allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f
write (u, "(A,9(1x,F10.7))") "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe1_3"

end subroutine sf_circe1_3

```

16.13 Lepton Collider Beamstrahlung and Photon collider: CIRCE2

```
<sf_circe2.f90>≡  
<File header>  
  
module sf_circe2  
  
  <Use kinds>  
  <Use strings>  
  use io_units  
  use format_defs, only: FMT_19  
  use numeric_utils  
  use diagnostics  
  use os_interface  
  use physics_defs, only: PHOTON, ELECTRON  
  use lorentz  
  use rng_base  
  use selectors  
  use pdg_arrays  
  use model_data  
  use flavors  
  use colors  
  use helicities  
  use quantum_numbers  
  use state_matrices  
  use polarizations  
  use sf_base  
  use circe2, circe2_rng_t => rng_type !NODEP!  
  
  <Standard module head>  
  
  <SF circe2: public>  
  
  <SF circe2: types>  
  
contains  
  
  <SF circe2: procedures>  
  
end module sf_circe2
```

16.13.1 Physics

CIRCE2 describes photon spectra Beamstrahlung is applied before ISR. The CIRCE2 implementation has a single structure function for both beams (which makes sense since it has to be switched on or off for both beams simultaneously).

16.13.2 The CIRCE2 data block

The CIRCE2 parameters are: file and collider specification, incoming (= outgoing) particles. The luminosity is returned by `circe2_luminosity`.

```

<SF circe2: public>≡
  public :: circe2_data_t

<SF circe2: types>≡
  type, extends (sf_data_t) :: circe2_data_t
    private
      class(model_data_t), pointer :: model => null ()
      type(flavor_t), dimension(2) :: flv_in
      integer, dimension(2) :: pdg_in
      real(default) :: sqrts = 0
      logical :: polarized = .false.
      logical :: beams_polarized = .false.
      class(rng_factory_t), allocatable :: rng_factory
      type(string_t) :: filename
      type(string_t) :: file
      type(string_t) :: design
      real(default) :: lumi = 0
      real(default), dimension(4) :: lumi_hel_frac = 0
      integer, dimension(0:4) :: h1 = [0, -1, -1, 1, 1]
      integer, dimension(0:4) :: h2 = [0, -1, 1, -1, 1]
      integer :: error = 1
    contains
      <SF circe2: circe2 data: TBP>
    end type circe2_data_t

<SF circe2: types>+≡
  type(circe2_state) :: circe2_global_state

<SF circe2: circe2 data: TBP>≡
  procedure :: init => circe2_data_init

<SF circe2: procedures>≡
  subroutine circe2_data_init (data, os_data, model, pdg_in, &
    sqrts, polarized, beam_pol, file, design)
    class(circe2_data_t), intent(out) :: data
    type(os_data_t), intent(in) :: os_data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), dimension(2), intent(in) :: pdg_in
    real(default), intent(in) :: sqrts
    logical, intent(in) :: polarized, beam_pol
    type(string_t), intent(in) :: file, design
    integer :: h
    data%model => model
    if (any (pdg_array_get_length (pdg_in) /= 1)) then
      call msg_fatal ("CIRCE2: incoming beam particles must be unique")
    end if
    call data%flv_in(1)%init (pdg_array_get (pdg_in(1), 1), model)
    call data%flv_in(2)%init (pdg_array_get (pdg_in(2), 1), model)
    data%pdg_in = data%flv_in%get_pdg ()
    data%sqrts = sqrts
    data%polarized = polarized
    data%beams_polarized = beam_pol
    data%filename = file
    data%design = design
  end subroutine

```

```

call data%check_file (os_data)
call circe2_load (circe2_global_state, trim (char(data%file)), &
    trim (char(data%design)), data%sqrts, data%error)
call data%check ()
data%lumi = circe2_luminosity (circe2_global_state, data%pdg_in, [0, 0])
if (vanishes (data%lumi)) then
    call msg_fatal ("CIRCE2: luminosity vanishes for specified beams.")
end if
if (data%polarized) then
    do h = 1, 4
        data%lumi_hel_frac(h) = &
            circe2_luminosity (circe2_global_state, data%pdg_in, &
                [data%h1(h), data%h2(h)]) &
            / data%lumi
    end do
end if
end subroutine circe2_data_init

```

Activate the generator mode. We import a RNG factory into the data type, which can then spawn RNG generator objects.

```

<SF circe2: circe2 data: TBP>+=
    procedure :: set_generator_mode => circe2_data_set_generator_mode

<SF circe2: procedures>+=
    subroutine circe2_data_set_generator_mode (data, rng_factory)
        class(circe2_data_t), intent(inout) :: data
        class(rng_factory_t), intent(inout), allocatable :: rng_factory
        call move_alloc (from = rng_factory, to = data%rng_factory)
    end subroutine circe2_data_set_generator_mode

```

Check whether the requested data file is in the system directory or in the current directory.

```

<SF circe2: circe2 data: TBP>+=
    procedure :: check_file => circe2_check_file

<SF circe2: procedures>+=
    subroutine circe2_check_file (data, os_data)
        class(circe2_data_t), intent(inout) :: data
        type(os_data_t), intent(in) :: os_data
        logical :: exist
        type(string_t) :: file
        file = data%filename
        if (file == "") &
            call msg_fatal ("CIRCE2: $circe2_file is not set")
        inquire (file = char (file), exist = exist)
        if (exist) then
            data%file = file
        else
            file = os_data%whizard_circe2path // "/" // data%filename
            inquire (file = char (file), exist = exist)
            if (exist) then
                data%file = file
            else
                call msg_fatal ("CIRCE2: data file '" // char (data%filename) &

```

```

        // '' not found")
    end if
end if
end subroutine circe2_check_file

```

Handle error conditions.

```

<SF circe2: circe2 data: TBP>+=
  procedure :: check => circe2_data_check

<SF circe2: procedures>+=
  subroutine circe2_data_check (data)
    class(circe2_data_t), intent(in) :: data
    type(flavor_t) :: flv_photon, flv_electron
    call flv_photon%init (PHOTON, data%model)
    if (.not. flv_photon%is_defined ()) then
      call msg_fatal ("CIRCE2: model must contain photon")
    end if
    call flv_electron%init (ELECTRON, data%model)
    if (.not. flv_electron%is_defined ()) then
      call msg_fatal ("CIRCE2: model must contain electron")
    end if
    if (any (abs (data%pdg_in) /= PHOTON .and. abs (data%pdg_in) /= ELECTRON)) &
      then
        call msg_fatal ("CIRCE2: applicable only for e+e- or photon collisions")
      end if
    select case (data%error)
    case (-1)
      call msg_fatal ("CIRCE2: data file not found.")
    case (-2)
      call msg_fatal ("CIRCE2: beam setup does not match data file.")
    case (-3)
      call msg_fatal ("CIRCE2: invalid format of data file.")
    case (-4)
      call msg_fatal ("CIRCE2: data file too large.")
    end select
  end subroutine circe2_data_check

```

Output

```

<SF circe2: circe2 data: TBP>+=
  procedure :: write => circe2_data_write

<SF circe2: procedures>+=
  subroutine circe2_data_write (data, unit, verbose)
    class(circe2_data_t), intent(in) :: data
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u, h
    logical :: verb
    verb = .false.; if (present (verbose)) verb = verbose
    u = given_output_unit (unit)
    write (u, "(1x,A)") "CIRCE2 data:"
    write (u, "(3x,A,A)") "file = ", char(data%filename)
    write (u, "(3x,A,A)") "design = ", char(data%design)
    write (u, "(3x,A," // FMT_19 // ")") "sqrts = ", data%sqrts

```

```

write (u, "(3x,A,A,A,A)") "prt_in = ", &
char (data%flv_in(1)%get_name ()), &
", ", char (data%flv_in(2)%get_name ())
write (u, "(3x,A,L1)") "polarized = ", data%polarized
write (u, "(3x,A,L1)") "beams pol. = ", data%beams_polarized
write (u, "(3x,A," // FMT_19 // ")") "luminosity = ", data%lumi
if (data%polarized) then
do h = 1, 4
write (u, "(6x,'(,I2,1x,I2,')',1x,'=',1x)", advance="no") &
data%h1(h), data%h2(h)
write (u, "(6x," // FMT_19 // ")") data%lumi_hel_frac(h)
end do
end if
if (verb) then
call data%rng_factory%write (u)
end if
end subroutine circe2_data_write

```

This is always in generator mode.

```

<SF circe2: circe2 data: TBP>+≡
procedure :: is_generator => circe2_data_is_generator
<SF circe2: procedures>+≡
function circe2_data_is_generator (data) result (flag)
class(circe2_data_t), intent(in) :: data
logical :: flag
flag = .true.
end function circe2_data_is_generator

```

The number of parameters is two, collinear splitting for the two beams.

```

<SF circe2: circe2 data: TBP>+≡
procedure :: get_n_par => circe2_data_get_n_par
<SF circe2: procedures>+≡
function circe2_data_get_n_par (data) result (n)
class(circe2_data_t), intent(in) :: data
integer :: n
n = 2
end function circe2_data_get_n_par

```

Return the outgoing particles PDG codes. They are equal to the incoming ones.

```

<SF circe2: circe2 data: TBP>+≡
procedure :: get_pdg_out => circe2_data_get_pdg_out
<SF circe2: procedures>+≡
subroutine circe2_data_get_pdg_out (data, pdg_out)
class(circe2_data_t), intent(in) :: data
type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
integer :: i, n
n = 2
do i = 1, n
pdg_out(i) = data%pdg_in(i)
end do
end subroutine circe2_data_get_pdg_out

```


Allocate the interaction record.

```

<SF circe2: circe2 data: TBP>+≡
  procedure :: allocate_sf_int => circe2_data_allocate_sf_int

<SF circe2: procedures>+≡
  subroutine circe2_data_allocate_sf_int (data, sf_int)
    class(circe2_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (circe2_t :: sf_int)
  end subroutine circe2_data_allocate_sf_int

```

Return the beam file.

```

<SF circe2: circe2 data: TBP>+≡
  procedure :: get_beam_file => circe2_data_get_beam_file

<SF circe2: procedures>+≡
  function circe2_data_get_beam_file (data) result (file)
    class(circe2_data_t), intent(in) :: data
    type(string_t) :: file
    file = "CIRCE2: " // data%filename
  end function circe2_data_get_beam_file

```

16.13.3 Random Number Generator for CIRCE

The CIRCE implementation now supports a generic random-number generator object that allows for a local state as a component. To support this, we must extend the abstract type provided by CIRCE and delegate the generator call to the (also abstract) RNG used by WHIZARD.

```

<SF circe2: types>+≡
  type, extends (circe2_rng_t) :: rng_obj_t
    class(rng_t), allocatable :: rng
  contains
    procedure :: generate => rng_obj_generate
  end type rng_obj_t

<SF circe2: procedures>+≡
  subroutine rng_obj_generate (rng_obj, u)
    class(rng_obj_t), intent(inout) :: rng_obj
    real(default), intent(out) :: u
    real(default) :: x
    call rng_obj%rng%generate (x)
    u = x
  end subroutine rng_obj_generate

```

16.13.4 The CIRCE2 object

For CIRCE2 spectra it does not make sense to describe the state matrix as a radiation interaction, even if photons originate from laser backscattering. Instead, it is a $2 \rightarrow 2$ interaction where the incoming particles are identical to the outgoing ones.

The current implementation of CIRCE2 does support polarization and classical correlations, but no entanglement, so the density matrix of the outgoing particles is diagonal. The incoming particles are unpolarized (user-defined polarization for beams is meaningless, since polarization is described by the data file). The outgoing particles are polarized or polarization-averaged, depending on user request.

When assigning matrix elements, we scan the previously initialized state matrix. For each entry, we extract helicity and call the structure function. In the unpolarized case, the helicity is undefined and replaced by value zero. In the polarized case, there are four entries. If the generator is used, only one entry is nonzero in each call. Which one, is determined by comparing with a previously (randomly, distributed by relative luminosity) selected pair of helicities.

```

<SF circe2: public>+≡
    public :: circe2_t

<SF circe2: types>+≡
    type, extends (sf_int_t) :: circe2_t
        type(circe2_data_t), pointer :: data => null ()
        type(rng_obj_t) :: rng_obj
        type(selector_t) :: selector
        integer :: h_sel = 0
    contains
        <SF circe2: circe2: TBP>
    end type circe2_t

```

Type string: show file and design of CIRCE2 structure function.

```

<SF circe2: circe2: TBP>≡
    procedure :: type_string => circe2_type_string

<SF circe2: procedures>+≡
    function circe2_type_string (object) result (string)
        class(circe2_t), intent(in) :: object
        type(string_t) :: string
        if (associated (object%data)) then
            string = "CIRCE2: " // object%data%design
        else
            string = "CIRCE2: [undefined]"
        end if
    end function circe2_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

<SF circe2: circe2: TBP>+≡
    procedure :: write => circe2_write

<SF circe2: procedures>+≡
    subroutine circe2_write (object, unit, testflag)
        class(circe2_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%data)) then
            call object%data%write (u)
        end if
    end subroutine circe2_write

```

```

        call object%base_write (u, testflag)
    else
        write (u, "(1x,A)") "CIRCE2 data: [undefined]"
    end if
end subroutine circe2_write

<SF circe2: circe2: TBP>+≡
procedure :: init => circe2_init

<SF circe2: procedures>+≡
subroutine circe2_init (sf_int, data)
    class(circe2_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    logical, dimension(4) :: mask_h
    real(default), dimension(2) :: m2_array
    real(default), dimension(0) :: null_array
    type(quantum_numbers_mask_t), dimension(4) :: mask
    type(quantum_numbers_t), dimension(4) :: qn
    type(helicity_t) :: hel
    type(color_t) :: col0
    integer :: h
    select type (data)
    type is (circe2_data_t)
        if (data%polarized .and. data%beams_polarized) then
            call msg_fatal ("CIRCE2: Beam polarization can't be set &
                &for polarized data file")
        else if (data%beams_polarized) then
            call msg_warning ("CIRCE2: User-defined beam polarization set &
                &for unpolarized CIRCE2 data file")
        end if
        mask_h(1:2) = .not. data%beams_polarized
        mask_h(3:4) = .not. (data%polarized .or. data%beams_polarized)
        mask = quantum_numbers_mask (.false., .false., mask_h)
        m2_array(:) = (data%flv_in(:)%get_mass ())*2
        call sf_int%base_init (mask, m2_array, null_array, m2_array)
        sf_int%data => data
        if (data%polarized) then
            if (vanishes (sum (data%lumi_hel_frac)) .or. &
                any (data%lumi_hel_frac < 0)) then
                call msg_fatal ("CIRCE2: Helicity-dependent lumi " &
                    // "fractions all vanish or", &
                    [var_str ("are negative: Please inspect the " &
                        // "CIRCE2 file or "), &
                    var_str ("switch off the polarized" // &
                        " option for CIRCE2.")])
            else
                call sf_int%selector%init (data%lumi_hel_frac)
            end if
        end if
        call col0%init ()
        if (data%beams_polarized) then
            do h = 1, 4
                call hel%init (data%h1(h))
                call qn(1)%init &

```

```

        (flv = data%flv_in(1), col = col0, hel = hel)
    call qn(3)%init &
        (flv = data%flv_in(1), col = col0, hel = hel)
    call hel%init (data%h2(h))
    call qn(2)%init &
        (flv = data%flv_in(2), col = col0, hel = hel)
    call qn(4)%init &
        (flv = data%flv_in(2), col = col0, hel = hel)
    call sf_int%add_state (qn)
end do
else if (data%polarized) then
    call qn(1)%init (flv = data%flv_in(1), col = col0)
    call qn(2)%init (flv = data%flv_in(2), col = col0)
    do h = 1, 4
        call hel%init (data%h1(h))
        call qn(3)%init &
            (flv = data%flv_in(1), col = col0, hel = hel)
        call hel%init (data%h2(h))
        call qn(4)%init &
            (flv = data%flv_in(2), col = col0, hel = hel)
        call sf_int%add_state (qn)
    end do
else
    call qn(1)%init (flv = data%flv_in(1), col = col0)
    call qn(2)%init (flv = data%flv_in(2), col = col0)
    call qn(3)%init (flv = data%flv_in(1), col = col0)
    call qn(4)%init (flv = data%flv_in(2), col = col0)
    call sf_int%add_state (qn)
end if
call sf_int%freeze ()
call sf_int%set_incoming ([1,2])
call sf_int%set_outgoing ([3,4])
call sf_int%data%rng_factory%make (sf_int%rng_obj%rng)
sf_int%status = SF_INITIAL
end select
end subroutine circe2_init

```

16.13.5 Kinematics

Refer to the data component.

```

<SF circe2: circe2: TBP>+≡
    procedure :: is_generator => circe2_is_generator

<SF circe2: procedures>+≡
    function circe2_is_generator (sf_int) result (flag)
        class(circe2_t), intent(in) :: sf_int
        logical :: flag
        flag = sf_int%data%is_generator ()
    end function circe2_is_generator

```

Generate free parameters. We first select a helicity, which we have to store, then generate x values for that helicity.

```

<SF circe2: circe2: TBP>+≡
  procedure :: generate_free => circe2_generate_whizard_free

<SF circe2: procedures>+≡
  subroutine circe2_generate_whizard_free (sf_int, r, rb, x_free)
    class(circe2_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: r, rb
    real(default), intent(inout) :: x_free
    integer :: h_sel
    if (sf_int%data%polarized) then
      call sf_int%selector%generate (sf_int%rng_obj%rng, h_sel)
    else
      h_sel = 0
    end if
    sf_int%h_sel = h_sel
    call circe2_generate_whizard (r, sf_int%data%pdg_in, &
      [sf_int%data%h1(h_sel), sf_int%data%h2(h_sel)], &
      sf_int%rng_obj)
    rb = 1 - r
    x_free = x_free * product (r)
  end subroutine circe2_generate_whizard_free

```

Generator mode: call the CIRCE2 generator for the given particles and helicities. (For unpolarized generation, helicities are zero.)

```

<SF circe2: procedures>+≡
  subroutine circe2_generate_whizard (x, pdg, hel, rng_obj)
    real(default), dimension(2), intent(out) :: x
    integer, dimension(2), intent(in) :: pdg
    integer, dimension(2), intent(in) :: hel
    class(rng_obj_t), intent(inout) :: rng_obj
    call circe2_generate (circe2_global_state, rng_obj, x, pdg, hel)
  end subroutine circe2_generate_whizard

```

Set kinematics. Trivial here.

```

<SF circe2: circe2: TBP>+≡
  procedure :: complete_kinematics => circe2_complete_kinematics

<SF circe2: procedures>+≡
  subroutine circe2_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(circe2_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    if (map) then
      call msg_fatal ("CIRCE2: map flag not supported")
    else
      x = r
      xb = rb
      f = 1
    end if
    call sf_int%reduce_momenta (x)

```

```
end subroutine circe2_complete_kinematics
```

Compute inverse kinematics.

```
<SF circe2: circe2: TBP>+≡
  procedure :: inverse_kinematics => circe2_inverse_kinematics

<SF circe2: procedures>+≡
  subroutine circe2_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(circe2_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta
    logical :: set_mom
    set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
    if (map) then
      call msg_fatal ("CIRCE2: map flag not supported")
    else
      r = x
      rb= xb
      f = 1
    end if
    if (set_mom) then
      call sf_int%reduce_momenta (x)
    end if
  end subroutine circe2_inverse_kinematics
```

16.13.6 CIRCE2 application

This function works on both beams. In polarized mode, we set only the selected helicity. In unpolarized mode, the interaction has only one entry, and the factor is unity.

```
<SF circe2: circe2: TBP>+≡
  procedure :: apply => circe2_apply

<SF circe2: procedures>+≡
  subroutine circe2_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(circe2_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    complex(default) :: f
    associate (data => sf_int%data)
      f = 1
      if (data%beams_polarized) then
        call sf_int%set_matrix_element (f)
      else if (data%polarized) then
        call sf_int%set_matrix_element (sf_int%h_sel, f)
      end if
    end associate
  end subroutine circe2_apply
```

```

        else
            call sf_int%set_matrix_element (1, f)
        end if
    end associate
    sf_int%status = SF_EVALUATED
end subroutine circe2_apply

```

16.13.7 Unit tests

Test module, followed by the corresponding implementation module.

`(sf_circe2_ut.f90)≡`
⟨File header⟩

```

module sf_circe2_ut
    use unit_tests
    use sf_circe2_uti

```

⟨Standard module head⟩

⟨SF circe2: public test⟩

contains

⟨SF circe2: test driver⟩

```

end module sf_circe2_ut

```

`(sf_circe2_uti.f90)≡`
⟨File header⟩

```

module sf_circe2_uti

```

⟨Use kinds⟩

⟨Use strings⟩

```

    use os_interface
    use physics_defs, only: PHOTON
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use rng_base
    use sf_aux
    use sf_base

```

```

    use sf_circe2

```

```

    use rng_base_ut, only: rng_test_factory_t

```

⟨Standard module head⟩

⟨SF circe2: test declarations⟩

contains

<SF circe2: tests>

end module sf_circe2_util

API: driver for the unit tests below.

<SF circe2: public test>≡

public :: sf_circe2_test

<SF circe2: test driver>≡

subroutine sf_circe2_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<SF circe2: execute tests>

end subroutine sf_circe2_test

Test structure function data

Construct and display a test structure function data object.

<SF circe2: execute tests>≡

call test (sf_circe2_1, "sf_circe2_1", &
"structure function configuration", &
u, results)

<SF circe2: test declarations>≡

public :: sf_circe2_1

<SF circe2: tests>≡

subroutine sf_circe2_1 (u)

integer, intent(in) :: u

type(os_data_t) :: os_data

type(model_data_t), target :: model

type(pdg_array_t), dimension(2) :: pdg_in

type(pdg_array_t), dimension(2) :: pdg_out

integer, dimension(:), allocatable :: pdg1, pdg2

class(sf_data_t), allocatable :: data

class(rng_factory_t), allocatable :: rng_factory

write (u, "(A)") "* Test output: sf_circe2_1"

write (u, "(A)") "* Purpose: initialize and display &
&CIRCE structure function data"

write (u, "(A)")

write (u, "(A)") "* Create empty data object"

write (u, "(A)")

call os_data%init ()

call model%init_qed_test ()

pdg_in(1) = PHOTON

pdg_in(2) = PHOTON

allocate (circe2_data_t :: data)

allocate (rng_test_factory_t :: rng_factory)


```

write (u, "(A)")
write (u, "(A)")  "* Initialize (unpolarized)"
write (u, "(A)")

select type (data)
type is (circe2_data_t)
  call data%init (os_data, model, pdg_in, &
    sqrts = 500._default, &
    polarized = .false., &
    beam_pol = .false., &
    file = var_str ("teslagg_500_polavg.circe"), &
    design = var_str ("TESLA/GG"))
  call data%set_generator_mode (rng_factory)
end select

call data%write (u, verbose = .true.)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
pdg2 = pdg_out(2)
write (u, "(2x,99(1x,I0))")  pdg1, pdg2

write (u, "(A)")
write (u, "(A)")  "* Initialize (polarized)"
write (u, "(A)")

allocate (rng_test_factory_t :: rng_factory)

select type (data)
type is (circe2_data_t)
  call data%init (os_data, model, pdg_in, &
    sqrts = 500._default, &
    polarized = .true., &
    beam_pol = .false., &
    file = var_str ("teslagg_500.circe"), &
    design = var_str ("TESLA/GG"))
  call data%set_generator_mode (rng_factory)
end select

call data%write (u, verbose = .true.)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe2_1"

end subroutine sf_circe2_1

```

Generator mode, unpolarized

Construct and evaluate a structure function object in generator mode.

```
<SF circe2: execute tests>+≡
  call test (sf_circe2_2, "sf_circe2_2", &
    "generator, unpolarized", &
    u, results)

<SF circe2: test declarations>+≡
  public :: sf_circe2_2

<SF circe2: tests>+≡
  subroutine sf_circe2_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(rng_factory_t), allocatable :: rng_factory
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, x_free

    write (u, "(A)")  "* Test output: sf_circe2_2"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &circe2 structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call os_data%init ()
    call model%init_qed_test ()
    call flv(1)%init (PHOTON, model)
    call flv(2)%init (PHOTON, model)
    pdg_in(1) = PHOTON
    pdg_in(2) = PHOTON

    call reset_interaction_counter ()

    allocate (circe2_data_t :: data)
    allocate (rng_test_factory_t :: rng_factory)
    select type (data)
    type is (circe2_data_t)
      call data%init (os_data, model, pdg_in, &
        sqrts = 500._default, &
        polarized = .false., &
        beam_pol = .false., &
        file = var_str ("teslagg_500_polavg.circe"), &
        design = var_str ("TESLA/GG"))
      call data%set_generator_mode (rng_factory)
    end select
```

```

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])
select type (sf_int)
type is (circe2_t)
    call sf_int%rng_obj%rng%init (3)
end select

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E,-sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Generate x"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe2_2"

end subroutine sf_circe2_2

```

Generator mode, polarized

Construct and evaluate a structure function object in generator mode.

```

<SF circe2: execute tests>+=
  call test (sf_circe2_3, "sf_circe2_3", &
    "generator, polarized", &
    u, results)

<SF circe2: test declarations>+=
  public :: sf_circe2_3

<SF circe2: tests>+=
  subroutine sf_circe2_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t), dimension(2) :: flv
    type(pdg_array_t), dimension(2) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(rng_factory_t), allocatable :: rng_factory
    class(sf_int_t), allocatable :: sf_int
    type(vector4_t) :: k1, k2
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f, x_free

    write (u, "(A)")  "* Test output: sf_circe2_3"
    write (u, "(A)")  "* Purpose: initialize and fill &
      &circe2 structure function object"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call os_data%init ()
    call model%init_qed_test ()
    call flv(1)%init (PHOTON, model)
    call flv(2)%init (PHOTON, model)
    pdg_in(1) = PHOTON
    pdg_in(2) = PHOTON

    call reset_interaction_counter ()

    allocate (circe2_data_t :: data)
    allocate (rng_test_factory_t :: rng_factory)
    select type (data)
    type is (circe2_data_t)
      call data%init (os_data, model, pdg_in, &
        sqrts = 500._default, &

```

```

        polarized = .true., &
        beam_pol = .false., &
        file = var_str ("teslagg_500.circe"), &
        design = var_str ("TESLA/GG"))
    call data%set_generator_mode (rng_factory)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1,2])
select type (sf_int)
type is (circe2_t)
    call sf_int%rng_obj%rng%init (3)
end select

write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 250
k1 = vector4_moving (E, sqrt (E**2 - flv(1)%get_mass ()**2), 3)
k2 = vector4_moving (E, -sqrt (E**2 - flv(2)%get_mass ()**2), 3)
call vector4_write (k1, u)
call vector4_write (k2, u)
call sf_int%seed_kinematics ([k1, k2])

write (u, "(A)")
write (u, "(A)")  "* Generate x"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0
rb = 0
x_free = 1
call sf_int%generate_free (r, rb, x_free)
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)

write (u, "(A,9(1x,F10.7))")  "x =", x
write (u, "(A,9(1x,F10.7))")  "xb=", xb
write (u, "(A,9(1x,F10.7))")  "f =", f
write (u, "(A,9(1x,F10.7))")  "xf=", x_free

write (u, "(A)")
write (u, "(A)")  "* Evaluate"
write (u, "(A)")

call sf_int%apply (scale = 0._default)
call sf_int%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_circe2_3"

end subroutine sf_circe2_3

```

16.14 HOPPET interface

Interface to the HOPPET wrapper necessary to perform the LO vs. NLO matching of processes containing an initial b quark.

```
<hoppet_interface.f90>≡  
  <File header>  
  
  module hoppet_interface  
    use lhpdf !NODEP!  
  
    <Standard module head>  
  
    public :: hoppet_init, hoppet_eval  
  
  contains  
  
    subroutine hoppet_init (pdf_builtin, pdf, pdf_id)  
      logical, intent(in) :: pdf_builtin  
      type(lhapdf_pdf_t), intent(inout), optional :: pdf  
      integer, intent(in), optional :: pdf_id  
      external InitForWhizard  
      call InitForWhizard (pdf_builtin, pdf, pdf_id)  
    end subroutine hoppet_init  
  
    subroutine hoppet_eval (x, q, f)  
      double precision, intent(in) :: x, q  
      double precision, intent(out) :: f(-6:6)  
      external EvalForWhizard  
      call EvalForWhizard (x, q, f)  
    end subroutine hoppet_eval  
  
  end module hoppet_interface
```

16.15 Builtin PDF sets

For convenience in order not to depend on the external package LHAPDF, we ship some PDFs with WHIZARD.

16.15.1 The module

```
<sf_pdf_builtin.f90>≡  
<File header>  
  
module sf_pdf_builtin  
  
  <Use kinds>  
    use kinds, only: double  
  <Use strings>  
    use io_units  
    use format_defs, only: FMT_17  
    use diagnostics  
    use os_interface  
    use physics_defs, only: PROTON, PHOTON, GLUON  
    use physics_defs, only: HADRON_REMNANT_SINGLET  
    use physics_defs, only: HADRON_REMNANT_TRIPLET  
    use physics_defs, only: HADRON_REMNANT_OCTET  
    use sm_qcd  
    use lorentz  
    use pdg_arrays  
    use model_data  
    use flavors  
    use colors  
    use quantum_numbers  
    use state_matrices  
    use polarizations  
    use sf_base  
    use pdf_builtin !NODEP!  
    use hoppet_interface  
  
  <Standard module head>  
  
  <SF pdf builtin: public>  
  
  <SF pdf builtin: types>  
  
  <SF pdf builtin: parameters>  
  
contains  
  
  <SF pdf builtin: procedures>  
  
end module sf_pdf_builtin
```

16.15.2 Codes for default PDF sets

```
<SF pdf builtin: parameters>≡
```



```

character(*), parameter :: PDF_BUILTIN_DEFAULT_PROTON = "CTEQ6L"
! character(*), parameter :: PDF_BUILTIN_DEFAULT_PION   = "NONE"
! character(*), parameter :: PDF_BUILTIN_DEFAULT_PHOTON = "MRST2004QEDp"

```

16.15.3 The PDF builtin data block

The data block holds the incoming flavor (which has to be proton, pion, or photon), the corresponding pointer to the global access data (1, 2, or 3), the flag `invert` which is set for an antiproton, the bounds as returned by LHAPDF for the specified set, and a mask that determines which partons will be actually in use.

```

<SF pdf builtin: public>≡
  public :: pdf_builtin_data_t

<SF pdf builtin: types>≡
  type, extends (sf_data_t) :: pdf_builtin_data_t
  private
    integer :: id = -1
    type (string_t) :: name
    class(model_data_t), pointer :: model => null ()
    type(flavor_t) :: flv_in
    logical :: invert
    logical :: has_photon
    logical :: photon
    logical, dimension(-6:6) :: mask
    logical :: mask_photon
    logical :: hoppet_b_matching = .false.
  contains
    <SF pdf builtin: pdf builtin data: TBP>
  end type pdf_builtin_data_t

```

Generate PDF data and initialize the requested set. Pion and photon PDFs are disabled at the moment until we ship appropriate structure functions. needed.

```

<SF pdf builtin: pdf builtin data: TBP>≡
  procedure :: init => pdf_builtin_data_init

<SF pdf builtin: procedures>≡
  subroutine pdf_builtin_data_init (data, &
    model, pdg_in, name, path, hoppet_b_matching)
    class(pdf_builtin_data_t), intent(out) :: data
    class(model_data_t), intent(in), target :: model
    type(pdg_array_t), intent(in) :: pdg_in
    type(string_t), intent(in) :: name
    type(string_t), intent(in) :: path
    logical, intent(in), optional :: hoppet_b_matching
    data%model => model
    if (pdg_array_get_length (pdg_in) /= 1) &
      call msg_fatal ("PDF: incoming particle must be unique")
    call data%flv_in%init (pdg_array_get (pdg_in, 1), model)
    data%mask = .true.
    data%mask_photon = .true.
    select case (pdg_array_get (pdg_in, 1))
    case (PROTON)

```

```

        data%name = var_str (PDF_BUILTIN_DEFAULT_PROTON)
        data%invert = .false.
        data%photon = .false.
    case (-PROTON)
        data%name = var_str (PDF_BUILTIN_DEFAULT_PROTON)
        data%invert = .true.
        data%photon = .false.
        ! case (PIPLUS)
        !     data%name = var_str (PDF_BUILTIN_DEFAULT_PION)
        !     data%invert = .false.
        !     data%photon = .false.
        ! case (-PIPLUS)
        !     data%name = var_str (PDF_BUILTIN_DEFAULT_PION)
        !     data%invert = .true.
        !     data%photon = .false.
        ! case (PHOTON)
        !     data%name = var_str (PDF_BUILTIN_DEFAULT_PHOTON)
        !     data%invert = .false.
        !     data%photon = .true.
    case default
        call msg_fatal ("PDF: " &
            // "incoming particle must either proton or antiproton.")
        return
    end select
    data%name = name
    data%id = pdf_get_id (data%name)
    if (data%id < 0) call msg_fatal ("unknown PDF set " // char (data%name))
    data%has_photon = pdf_provides_photon (data%id)
    if (present (hoppet_b_matching)) data%hoppet_b_matching = hoppet_b_matching
    call pdf_init (data%id, path)
    if (data%hoppet_b_matching) call hoppet_init (.true., pdf_id = data%id)
end subroutine pdf_builtin_data_init

```

Enable/disable partons explicitly. If a mask entry is true, applying the PDF will generate the corresponding flavor on output.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
    procedure :: set_mask => pdf_builtin_data_set_mask

<SF pdf builtin: procedures>+≡
    subroutine pdf_builtin_data_set_mask (data, mask)
        class(pdf_builtin_data_t), intent(inout) :: data
        logical, dimension(-6:6), intent(in) :: mask
        data%mask = mask
    end subroutine pdf_builtin_data_set_mask

```

Output.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
    procedure :: write => pdf_builtin_data_write

<SF pdf builtin: procedures>+≡
    subroutine pdf_builtin_data_write (data, unit, verbose)
        class(pdf_builtin_data_t), intent(in) :: data
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
    end subroutine pdf_builtin_data_write

```

```

integer :: u
u = given_output_unit (unit); if (u < 0) return
write (u, "(1x,A)") "PDF builtin data:"
if (data%id < 0) then
  write (u, "(3x,A)") "[undefined]"
  return
end if
write (u, "(3x,A)", advance="no") "flavor      = "
call data%flv_in%write (u); write (u, *)
write (u, "(3x,A,A)") "name      = ", char (data%name)
write (u, "(3x,A,L1)") "invert    = ", data%invert
write (u, "(3x,A,L1)") "has photon = ", data%has_photon
write (u, "(3x,A,6(1x,L1),1x,A,1x,L1,1x,A,6(1x,L1))") &
  "mask      = ", &
  data%mask(-6:-1), " ", data%mask(0), " ", data%mask(1:6)
write (u, "(3x,A,L1)") "photon mask = ", data%mask_photon
write (u, "(3x,A,L1)") "hoppet_b   = ", data%hoppet_b_matching
end subroutine pdf_builtin_data_write

```

The number of parameters is one. We do not generate transverse momentum.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
procedure :: get_n_par => pdf_builtin_data_get_n_par

<SF pdf builtin: procedures>+≡
function pdf_builtin_data_get_n_par (data) result (n)
  class(pdf_builtin_data_t), intent(in) :: data
  integer :: n
  n = 1
end function pdf_builtin_data_get_n_par

```

Return the outgoing particle PDG codes. This is based on the mask.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
procedure :: get_pdg_out => pdf_builtin_data_get_pdg_out

<SF pdf builtin: procedures>+≡
subroutine pdf_builtin_data_get_pdg_out (data, pdg_out)
  class(pdf_builtin_data_t), intent(in) :: data
  type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
  integer, dimension(:), allocatable :: pdg1
  integer :: n, np, i
  n = count (data%mask)
  np = 0; if (data%has_photon .and. data%mask_photon) np = 1
  allocate (pdg1 (n + np))
  pdg1(1:n) = pack ([i, i = -6, 6], data%mask)
  if (np == 1) pdg1(n+np) = PHOTON
  pdg_out(1) = pdg1
end subroutine pdf_builtin_data_get_pdg_out

```

Allocate the interaction record.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
procedure :: allocate_sf_int => pdf_builtin_data_allocate_sf_int

```

```

<SF pdf builtin: procedures>+≡
  subroutine pdf_builtin_data_allocate_sf_int (data, sf_int)
    class(pdf_builtin_data_t), intent(in) :: data
    class(sf_int_t), intent(inout), allocatable :: sf_int
    allocate (pdf_builtin_t :: sf_int)
  end subroutine pdf_builtin_data_allocate_sf_int

```

Return the numerical PDF set index.

```

<SF pdf builtin: pdf builtin data: TBP>+≡
  procedure :: get_pdf_set => pdf_builtin_data_get_pdf_set

<SF pdf builtin: procedures>+≡
  elemental function pdf_builtin_data_get_pdf_set (data) result (pdf_set)
    class(pdf_builtin_data_t), intent(in) :: data
    integer :: pdf_set
    pdf_set = data%id
  end function pdf_builtin_data_get_pdf_set

```

16.15.4 The PDF object

The PDF $1 \rightarrow 2$ interaction which describes the splitting of an (anti)proton into a parton and a beam remnant. We stay in the strict forward-splitting limit, but allow some invariant mass for the beam remnant such that the outgoing parton is exactly massless. For a real event, we would replace this by a parton cascade, where the outgoing partons have virtuality as dictated by parton-shower kinematics, and transverse momentum is generated.

The PDF application is a $1 \rightarrow 2$ splitting process, where the particles are ordered as (hadron, remnant, parton).

Polarization is ignored completely. The beam particle is colorless, while partons and beam remnant carry color. The remnant gets a special flavor code.

```

<SF pdf builtin: public>+≡
  public :: pdf_builtin_t

<SF pdf builtin: types>+≡
  type, extends (sf_int_t) :: pdf_builtin_t
    type(pdf_builtin_data_t), pointer :: data => null ()
    real(default) :: x = 0
    real(default) :: q = 0
  contains
    <SF pdf builtin: pdf builtin: TBP>
  end type pdf_builtin_t

```

Type string: display the chosen PDF set.

```

<SF pdf builtin: pdf builtin: TBP>≡
  procedure :: type_string => pdf_builtin_type_string

<SF pdf builtin: procedures>+≡
  function pdf_builtin_type_string (object) result (string)
    class(pdf_builtin_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "PDF builtin: " // object%data%name
    end if
  end function pdf_builtin_type_string

```

```

else
  string = "PDF builtin: [undefined]"
end if
end function pdf_builtin_type_string

```

Output. Call the interaction routine after displaying the configuration.

```

⟨SF pdf builtin: pdf builtin: TBP⟩+≡
  procedure :: write => pdf_builtin_write

⟨SF pdf builtin: procedures⟩+≡
  subroutine pdf_builtin_write (object, unit, testflag)
    class(pdf_builtin_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      if (object%status >= SF_DONE_KINEMATICS) then
        write (u, "(1x,A)") "SF parameters:"
        write (u, "(3x,A," // FMT_17 // ")") "x =", object%x
        if (object%status >= SF_FAILED_EVALUATION) then
          write (u, "(3x,A," // FMT_17 // ")") "Q =", object%q
        end if
      end if
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "PDF builtin data: [undefined]"
    end if
  end subroutine pdf_builtin_write

```

Initialize. We know that `data` will be of concrete type `sf_test_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass, but keep the radiated mass zero.

Optionally, we can provide minimum and maximum values for the momentum transfer.

```

⟨SF pdf builtin: pdf builtin: TBP⟩+≡
  procedure :: init => pdf_builtin_init

⟨SF pdf builtin: procedures⟩+≡
  subroutine pdf_builtin_init (sf_int, data)
    class(pdf_builtin_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(3) :: mask
    type(flavor_t) :: flv, flv_remnant
    type(color_t) :: col0
    type(quantum_numbers_t), dimension(3) :: qn
    integer :: i
    select type (data)
    type is (pdf_builtin_data_t)
      mask = quantum_numbers_mask (.false., .false., .true.)
      call col0%init ()

```

```

call sf_int%base_init (mask, [0._default], [0._default], [0._default])
sf_int%data => data
do i = -6, 6
  if (data%mask(i)) then
    call qn(1)%init (data%flv_in, col = col0)
    if (i == 0) then
      call flv%init (GLUON, data%model)
      call flv_remnant%init (HADRON_REMNANT_OCTET, data%model)
    else
      call flv%init (i, data%model)
      call flv_remnant%init &
        (sign (HADRON_REMNANT_TRIPLET, -i), data%model)
    end if
    call qn(2)%init ( &
      flv = flv_remnant, col = color_from_flavor (flv_remnant, 1))
    call qn(2)%tag_radiated ()
    call qn(3)%init ( &
      flv = flv, col = color_from_flavor (flv, 1, reverse=.true.))
    call sf_int%add_state (qn)
  end if
end do
if (data%has_photon .and. data%mask_photon) then
  call flv%init (PHOTON, data%model)
  call flv_remnant%init (HADRON_REMNANT_SINGLET, data%model)
  call qn(2)%init (flv = flv_remnant, &
    col = color_from_flavor (flv_remnant, 1))
  call qn(2)%tag_radiated ()
  call qn(3)%init (flv = flv, &
    col = color_from_flavor (flv, 1, reverse = .true.))
  call sf_int%add_state (qn)
end if
call sf_int%freeze ()
call sf_int%set_incoming ([1])
call sf_int%set_radiated ([2])
call sf_int%set_outgoing ([3])
sf_int%status = SF_INITIAL
end select
end subroutine pdf_builtin_init

```

16.15.5 Kinematics

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, we are asked to provide an efficient mapping. For the test case, we set $x = r^2$ and consequently $f(r) = 2r$.

(SF pdf builtin: pdf builtin: TBP) +≡

```
procedure :: complete_kinematics => pdf_builtin_complete_kinematics
```

(SF pdf builtin: procedures) +≡

```

subroutine pdf_builtin_complete_kinematics (sf_int, x, xb, f, r, rb, map)
  class(pdf_builtin_t), intent(inout) :: sf_int
  real(default), dimension(:), intent(out) :: x
  real(default), dimension(:), intent(out) :: xb

```

```

real(default), intent(out) :: f
real(default), dimension(:), intent(in) :: r
real(default), dimension(:), intent(in) :: rb
logical, intent(in) :: map
if (map) then
  call msg_fatal ("PDF builtin: map flag not supported")
else
  x(1) = r(1)
  xb(1) = rb(1)
  f = 1
end if
call sf_int%split_momentum (x, xb)
select case (sf_int%status)
case (SF_DONE_KINEMATICS)
  sf_int%x = x(1)
case (SF_FAILED_KINEMATICS)
  sf_int%x = 0
  f = 0
end select
end subroutine pdf_builtin_complete_kinematics

```

Overriding the default method: we compute the x value from the momentum configuration. In this specific case, we also set the internally stored x value, so it can be used in the following routine.

```

⟨SF pdf builtin: pdf builtin: TBP⟩+≡
  procedure :: recover_x => pdf_builtin_recover_x

⟨SF pdf builtin: procedures⟩+≡
  subroutine pdf_builtin_recover_x (sf_int, x, xb, x_free)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb, x_free)
    sf_int%x = x(1)
  end subroutine pdf_builtin_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

⟨SF pdf builtin: pdf builtin: TBP⟩+≡
  procedure :: inverse_kinematics => pdf_builtin_inverse_kinematics

⟨SF pdf builtin: procedures⟩+≡
  subroutine pdf_builtin_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(in) :: x
    real(default), dimension(:), intent(in) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(out) :: r
    real(default), dimension(:), intent(out) :: rb
    logical, intent(in) :: map
    logical, intent(in), optional :: set_momenta

```

```

logical :: set_mom
set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
if (map) then
  call msg_fatal ("PDF builtin: map flag not supported")
else
  r(1) = x(1)
  rb(1)= xb(1)
  f = 1
end if
if (set_mom) then
  call sf_int%split_momentum (x, xb)
  select case (sf_int%status)
  case (SF_FAILED_KINEMATICS); f = 0
  end select
end if
end subroutine pdf_builtin_inverse_kinematics

```

16.15.6 Structure function

Once the scale is also known, we can actually call the PDF and set the values. Contrary to LHAPDF, the wrapper already takes care of adjusting to the x and Q bounds. Account for the Jacobian.

The parameter `negative_sf` is necessary to determine if we allow for negative PDF values. The class `rescale` gives rescaling prescription for NLO convolution of the structure function in combination with `i_sub`.

```

⟨SF pdf builtin: pdf builtin: TBP⟩+≡
  procedure :: apply => pdf_builtin_apply

⟨SF pdf builtin: procedures⟩+≡
  subroutine pdf_builtin_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(pdf_builtin_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default), dimension(-6:6) :: ff
    real(double), dimension(-6:6) :: ff_dbl
    real(default) :: x, fph
    real(double) :: xx, qq
    complex(default), dimension(:), allocatable :: fc
    integer :: i, j_sub, i_sub_opt
    logical :: negative_sf_opt
    i_sub_opt = 0; if (present (i_sub)) i_sub_opt = i_sub
    negative_sf_opt = .false.; if (present(negative_sf)) negative_sf_opt = negative_sf
    associate (data => sf_int%data)
      sf_int%q = scale
      x = sf_int%x
      if (present (rescale)) call rescale%apply (x)
      if (debug2_active (D_BEAMS)) then
        call msg_debug2 (D_BEAMS, "pdf_builtin_apply")
        call msg_debug2 (D_BEAMS, "rescale: ", present(rescale))
        call msg_debug2 (D_BEAMS, "i_sub: ", i_sub_opt)
      end if
    end associate
  end subroutine pdf_builtin_apply

```



```

        call msg_debug2 (D_BEAMS, "x: ", x)
    end if
    xx = x
    qq = scale
    if (data%invert) then
        if (data%has_photon) then
            call pdf_evolve (data%id, x, scale, ff(6:-6:-1), fph)
        else
            if (data%hoppet_b_matching) then
                call hoppet_eval (xx, qq, ff_dbl(6:-6:-1))
                ff = ff_dbl
            else
                call pdf_evolve (data%id, x, scale, ff(6:-6:-1))
            end if
        end if
    else
        if (data%has_photon) then
            call pdf_evolve (data%id, x, scale, ff, fph)
        else
            if (data%hoppet_b_matching) then
                call hoppet_eval (xx, qq, ff_dbl)
                ff = ff_dbl
            else
                call pdf_evolve (data%id, x, scale, ff)
            end if
        end if
    end if
    if (data%has_photon) then
        allocate (fc (count ([data%mask, data%mask_photon])))
        if (negative_sf_opt) then
            fc = pack ([ff, fph], [data%mask, data%mask_photon])
        else
            fc = max( pack ([ff, fph], [data%mask, data%mask_photon]), 0._default)
        end if
    else
        allocate (fc (count (data%mask)))
        if (negative_sf_opt) then
            fc = pack (ff, data%mask)
        else
            fc = max( pack (ff, data%mask), 0._default)
        end if
    end if
    end associate
    if (debug_active (D_BEAMS)) print *, 'Set pdfs: ', real (fc)
    call sf_int%set_matrix_element (fc, [(i_sub_opt * size(fc) + i, i = 1, size(fc))])
    sf_int%status = SF_EVALUATED
end subroutine pdf_builtin_apply

```

16.15.7 Strong Coupling

Since the PDF codes provide a function for computing the running α_s value, we make this available as an implementation of the abstract `alpha_qcd_t` type,

which is used for matrix element evaluation.

```

<SF pdf builtin: public>+≡
    public :: alpha_qcd_pdf_builtin_t

<SF pdf builtin: types>+≡
    type, extends (alpha_qcd_t) :: alpha_qcd_pdf_builtin_t
    type(string_t) :: pdfset_name
    integer :: pdfset_id = -1
    contains
    <SF pdf builtin: alpha qcd: TBP>
    end type alpha_qcd_pdf_builtin_t

```

Output.

```

<SF pdf builtin: alpha qcd: TBP>≡
    procedure :: write => alpha_qcd_pdf_builtin_write

<SF pdf builtin: procedures>+≡
    subroutine alpha_qcd_pdf_builtin_write (object, unit)
        class(alpha_qcd_pdf_builtin_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A)") "QCD parameters (pdf_builtin):"
        write (u, "(5x,A,A)") "PDF set = ", char (object%pdfset_name)
        write (u, "(5x,A,I0)") "PDF ID = ", object%pdfset_id
    end subroutine alpha_qcd_pdf_builtin_write

```

Calculation: the numeric ID selects the correct PDF set, which must be properly initialized.

```

<SF pdf builtin: alpha qcd: TBP>+≡
    procedure :: get => alpha_qcd_pdf_builtin_get

<SF pdf builtin: procedures>+≡
    function alpha_qcd_pdf_builtin_get (alpha_qcd, scale) result (alpha)
        class(alpha_qcd_pdf_builtin_t), intent(in) :: alpha_qcd
        real(default), intent(in) :: scale
        real(default) :: alpha
        alpha = pdf_alphas (alpha_qcd%pdfset_id, scale)
    end function alpha_qcd_pdf_builtin_get

```

Initialization. We need to access the global initialization status.

```

<SF pdf builtin: alpha qcd: TBP>+≡
    procedure :: init => alpha_qcd_pdf_builtin_init

<SF pdf builtin: procedures>+≡
    subroutine alpha_qcd_pdf_builtin_init (alpha_qcd, name, path)
        class(alpha_qcd_pdf_builtin_t), intent(out) :: alpha_qcd
        type(string_t), intent(in) :: name
        type(string_t), intent(in) :: path
        alpha_qcd%pdfset_name = name
        alpha_qcd%pdfset_id = pdf_get_id (name)
        if (alpha_qcd%pdfset_id < 0) &
            call msg_fatal ("QCD parameter initialization: PDF set " &
                // char (name) // " is unknown")
    end subroutine alpha_qcd_pdf_builtin_init

```

```

        call pdf_init (alpha_qcd%pdfset_id, path)
    end subroutine alpha_qcd_pdf_builtin_init

```

16.15.8 Unit tests

Test module, followed by the corresponding implementation module.

```

<sf_pdf_builtin_ut.f90>≡
  <File header>

  module sf_pdf_builtin_ut
    use unit_tests
    use sf_pdf_builtin_ut

    <Standard module head>

    <SF pdf builtin: public test>

    contains

    <SF pdf builtin: test driver>

  end module sf_pdf_builtin_ut

<sf_pdf_builtin_util.f90>≡
  <File header>

  module sf_pdf_builtin_util

    <Use kinds>
    <Use strings>
    use os_interface
    use physics_defs, only: PROTON
    use sm_qcd
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data
    use sf_base

    use sf_pdf_builtin

    <Standard module head>

    <SF pdf builtin: test declarations>

    contains

    <SF pdf builtin: tests>

  end module sf_pdf_builtin_util

```

API: driver for the unit tests below.

```
<SF pdf builtin: public test>≡
  public :: sf_pdf_builtin_test

<SF pdf builtin: test driver>≡
  subroutine sf_pdf_builtin_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <SF pdf builtin: execute tests>
  end subroutine sf_pdf_builtin_test
```

Test structure function data

Construct and display a test structure function data object.

```
<SF pdf builtin: execute tests>≡
  call test (sf_pdf_builtin_1, "sf_pdf_builtin_1", &
    "structure function configuration", &
    u, results)

<SF pdf builtin: test declarations>≡
  public :: sf_pdf_builtin_1

<SF pdf builtin: tests>≡
  subroutine sf_pdf_builtin_1 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(pdg_array_t) :: pdg_in
    type(pdg_array_t), dimension(1) :: pdg_out
    integer, dimension(:), allocatable :: pdg1
    class(sf_data_t), allocatable :: data
    type(string_t) :: name

    write (u, "(A)")  "* Test output: sf_pdf_builtin_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &test structure function data"
    write (u, "(A)")

    write (u, "(A)")  "* Create empty data object"
    write (u, "(A)")

    call os_data%init ()

    call model%init_sm_test ()
    pdg_in = PROTON

    allocate (pdf_builtin_data_t :: data)
    call data%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize"
    write (u, "(A)")

    name = "CTEQ6L"
```

```

select type (data)
type is (pdf_builtin_data_t)
  call data%init (model, pdg_in, name, &
    os_data%pdf_builtin_datapath)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)") "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))") pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_pdf_builtin_1"

end subroutine sf_pdf_builtin_1

```

Test and probe structure function

Construct and display a structure function object based on the PDF builtin structure function.

```

<SF pdf builtin: execute tests>+≡
  call test (sf_pdf_builtin_2, "sf_pdf_builtin_2", &
    "structure function instance", &
    u, results)

<SF pdf builtin: test declarations>+≡
  public :: sf_pdf_builtin_2

<SF pdf builtin: tests>+≡
  subroutine sf_pdf_builtin_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    class(sf_int_t), allocatable :: sf_int
    type(string_t) :: name
    type(vector4_t) :: k
    type(vector4_t), dimension(2) :: q
    real(default) :: E
    real(default), dimension(:), allocatable :: r, rb, x, xb
    real(default) :: f

    write (u, "(A)")  "* Test output: sf_pdf_builtin_2"
    write (u, "(A)")  "* Purpose: initialize and fill &

```

```

        &test structure function object"
write (u, "(A)")

write (u, "(A)")  "* Initialize configuration data"
write (u, "(A)")

call os_data%init ()
call model%init_sm_test ()
call flv%init (PROTON, model)
pdg_in = PROTON

call reset_interaction_counter ()

name = "CTEQ6L"

allocate (pdf_builtin_data_t :: data)
select type (data)
type is (pdf_builtin_data_t)
    call data%init (model, pdg_in, name, &
        os_data%pdf_builtin_datapath)
end select

write (u, "(A)")  "* Initialize structure-function object"
write (u, "(A)")

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize incoming momentum with E=500"
write (u, "(A)")
E = 500
k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
call vector4_write (k, u)
call sf_int%seed_kinematics ([k])

write (u, "(A)")
write (u, "(A)")  "* Set kinematics for x=0.5"
write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.5_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")

```

```

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)")  "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)")  "* Evaluate for Q = 100 GeV"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale = 100._default)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_pdf_builtin_2"

end subroutine sf_pdf_builtin_2

```

Strong Coupling

Test α_s as an implementation of the `alpha_qcd.t` abstract type.

```

<SF pdf builtin: execute tests>+≡
  call test (sf_pdf_builtin_3, "sf_pdf_builtin_3", &
    "running alpha_s", &
    u, results)

<SF pdf builtin: test declarations>+≡
  public :: sf_pdf_builtin_3

```

```

<SF pdf builtin: tests>+≡
subroutine sf_pdf_builtin_3 (u)
  integer, intent(in) :: u
  type(os_data_t) :: os_data
  type(qcd_t) :: qcd
  type(string_t) :: name

  write (u, "(A)")  "* Test output: sf_pdf_builtin_3"
  write (u, "(A)")  "* Purpose: initialize and evaluate alpha_s"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize configuration data"
  write (u, "(A)")

  call os_data%init ()

  name = "CTEQ6L"

  write (u, "(A)")  "* Initialize qcd object"
  write (u, "(A)")

  allocate (alpha_qcd_pdf_builtin_t :: qcd%alpha)
  select type (alpha => qcd%alpha)
  type is (alpha_qcd_pdf_builtin_t)
    call alpha%init (name, os_data%pdf_builtin_datapath)
  end select
  call qcd%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Evaluate for Q = 100"
  write (u, "(A)")

  write (u, "(1x,A,F8.5)")  "alpha = ", qcd%alpha%get (100._default)

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: sf_pdf_builtin_3"

end subroutine sf_pdf_builtin_3

```


16.16 LHAPDF

Parton distribution functions (PDFs) are available via an interface to the LHAPDF standard library.

16.16.1 The module

```
<sf_lhapdf.f90>≡  
<File header>  
  
module sf_lhapdf  
  
  <Use kinds>  
  <Use strings>  
  use format_defs, only: FMT_17, FMT_19  
  use io_units  
  use system_dependencies, only: LHAPDF_PDFSETS_PATH  
  use system_dependencies, only: LHAPDF5_AVAILABLE  
  use system_dependencies, only: LHAPDF6_AVAILABLE  
  use diagnostics  
  use physics_defs, only: PROTON, PHOTON, PIPLUS, GLUON  
  use physics_defs, only: HADRON_REMNANT_SINGLET  
  use physics_defs, only: HADRON_REMNANT_TRIPLET  
  use physics_defs, only: HADRON_REMNANT_OCTET  
  use lorentz  
  use sm_qcd  
  use pdg_arrays  
  use model_data  
  use flavors  
  use colors  
  use quantum_numbers  
  use state_matrices  
  use polarizations  
  use sf_base  
  use lhapdf !NODEP!  
  use hoppet_interface  
  
  <Standard module head>  
  
  <SF lhapdf: public>  
  
  <SF lhapdf: types>  
  
  <SF lhapdf: parameters>  
  
  <SF lhapdf: variables>  
  
  <SF lhapdf: interfaces>  
  
contains  
  
  <SF lhapdf: procedures>  
  
end module sf_lhapdf
```

16.16.2 Codes for default PDF sets

The default PDF for protons set is chosen to be CTEQ6ll (LO fit with LO α_s).

```
<SF lhpdf: parameters>≡  
  character(*), parameter :: LHAPDF5_DEFAULT_PROTON = "cteq6ll.LHpdf"  
  character(*), parameter :: LHAPDF5_DEFAULT_PION   = "ABFKWPI.LHgrid"  
  character(*), parameter :: LHAPDF5_DEFAULT_PHOTON = "GSG960.LHgrid"  
  character(*), parameter :: LHAPDF6_DEFAULT_PROTON = "CT10"
```

16.16.3 LHAPDF library interface

Here we specify explicit interfaces for all LHAPDF routines that we use below.

```
<SF lhpdf: interfaces>≡  
  interface  
    subroutine InitPDFsetM (set, file)  
      integer, intent(in) :: set  
      character(*), intent(in) :: file  
    end subroutine InitPDFsetM  
  end interface  
  
<SF lhpdf: interfaces>+≡  
  interface  
    subroutine InitPDFM (set, mem)  
      integer, intent(in) :: set, mem  
    end subroutine InitPDFM  
  end interface  
  
<SF lhpdf: interfaces>+≡  
  interface  
    subroutine numberPDFM (set, n_members)  
      integer, intent(in) :: set  
      integer, intent(out) :: n_members  
    end subroutine numberPDFM  
  end interface  
  
<SF lhpdf: interfaces>+≡  
  interface  
    subroutine evolvePDFM (set, x, q, ff)  
      integer, intent(in) :: set  
      double precision, intent(in) :: x, q  
      double precision, dimension(-6:6), intent(out) :: ff  
    end subroutine evolvePDFM  
  end interface  
  
<SF lhpdf: interfaces>+≡  
  interface  
    subroutine evolvePDFphotonM (set, x, q, ff, fphot)  
      integer, intent(in) :: set  
      double precision, intent(in) :: x, q  
      double precision, dimension(-6:6), intent(out) :: ff  
      double precision, intent(out) :: fphot  
    end subroutine evolvePDFphotonM
```

```

end interface

<SF lhpdf: interfaces>+≡
interface
  subroutine evolvePDFpM (set, x, q, s, scheme, ff)
    integer, intent(in) :: set
    double precision, intent(in) :: x, q, s
    integer, intent(in) :: scheme
    double precision, dimension(-6:6), intent(out) :: ff
  end subroutine evolvePDFpM
end interface

<SF lhpdf: interfaces>+≡
interface
  subroutine GetXminM (set, mem, xmin)
    integer, intent(in) :: set, mem
    double precision, intent(out) :: xmin
  end subroutine GetXminM
end interface

<SF lhpdf: interfaces>+≡
interface
  subroutine GetXmaxM (set, mem, xmax)
    integer, intent(in) :: set, mem
    double precision, intent(out) :: xmax
  end subroutine GetXmaxM
end interface

<SF lhpdf: interfaces>+≡
interface
  subroutine GetQ2minM (set, mem, q2min)
    integer, intent(in) :: set, mem
    double precision, intent(out) :: q2min
  end subroutine GetQ2minM
end interface

<SF lhpdf: interfaces>+≡
interface
  subroutine GetQ2maxM (set, mem, q2max)
    integer, intent(in) :: set, mem
    double precision, intent(out) :: q2max
  end subroutine GetQ2maxM
end interface

<SF lhpdf: interfaces>+≡
interface
  function has_photon () result(flag)
    logical :: flag
  end function has_photon
end interface

```

16.16.4 The LHAPDF status

This type holds the initialization status of the LHAPDF system. Entry 1 is for proton PDFs, entry 2 for pion PDFs, entry 3 for photon PDFs.

Since it is connected to the external LHAPDF library, this is a truly global object. We implement it as a private module variable. To access it from elsewhere, the caller has to create and initialize an object of type `lhapdf_status_t`, which acts as a proxy.

```

<SF lhapdf: types>≡
  type :: lhapdf_global_status_t
    private
      logical, dimension(3) :: initialized = .false.
    end type lhapdf_global_status_t

<SF lhapdf: variables>≡
  type(lhapdf_global_status_t), save :: lhapdf_global_status

<SF lhapdf: procedures>≡
  function lhapdf_global_status_is_initialized (set) result (flag)
    logical :: flag
    integer, intent(in), optional :: set
    if (present (set)) then
      select case (set)
        case (1:3);   flag = lhapdf_global_status%initialized(set)
        case default; flag = .false.
      end select
    else
      flag = any (lhapdf_global_status%initialized)
    end if
  end function lhapdf_global_status_is_initialized

<SF lhapdf: procedures>+≡
  subroutine lhapdf_global_status_set_initialized (set)
    integer, intent(in) :: set
    lhapdf_global_status%initialized(set) = .true.
  end subroutine lhapdf_global_status_set_initialized

```

This is the only public procedure, it tells the system to forget about previous initialization, allowing for changing the chosen PDF set. Note that such a feature works only if the global program flow is serial, so no two distinct sets are accessed simultaneously. But this applies to LHAPDF anyway.

```

<SF lhapdf: public>≡
  public :: lhapdf_global_reset

<SF lhapdf: procedures>+≡
  subroutine lhapdf_global_reset ()
    lhapdf_global_status%initialized = .false.
  end subroutine lhapdf_global_reset

```

16.16.5 LHAPDF initialization

Before using LHAPDF, we have to initialize it with a particular data set and member. This applies not just if we use structure functions, but also if we just use an α_s formula. The integer `set` should be 1 for proton, 2 for pion, and 3 for photon, but this is just convention.

It appears as if LHAPDF does not allow for multiple data sets being used concurrently (?), so multi-threaded usage with different sets (e.g., a scan) is excluded. The current setup with a global flag that indicates initialization is fine as long as Whizard itself is run in serial mode at the Sindarin level. If we introduce multithreading in any form from Sindarin, we have to rethink the implementation of the LHAPDF interface. (The same considerations apply to builtin PDFs.)

If the particular set has already been initialized, do nothing. This implies that whenever we want to change the setup for a particular set, we have to reset the LHAPDF status. `lhpdf_initialize` has an obvious name clash with `lhpdf_init`, the reason it works for `pdf.builtin` is that these things are outsourced to a separate module (inc. `lhpdf.status` etc.).

```

<SF lhpdf: public>+≡
  public :: lhpdf_initialize

<SF lhpdf: procedures>+≡
  subroutine lhpdf_initialize (set, prefix, file, member, pdf, b_match)
    integer, intent(in) :: set
    type(string_t), intent(inout) :: prefix
    type(string_t), intent(inout) :: file
    type(lhpdf_pdf_t), intent(inout), optional :: pdf
    integer, intent(inout) :: member
    logical, intent(in), optional :: b_match
    if (prefix == "") prefix = LHAPDF_PDFSETS_PATH
    if (LHAPDF5_AVAILABLE) then
      if (lhpdf_global_status_is_initialized (set)) return
      if (file == "") then
        select case (set)
          case (1); file = LHAPDF5_DEFAULT_PROTON
          case (2); file = LHAPDF5_DEFAULT_PION
          case (3); file = LHAPDF5_DEFAULT_PHOTON
        end select
      end if
      if (data_file_exists (prefix // "/" // file)) then
        call InitPDFsetM (set, char (prefix // "/" // file))
      else
        call msg_fatal ("LHAPDF: Data file '" &
          // char (file) // "' not found in '" // char (prefix) // "'")
        return
      end if
      if (.not. dataset_member_exists (set, member)) then
        call msg_error (" LHAPDF: Chosen member does not exist for set '" &
          // char (file) // "', using default.")
        member = 0
      end if
      call InitPDFM (set, member)
    else if (LHAPDF6_AVAILABLE) then

```

```

! TODO: (bcn 2015-07-07) we should have a closer look why this global
!           check must not be executed
!   if (lhpdf_global_status_is_initialized (set) .and. &
!       pdf%is_associated ()) return
!   if (file == "") then
!       select case (set)
!       case (1); file = LHAPDF6_DEFAULT_PROTON
!       case (2);
!           call msg_fatal ("LHAPDF6: no pion PDFs supported")
!       case (3);
!           call msg_fatal ("LHAPDF6: no photon PDFs supported")
!       end select
!   end if
!   if (data_file_exists (prefix // "/" // file // "/" // file // ".info")) then
!       call pdf%init (char (file), member)
!   else
!       call msg_fatal ("LHAPDF: Data file '" &
!           // char (file) // "' not found in '" // char (prefix) // "'.")
!       return
!   end if
! end if
! if (present (b_match)) then
!   if (b_match) then
!     if (LHAPDF5_AVAILABLE) then
!       call hoppet_init (.false.)
!     else if (LHAPDF6_AVAILABLE) then
!       call hoppet_init (.false., pdf)
!     end if
!   end if
! end if
! call lhpdf_global_status_set_initialized (set)
contains
function data_file_exists (fq_name) result (exist)
  type(string_t), intent(in) :: fq_name
  logical :: exist
  inquire (file = char(fq_name), exist = exist)
end function data_file_exists
function dataset_member_exists (set, member) result (exist)
  integer, intent(in) :: set, member
  logical :: exist
  integer :: n_members
  call numberPDFM (set, n_members)
  exist = member >= 0 .and. member <= n_members
end function dataset_member_exists
end subroutine lhpdf_initialize

```

16.16.6 Kinematics

Set kinematics. If `map` is unset, the r and x values coincide, and the Jacobian $f(r)$ is trivial.

If `map` is set, we are asked to provide an efficient mapping. For the test case, we set $x = r^2$ and consequently $f(r) = 2r$.

```

<SF lhpdf: lhpdf: TBP>≡
  procedure :: complete_kinematics => lhpdf_complete_kinematics

<SF lhpdf: procedures>+≡
  subroutine lhpdf_complete_kinematics (sf_int, x, xb, f, r, rb, map)
    class(lhpdf_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(out) :: f
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), intent(in) :: rb
    logical, intent(in) :: map
    if (map) then
      call msg_fatal ("LHAPDF: map flag not supported")
    else
      x(1) = r(1)
      xb(1) = rb(1)
      f = 1
    end if
    call sf_int%split_momentum (x, xb)
    select case (sf_int%status)
    case (SF_DONE_KINEMATICS)
      sf_int%x = x(1)
    case (SF_FAILED_KINEMATICS)
      sf_int%x = 0
      f = 0
    end select
  end subroutine lhpdf_complete_kinematics

```

Overriding the default method: we compute the x value from the momentum configuration. In this specific case, we also set the internally stored x value, so it can be used in the following routine.

```

<SF lhpdf: lhpdf: TBP>+≡
  procedure :: recover_x => lhpdf_recover_x

<SF lhpdf: procedures>+≡
  subroutine lhpdf_recover_x (sf_int, x, xb, x_free)
    class(lhpdf_t), intent(inout) :: sf_int
    real(default), dimension(:), intent(out) :: x
    real(default), dimension(:), intent(out) :: xb
    real(default), intent(inout), optional :: x_free
    call sf_int%base_recover_x (x, xb, x_free)
    sf_int%x = x(1)
  end subroutine lhpdf_recover_x

```

Compute inverse kinematics. Here, we start with the x array and compute the “input” r values and the Jacobian f . After this, we can set momenta by the same formula as for normal kinematics.

```

<SF lhpdf: lhpdf: TBP>+≡
  procedure :: inverse_kinematics => lhpdf_inverse_kinematics

<SF lhpdf: procedures>+≡
  subroutine lhpdf_inverse_kinematics (sf_int, x, xb, f, r, rb, map, set_momenta)
    class(lhpdf_t), intent(inout) :: sf_int

```

```

real(default), dimension(:), intent(in) :: x
real(default), dimension(:), intent(in) :: xb
real(default), intent(out) :: f
real(default), dimension(:), intent(out) :: r
real(default), dimension(:), intent(out) :: rb
logical, intent(in) :: map
logical, intent(in), optional :: set_momenta
logical :: set_mom
set_mom = .false.; if (present (set_momenta)) set_mom = set_momenta
if (map) then
    call msg_fatal ("LHAPDF: map flag not supported")
else
    r(1) = x(1)
    rb(1) = xb(1)
    f = 1
end if
if (set_mom) then
    call sf_int%split_momentum (x, xb)
    select case (sf_int%status)
    case (SF_FAILED_KINEMATICS); f = 0
    end select
end if
end subroutine lhapdf_inverse_kinematics

```

16.16.7 The LHAPDF data block

The data block holds the incoming flavor (which has to be proton, pion, or photon), the corresponding pointer to the global access data (1, 2, or 3), the flag `invert` which is set for an antiproton, the bounds as returned by LHAPDF for the specified set, and a mask that determines which partons will be actually in use.

```

<SF lhapdf: public>+≡
    public :: lhapdf_data_t

<SF lhapdf: types>+≡
    type, extends (sf_data_t) :: lhapdf_data_t
    private
    type(string_t) :: prefix
    type(string_t) :: file
    type(lhapdf_pdf_t) :: pdf
    integer :: member = 0
    class(model_data_t), pointer :: model => null ()
    type(flavor_t) :: flv_in
    integer :: set = 0
    logical :: invert = .false.
    logical :: photon = .false.
    logical :: has_photon = .false.
    integer :: photon_scheme = 0
    real(default) :: xmin = 0, xmax = 0
    real(default) :: qmin = 0, qmax = 0
    logical, dimension(-6:6) :: mask = .true.
    logical :: mask_photon = .true.

```



```

        logical :: hoppet_b_matching = .false.
contains
    <SF lhpdf: lhpdf data: TBP>
end type lhpdf_data_t

```

Generate PDF data. This is provided as a function, but it has the side-effect of initializing the requested PDF set. A finalizer is not needed.

The library uses double precision, so since the default precision may be extended or quadruple, we use auxiliary variables for type casting.

```

<SF lhpdf: lhpdf data: TBP>≡
    procedure :: init => lhpdf_data_init

<SF lhpdf: procedures>+≡
    subroutine lhpdf_data_init &
        (data, model, pdg_in, prefix, file, member, photon_scheme, &
         hoppet_b_matching)
        class(lhpdf_data_t), intent(out) :: data
        class(model_data_t), intent(in), target :: model
        type(pdg_array_t), intent(in) :: pdg_in
        type(string_t), intent(in), optional :: prefix, file
        integer, intent(in), optional :: member
        integer, intent(in), optional :: photon_scheme
        logical, intent(in), optional :: hoppet_b_matching
        double precision :: xmin, xmax, q2min, q2max
        external :: InitPDFsetM, InitPDFM, numberPDFM
        external :: GetXminM, GetXmaxM, GetQ2minM, GetQ2maxM
        if (.not. LHAPDF5_AVAILABLE .and. .not. LHAPDF6_AVAILABLE) then
            call msg_fatal ("LHAPDF requested but library is not linked")
            return
        end if
        data%model => model
        if (pdg_array_get_length (pdg_in) /= 1) &
            call msg_fatal ("PDF: incoming particle must be unique")
        call data%flv_in%init (pdg_array_get (pdg_in, 1), model)
        select case (pdg_array_get (pdg_in, 1))
        case (PROTON)
            data%set = 1
        case (-PROTON)
            data%set = 1
            data%invert = .true.
        case (PIPLUS)
            data%set = 2
        case (-PIPLUS)
            data%set = 2
            data%invert = .true.
        case (PHOTON)
            data%set = 3
            data%photon = .true.
            if (present (photon_scheme)) data%photon_scheme = photon_scheme
        case default
            call msg_fatal (" LHAPDF: " &
                // "incoming particle must be (anti)proton, pion, or photon.")
            return
        end select
    end subroutine

```

```

if (present (prefix)) then
  data%prefix = prefix
else
  data%prefix = ""
end if
if (present (file)) then
  data%file = file
else
  data%file = ""
end if
if (present (hoppet_b_matching)) data%hoppet_b_matching = hoppet_b_matching
if (LHAPDF5_AVAILABLE) then
  call lhpdf_initialize (data%set, &
    data%prefix, data%file, data%member, &
    b_match = data%hoppet_b_matching)
  call GetXminM (data%set, data%member, xmin)
  call GetXmaxM (data%set, data%member, xmax)
  call GetQ2minM (data%set, data%member, q2min)
  call GetQ2maxM (data%set, data%member, q2max)
  data%xmin = xmin
  data%xmax = xmax
  data%qmin = sqrt (q2min)
  data%qmax = sqrt (q2max)
  data%has_photon = has_photon ()
else if (LHAPDF6_AVAILABLE) then
  call lhpdf_initialize (data%set, &
    data%prefix, data%file, data%member, &
    data%pdf, data%hoppet_b_matching)
  data%xmin = data%pdf%getxmin ()
  data%xmax = data%pdf%getxmax ()
  data%qmin = sqrt(data%pdf%getq2min ())
  data%qmax = sqrt(data%pdf%getq2max ())
  data%has_photon = data%pdf%has_photon ()
end if
end subroutine lhpdf_data_init

```

Enable/disable partons explicitly. If a mask entry is true, applying the PDF will generate the corresponding flavor on output.

```

<LHAPDF: lhpdf data: TBP>≡
  procedure :: set_mask => lhpdf_data_set_mask

<LHAPDF: procedures>≡
  subroutine lhpdf_data_set_mask (data, mask)
    class(lhpdf_data_t), intent(inout) :: data
    logical, dimension(-6:6), intent(in) :: mask
    data%mask = mask
  end subroutine lhpdf_data_set_mask

```

Return the public part of the data set.

```

<LHAPDF: public>≡
  public :: lhpdf_data_get_public_info

<LHAPDF: procedures>+≡
  subroutine lhpdf_data_get_public_info &

```

```

        (data, lhapdf_dir, lhapdf_file, lhapdf_member)
type(lhapdf_data_t), intent(in) :: data
type(string_t), intent(out) :: lhapdf_dir, lhapdf_file
integer, intent(out) :: lhapdf_member
lhapdf_dir = data%prefix
lhapdf_file = data%file
lhapdf_member = data%member
end subroutine lhapdf_data_get_public_info

```

Return the number of the member of the data set.

```

<LHAPDF: public>+≡
    public :: lhapdf_data_get_set

<LHAPDF: procedures>+≡
    function lhapdf_data_get_set(data) result(set)
        type(lhapdf_data_t), intent(in) :: data
        integer :: set
        set = data%set
    end function lhapdf_data_get_set

```

Output

```

<SF lhapdf: lhapdf data: TBP>+≡
    procedure :: write => lhapdf_data_write

<SF lhapdf: procedures>+≡
    subroutine lhapdf_data_write (data, unit, verbose)
        class(lhapdf_data_t), intent(in) :: data
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        logical :: verb
        integer :: u
        if (present (verbose)) then
            verb = verbose
        else
            verb = .false.
        end if
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1x,A)") "LHAPDF data:"
        if (data%set /= 0) then
            write (u, "(3x,A)", advance="no") "flavor          = "
            call data%flv_in%write (u); write (u, *)
            if (verb) then
                write (u, "(3x,A,A)"          " prefix          = ", char (data%prefix)
            else
                write (u, "(3x,A,A)"          " prefix          = ", &
                    " <empty (non-verbose version)>")
            end if
            write (u, "(3x,A,A)"          " file              = ", char (data%file)
            write (u, "(3x,A,I3)"          " member             = ", data%member
            write (u, "(3x,A," // FMT_19 // ")") " x(min)              = ", data%xmin
            write (u, "(3x,A," // FMT_19 // ")") " x(max)              = ", data%xmax
            write (u, "(3x,A," // FMT_19 // ")") " Q(min)              = ", data%qmin
            write (u, "(3x,A," // FMT_19 // ")") " Q(max)              = ", data%qmax
            write (u, "(3x,A,L1)"          " invert              = ", data%invert

```

```

        if (data%photon) write (u, "(3x,A,I3)") &
            " IP2 (scheme) = ", data%photon_scheme
        write (u, "(3x,A,6(1x,L1),1x,A,1x,L1,1x,A,6(1x,L1))") &
            " mask = ", &
            data%mask(-6:-1), "*", data%mask(0), "*", data%mask(1:6)
        write (u, "(3x,A,L1)") " photon mask = ", data%mask_photon
        if (data%set == 1) write (u, "(3x,A,L1)") &
            " hoppet_b = ", data%hoppet_b_matching
    else
        write (u, "(3x,A)") "[undefined]"
    end if
end subroutine lhpdf_data_write

```

The number of parameters is one. We do not generate transverse momentum.

```

<SF lhpdf: lhpdf data: TBP>+≡
    procedure :: get_n_par => lhpdf_data_get_n_par

<SF lhpdf: procedures>+≡
    function lhpdf_data_get_n_par (data) result (n)
        class(lhpdf_data_t), intent(in) :: data
        integer :: n
        n = 1
    end function lhpdf_data_get_n_par

```

Return the outgoing particle PDG codes. This is based on the mask.

```

<SF lhpdf: lhpdf data: TBP>+≡
    procedure :: get_pdg_out => lhpdf_data_get_pdg_out

<SF lhpdf: procedures>+≡
    subroutine lhpdf_data_get_pdg_out (data, pdg_out)
        class(lhpdf_data_t), intent(in) :: data
        type(pdg_array_t), dimension(:), intent(inout) :: pdg_out
        integer, dimension(:), allocatable :: pdg1
        integer :: n, np, i
        n = count (data%mask)
        np = 0; if (data%has_photon .and. data%mask_photon) np = 1
        allocate (pdg1 (n + np))
        pdg1(1:n) = pack ([i, i = -6, 6], data%mask)
        if (np == 1) pdg1(n+np) = PHOTON
        pdg_out(1) = pdg1
    end subroutine lhpdf_data_get_pdg_out

```

Allocate the interaction record.

```

<SF lhpdf: lhpdf data: TBP>+≡
    procedure :: allocate_sf_int => lhpdf_data_allocate_sf_int

<SF lhpdf: procedures>+≡
    subroutine lhpdf_data_allocate_sf_int (data, sf_int)
        class(lhpdf_data_t), intent(in) :: data
        class(sf_int_t), intent(inout), allocatable :: sf_int
        allocate (lhpdf_t :: sf_int)
    end subroutine lhpdf_data_allocate_sf_int

```

Return the numerical PDF set index.

```

<SF lhpdf: lhpdf data: TBP>+≡
  procedure :: get_pdf_set => lhpdf_data_get_pdf_set

<SF lhpdf: procedures>+≡
  elemental function lhpdf_data_get_pdf_set (data) result (pdf_set)
    class(lhpdf_data_t), intent(in) :: data
    integer :: pdf_set
    pdf_set = data%set
  end function lhpdf_data_get_pdf_set

```

16.16.8 The LHAPDF object

The `lhpdf_t` data type is a $1 \rightarrow 2$ interaction which describes the splitting of an (anti)proton into a parton and a beam remnant. We stay in the strict forward-splitting limit, but allow some invariant mass for the beam remnant such that the outgoing parton is exactly massless. For a real event, we would replace this by a parton cascade, where the outgoing partons have virtuality as dictated by parton-shower kinematics, and transverse momentum is generated.

This is the LHAPDF object which holds input data together with the interaction. We also store the x momentum fraction and the scale, since kinematics and function value are requested at different times.

The PDF application is a $1 \rightarrow 2$ splitting process, where the particles are ordered as (hadron, remnant, parton).

Polarization is ignored completely. The beam particle is colorless, while partons and beam remnant carry color. The remnant gets a special flavor code.

```

<SF lhpdf: public>+≡
  public :: lhpdf_t

<SF lhpdf: types>+≡
  type, extends (sf_int_t) :: lhpdf_t
    type(lhpdf_data_t), pointer :: data => null ()
    real(default) :: x = 0
    real(default) :: q = 0
    real(default) :: s = 0
  contains
    <SF lhpdf: lhpdf: TBP>
  end type lhpdf_t

```

Type string: display the chosen PDF set.

```

<SF lhpdf: lhpdf: TBP>+≡
  procedure :: type_string => lhpdf_type_string

<SF lhpdf: procedures>+≡
  function lhpdf_type_string (object) result (string)
    class(lhpdf_t), intent(in) :: object
    type(string_t) :: string
    if (associated (object%data)) then
      string = "LHAPDF: " // object%data%file
    else
      string = "LHAPDF: [undefined]"
    end if
  end function

```

```
end function lhapdf_type_string
```

Output. Call the interaction routine after displaying the configuration.

```
<SF lhapdf: lhapdf: TBP>+≡
  procedure :: write => lhapdf_write

<SF lhapdf: procedures>+≡
  subroutine lhapdf_write (object, unit, testflag)
    class(lhapdf_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%data)) then
      call object%data%write (u)
      if (object%status >= SF_DONE_KINEMATICS) then
        write (u, "(1x,A)") "SF parameters:"
        write (u, "(3x,A," // FMT_17 // ")") "x =", object%x
        if (object%status >= SF_FAILED_EVALUATION) then
          write (u, "(3x,A," // FMT_17 // ")") "Q =", object%q
        end if
      end if
      call object%base_write (u, testflag)
    else
      write (u, "(1x,A)") "LHAPDF data: [undefined]"
    end if
  end subroutine lhapdf_write
```

Initialize. We know that `data` will be of concrete type `sf_lhapdf_data_t`, but we have to cast this explicitly.

For this implementation, we set the incoming and outgoing masses equal to the physical particle mass, but keep the radiated mass zero.

```
<SF lhapdf: lhapdf: TBP>+≡
  procedure :: init => lhapdf_init

<SF lhapdf: procedures>+≡
  subroutine lhapdf_init (sf_int, data)
    class(lhapdf_t), intent(out) :: sf_int
    class(sf_data_t), intent(in), target :: data
    type(quantum_numbers_mask_t), dimension(3) :: mask
    type(flavor_t) :: flv, flv_remnant
    type(color_t) :: col0
    type(quantum_numbers_t), dimension(3) :: qn
    integer :: i
    select type (data)
    type is (lhapdf_data_t)
      mask = quantum_numbers_mask (.false., .false., .true.)
      call col0%init ()
      call sf_int%base_init (mask, [0._default], [0._default], [0._default])
      sf_int%data => data
      do i = -6, 6
        if (data%mask(i)) then
          call qn(1)%init (data%flv_in, col = col0)
          if (i == 0) then
```

```

        call flv%init (GLUON, data%model)
        call flv_remnant%init (HADRON_REMNANT_OCTET, data%model)
    else
        call flv%init (i, data%model)
        call flv_remnant%init &
            (sign (HADRON_REMNANT_TRIPLET, -i), data%model)
    end if
    call qn(2)%init ( &
        flv = flv_remnant, col = color_from_flavor (flv_remnant, 1))
    call qn(2)%tag_radiated ()
    call qn(3)%init ( &
        flv = flv, col = color_from_flavor (flv, 1, reverse=.true.))
    call sf_int%add_state (qn)
end if
end do
if (data%has_photon .and. data%mask_photon) then
    call flv%init (PHOTON, data%model)
    call flv_remnant%init (HADRON_REMNANT_SINGLET, data%model)
    call qn(2)%init (flv = flv_remnant, &
        col = color_from_flavor (flv_remnant, 1))
    call qn(2)%tag_radiated ()
    call qn(3)%init (flv = flv, &
        col = color_from_flavor (flv, 1, reverse=.true.))
    call sf_int%add_state (qn)
end if
call sf_int%freeze ()
call sf_int%set_incoming ([1])
call sf_int%set_radiated ([2])
call sf_int%set_outgoing ([3])
sf_int%status = SF_INITIAL
end select
end subroutine lhpdf_init

```

16.16.9 Structure function

We have to cast the LHAPDF arguments to/from double precision (possibly from/to extended/quadruple precision), if necessary. Some structure functions can yield negative results (sea quarks close to $x = 1$). In an NLO computation, this is perfectly fine and we keep negative values. Unlike total cross sections, PDFs do not have to be positive definite. For LO however, negative PDFs would cause negative event weights so we set these values to zero instead.

<SF lhpdf: lhpdf: TBP>+≡

```
procedure :: apply => lhpdf_apply
```

<SF lhpdf: procedures>+≡

```

subroutine lhpdf_apply (sf_int, scale, negative_sf, rescale, i_sub)
    class(lhpdf_t), intent(inout) :: sf_int
    real(default), intent(in) :: scale
    logical, intent(in), optional :: negative_sf
    class(sf_rescale_t), intent(in), optional :: rescale
    integer, intent(in), optional :: i_sub
    real(default) :: x, s

```

```

double precision :: xx, qq, ss
double precision, dimension(-6:6) :: ff
double precision :: fphot
complex(default), dimension(:), allocatable :: fc
integer :: i, i_sub_opt, j_sub
logical :: negative_sf_opt
external :: evolvePDFM, evolvePDFpM
i_sub_opt = 0; if (present (i_sub)) i_sub_opt = i_sub
negative_sf_opt = .false.; if (present(negative_sf)) negative_sf_opt = negative_sf
associate (data => sf_int%data)
    sf_int%q = scale
    x = sf_int%x
    if (present (rescale)) call rescale%apply (x)
    s = sf_int%s
    xx = x
    if (debug2_active (D_BEAMS)) then
        call msg_debug2 (D_BEAMS, "lhpdf_apply")
        call msg_debug2 (D_BEAMS, "rescale: ", present(rescale))
        call msg_debug2 (D_BEAMS, "i_sub: ", i_sub_opt)
        call msg_debug2 (D_BEAMS, "x: ", x)
    end if
    qq = min (data%qmax, scale)
    qq = max (data%qmin, qq)
    if (.not. data%photon) then
        if (data%invert) then
            if (data%has_photon) then
                if (LHAPDF5_AVAILABLE) then
                    call evolvePDFphotonM &
                        (data%set, xx, qq, ff(6:-6:-1), fphot)
                else if (LHAPDF6_AVAILABLE) then
                    call data%pdf%evolve_pdfphotonm &
                        (xx, qq, ff(6:-6:-1), fphot)
                end if
            else
                if (data%hoppet_b_matching) then
                    call hoppet_eval (xx, qq, ff(6:-6:-1))
                else
                    if (LHAPDF5_AVAILABLE) then
                        call evolvePDFM (data%set, xx, qq, ff(6:-6:-1))
                    else if (LHAPDF6_AVAILABLE) then
                        call data%pdf%evolve_pdfm (xx, qq, ff(6:-6:-1))
                    end if
                end if
            end if
        else
            if (data%has_photon) then
                if (LHAPDF5_AVAILABLE) then
                    call evolvePDFphotonM (data%set, xx, qq, ff, fphot)
                else if (LHAPDF6_AVAILABLE) then
                    call data%pdf%evolve_pdfphotonm (xx, qq, ff, fphot)
                end if
            else
                if (data%hoppet_b_matching) then
                    call hoppet_eval (xx, qq, ff)
                end if
            end if
        end if
    end if
end associate

```



```

        else
            if (LHAPDF5_AVAILABLE) then
                call evolvePDFM (data%set, xx, qq, ff)
            else if (LHAPDF6_AVAILABLE) then
                call data%pdf%evolve_pdfm (xx, qq, ff)
            end if
        end if
    end if
end if
else
    ss = s
    if (LHAPDF5_AVAILABLE) then
        call evolvePDFpM (data%set, xx, qq, &
            ss, data%photon_scheme, ff)
    else if (LHAPDF6_AVAILABLE) then
        call data%pdf%evolve_pdfpm (xx, qq, ss, &
            data%photon_scheme, ff)
    end if
end if
if (data%has_photon) then
    allocate (fc (count ([data%mask, data%mask_photon])))
    if (negative_sf_opt) then
        fc = pack ([ff, fphot] / x, [data%mask, data%mask_photon])
    else
        fc = max( pack ([ff, fphot] / x, [data%mask, data%mask_photon]), 0._default)
    end if
else
    allocate (fc (count (data%mask)))
    if (negative_sf_opt) then
        fc = pack (ff / x, data%mask)
    else
        fc = max( pack (ff / x, data%mask), 0._default)
    end if
end if
end associate
if (debug_active (D_BEAMS)) print *, 'Set pdfs: ', real (fc)
call sf_int%set_matrix_element (fc, [(i_sub_opt * size(fc) + i, i = 1, size(fc))])
sf_int%status = SF_EVALUATED
end subroutine lhpdf_apply

```

16.16.10 Strong Coupling

Since the PDF codes provide a function for computing the running α_s value, we make this available as an implementation of the abstract `alpha_qcd_t` type, which is used for matrix element evaluation.

```

<SF lhpdf: public>+≡
    public :: alpha_qcd_lhpdf_t

<SF lhpdf: types>+≡
    type, extends (alpha_qcd_t) :: alpha_qcd_lhpdf_t
        type(string_t) :: pdfset_dir
        type(string_t) :: pdfset_file
        integer :: pdfset_member = -1

```

```

        type(lhapdf_pdf_t) :: pdf
    contains
        <SF lhpdf: alpha qcd: TBP>
    end type alpha_qcd_lhapdf_t

```

Output. As in earlier versions we leave the LHAPDF path out.

```

<SF lhpdf: alpha qcd: TBP>≡
    procedure :: write => alpha_qcd_lhapdf_write

<SF lhpdf: procedures>+≡
    subroutine alpha_qcd_lhapdf_write (object, unit)
        class(alpha_qcd_lhapdf_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A)") "QCD parameters (lhpdf):"
        write (u, "(5x,A,A)") "PDF set      = ", char (object%pdfset_file)
        write (u, "(5x,A,I0)") "PDF member = ", object%pdfset_member
    end subroutine alpha_qcd_lhapdf_write

```

Calculation: the numeric member ID selects the correct PDF set, which must be properly initialized.

```

<SF lhpdf: interfaces>+≡
    interface
        double precision function alphasPDF (Q)
            double precision, intent(in) :: Q
        end function alphasPDF
    end interface

<SF lhpdf: alpha qcd: TBP>+≡
    procedure :: get => alpha_qcd_lhapdf_get

<SF lhpdf: procedures>+≡
    function alpha_qcd_lhapdf_get (alpha_qcd, scale) result (alpha)
        class(alpha_qcd_lhapdf_t), intent(in) :: alpha_qcd
        real(default), intent(in) :: scale
        real(default) :: alpha
        if (LHAPDF5_AVAILABLE) then
            alpha = alphasPDF (dble (scale))
        else if (LHAPDF6_AVAILABLE) then
            alpha = alpha_qcd%pdf%alphas_pdf (dble (scale))
        end if
    end function alpha_qcd_lhapdf_get

```

Initialization. We need to access the (quasi-global) initialization status.

```

<SF lhpdf: alpha qcd: TBP>+≡
    procedure :: init => alpha_qcd_lhapdf_init

<SF lhpdf: procedures>+≡
    subroutine alpha_qcd_lhapdf_init (alpha_qcd, file, member, path)
        class(alpha_qcd_lhapdf_t), intent(out) :: alpha_qcd
        type(string_t), intent(inout) :: file
        integer, intent(inout) :: member
    end subroutine alpha_qcd_lhapdf_init

```

```

type(string_t), intent(inout) :: path
alpha_qcd%pdfset_file = file
alpha_qcd%pdfset_member = member
if (alpha_qcd%pdfset_member < 0) &
    call msg_fatal ("QCD parameter initialization: PDF set " &
        // char (file) // " is unknown")
if (LHAPDF5_AVAILABLE) then
    call lhpdf_initialize (1, path, file, member)
else if (LHAPDF6_AVAILABLE) then
    call lhpdf_initialize &
        (1, path, file, member, alpha_qcd%pdf)
end if
end subroutine alpha_qcd_lhpdf_init

```

16.16.11 Unit tests

Test module, followed by the corresponding implementation module.

<sf_lhpdf_ut.f90>≡
<File header>

```

module sf_lhpdf_ut
    use unit_tests
    use system_dependencies, only: LHAPDF5_AVAILABLE
    use system_dependencies, only: LHAPDF6_AVAILABLE
    use sf_lhpdf_uti

```

<Standard module head>

<SF lhpdf: public test>

contains

<SF lhpdf: test driver>

end module sf_lhpdf_ut

<sf_lhpdf_uti.f90>≡
<File header>

```

module sf_lhpdf_uti

```

<Use kinds>

<Use strings>

```

    use system_dependencies, only: LHAPDF5_AVAILABLE
    use system_dependencies, only: LHAPDF6_AVAILABLE
    use os_interface
    use physics_defs, only: PROTON
    use sm_qcd
    use lorentz
    use pdg_arrays
    use flavors
    use interactions, only: reset_interaction_counter
    use model_data

```

```

    use sf_base

    use sf_lhapdf

    <Standard module head>

    <SF lhpdf: test declarations>

    contains

    <SF lhpdf: tests>

    end module sf_lhapdf_util
API: driver for the unit tests below.
<SF lhpdf: public test>≡
    public :: sf_lhapdf_test
<SF lhpdf: test driver>≡
    subroutine sf_lhapdf_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <SF lhpdf: execute tests>
    end subroutine sf_lhapdf_test

```

Test structure function data

Construct and display a test structure function data object.

```

<SF lhpdf: execute tests>≡
    if (LHAPDF5_AVAILABLE) then
        call test (sf_lhapdf_1, "sf_lhapdf5_1", &
            "structure function configuration", &
            u, results)
    else if (LHAPDF6_AVAILABLE) then
        call test (sf_lhapdf_1, "sf_lhapdf6_1", &
            "structure function configuration", &
            u, results)
    end if

<SF lhpdf: test declarations>≡
    public :: sf_lhapdf_1

<SF lhpdf: tests>≡
    subroutine sf_lhapdf_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(pdg_array_t) :: pdg_in
        type(pdg_array_t), dimension(1) :: pdg_out
        integer, dimension(:), allocatable :: pdg1
        class(sf_data_t), allocatable :: data

        write (u, "(A)")  "* Test output: sf_lhapdf_1"
        write (u, "(A)")  "* Purpose: initialize and display &
            &test structure function data"
        write (u, "(A)")
    end subroutine sf_lhapdf_1

```

```

write (u, "(A)")  "* Create empty data object"
write (u, "(A)")

call model%init_sm_test ()
pdg_in = PROTON

allocate (lhpdf_data_t :: data)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

select type (data)
type is (lhpdf_data_t)
    call data%init (model, pdg_in)
end select

call data%write (u)

write (u, "(A)")

write (u, "(1x,A)")  "Outgoing particle codes:"
call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(2x,99(1x,I0))")  pdg1

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_lhpdf_1"

end subroutine sf_lhpdf_1

```

Test and probe structure function

Construct and display a structure function object based on the PDF builtin structure function.

```

<SF lhpdf: execute tests>+≡
  if (LHAPDF5_AVAILABLE) then
    call test (sf_lhpdf_2, "sf_lhpdf5_2", &
      "structure function instance", &
      u, results)
  else if (LHAPDF6_AVAILABLE) then
    call test (sf_lhpdf_2, "sf_lhpdf6_2", &
      "structure function instance", &
      u, results)
  end if
<SF lhpdf: test declarations>+≡
  public :: sf_lhpdf_2

```

```

<SF lhpdf: tests>+≡
subroutine sf_lhapdf_2 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t) :: flv
  type(pdg_array_t) :: pdg_in
  class(sf_data_t), allocatable, target :: data
  class(sf_int_t), allocatable :: sf_int
  type(vector4_t) :: k
  type(vector4_t), dimension(2) :: q
  real(default) :: E
  real(default), dimension(:), allocatable :: r, rb, x, xb
  real(default) :: f

  write (u, "(A)")  "* Test output: sf_lhapdf_2"
  write (u, "(A)")  "* Purpose: initialize and fill &
    &test structure function object"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize configuration data"
  write (u, "(A)")

  call model%init_sm_test ()
  call flv%init (PROTON, model)
  pdg_in = PROTON
  call lhpdf_global_reset ()

  call reset_interaction_counter ()

  allocate (lhpdf_data_t :: data)
  select type (data)
  type is (lhpdf_data_t)
    call data%init (model, pdg_in)
  end select

  write (u, "(A)")  "* Initialize structure-function object"
  write (u, "(A)")

  call data%allocate_sf_int (sf_int)
  call sf_int%init (data)
  call sf_int%set_beam_index ([1])

  call sf_int%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Initialize incoming momentum with E=500"
  write (u, "(A)")
  E = 500
  k = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
  call vector4_write (k, u)
  call sf_int%seed_kinematics ([k])

  write (u, "(A)")
  write (u, "(A)")  "* Set kinematics for x=0.5"

```

```

write (u, "(A)")

allocate (r (data%get_n_par ()))
allocate (rb(size (r)))
allocate (x (size (r)))
allocate (xb(size (r)))

r = 0.5_default
rb = 1 - r
call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%write (u)

write (u, "(A)")
write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb
write (u, "(A,9(1x,F10.7))") "f =", f

write (u, "(A)")
write (u, "(A)") "* Recover x from momenta"
write (u, "(A)")

q = sf_int%get_momenta (outgoing=.true.)
call sf_int%final ()
deallocate (sf_int)

call data%allocate_sf_int (sf_int)
call sf_int%init (data)
call sf_int%set_beam_index ([1])

call sf_int%seed_kinematics ([k])
call sf_int%set_momenta (q, outgoing=.true.)
call sf_int%recover_x (x, xb)

write (u, "(A,9(1x,F10.7))") "x =", x
write (u, "(A,9(1x,F10.7))") "xb=", xb

write (u, "(A)")
write (u, "(A)") "* Evaluate for Q = 100 GeV"
write (u, "(A)")

call sf_int%complete_kinematics (x, xb, f, r, rb, map=.false.)
call sf_int%apply (scale = 100._default)
call sf_int%write (u, testflag = .true.)

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call sf_int%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: sf_lhapdf_2"

```

```
end subroutine sf_lhapdf_2
```

Strong Coupling

Test α_s as an implementation of the `alpha_qcd_t` abstract type.

```
<SF lhpdf: execute tests>+≡
  if (LHAPDF5_AVAILABLE) then
    call test (sf_lhapdf_3, "sf_lhapdf5_3", &
      "running alpha_s", &
      u, results)
  else if (LHAPDF6_AVAILABLE) then
    call test (sf_lhapdf_3, "sf_lhapdf6_3", &
      "running alpha_s", &
      u, results)
  end if

<SF lhpdf: test declarations>+≡
  public :: sf_lhapdf_3

<SF lhpdf: tests>+≡
  subroutine sf_lhapdf_3 (u)
    integer, intent(in) :: u
    type(qcd_t) :: qcd
    type(string_t) :: name, path
    integer :: member

    write (u, "(A)")  "* Test output: sf_lhapdf_3"
    write (u, "(A)")  "* Purpose: initialize and evaluate alpha_s"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize configuration data"
    write (u, "(A)")

    call lhpdf_global_reset ()

    if (LHAPDF5_AVAILABLE) then
      name = "cteq6ll.LHpdf"
      member = 1
      path = ""
    else if (LHAPDF6_AVAILABLE) then
      name = "CT10"
      member = 1
      path = ""
    end if

    write (u, "(A)")  "* Initialize qcd object"
    write (u, "(A)")

    allocate (alpha_qcd_lhapdf_t :: qcd%alpha)
    select type (alpha => qcd%alpha)
    type is (alpha_qcd_lhapdf_t)
      call alpha%init (name, member, path)
    end select
    call qcd%write (u)
```



```

write (u, "(A)")
write (u, "(A)")  "* Evaluate for Q = 100"
write (u, "(A)")

write (u, "(1x,A,F8.5)")  "alpha = ", qcd%alpha%get (100._default)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

write (u, "(A)")
write (u, "(A)")  "* Test output end: sf_lhapdf_3"

end subroutine sf_lhapdf_3

```

16.17 Easy PDF Access

For the shower, subtraction and matching, it is very useful to have direct access to $f(x, Q)$ independently of the used library.

```

⟨pdf.f90⟩≡
  ⟨File header⟩

  module pdf

    ⟨Use kinds with double⟩
    use io_units
    use system_dependencies, only: LHAPDF5_AVAILABLE, LHAPDF6_AVAILABLE
    use diagnostics
    use beam_structures
    use lhapdf !NODEP!
    use pdf_builtin !NODEP!

    ⟨Standard module head⟩

    ⟨PDF: public⟩

    ⟨PDF: parameters⟩

    ⟨PDF: types⟩

    contains

    ⟨PDF: procedures⟩

  end module pdf

```

We support the following implementations:

```

⟨PDF: parameters⟩≡
  integer, parameter, public :: STRF_NONE = 0
  integer, parameter, public :: STRF_LHAPDF6 = 1
  integer, parameter, public :: STRF_LHAPDF5 = 2
  integer, parameter, public :: STRF_PDF_BUILTIN = 3

```

A container to bundle all necessary PDF data. Could be moved to a more central location.

$\langle PDF: public \rangle \equiv$

```
public :: pdf_data_t
```

$\langle PDF: types \rangle \equiv$

```
type :: pdf_data_t
type(lhapdf_pdf_t) :: pdf
real(default) :: xmin, xmax, qmin, qmax
integer :: type = STRF_NONE
integer :: set = 0
contains
   $\langle PDF: pdf\ data: TBP \rangle$ 
end type pdf_data_t
```

$\langle PDF: pdf\ data: TBP \rangle \equiv$

```
procedure :: init => pdf_data_init
```

$\langle PDF: procedures \rangle \equiv$

```
subroutine pdf_data_init (pdf_data, pdf_data_in)
  class(pdf_data_t), intent(out) :: pdf_data
  type(pdf_data_t), target, intent(in) :: pdf_data_in
  pdf_data%xmin = pdf_data_in%xmin
  pdf_data%xmax = pdf_data_in%xmax
  pdf_data%qmin = pdf_data_in%qmin
  pdf_data%qmax = pdf_data_in%qmax
  pdf_data%set = pdf_data_in%set
  pdf_data%type = pdf_data_in%type
  if (pdf_data%type == STRF_LHAPDF6) then
    if (pdf_data_in%pdf%is_associated ()) then
      call lhapdf_copy_pointer (pdf_data_in%pdf, pdf_data%pdf)
    else
      call msg_bug ('pdf_data_init: pdf_data%pdf was not associated!')
    end if
  end if
end subroutine pdf_data_init
```

$\langle PDF: pdf\ data: TBP \rangle + \equiv$

```
procedure :: write => pdf_data_write
```

$\langle PDF: procedures \rangle + \equiv$

```
subroutine pdf_data_write (pdf_data, unit)
  class(pdf_data_t), intent(in) :: pdf_data
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(3x,A,I0)") "PDF set = ", pdf_data%set
  write (u, "(3x,A,I0)") "PDF type = ", pdf_data%type
end subroutine pdf_data_write
```

$\langle PDF: pdf\ data: TBP \rangle + \equiv$

```
procedure :: setup => pdf_data_setup
```

<PDF: procedures>+≡

```

subroutine pdf_data_setup (pdf_data, caller, beam_structure, lhpdf_member, set)
  class(pdf_data_t), intent(inout) :: pdf_data
  character(len=*), intent(in) :: caller
  type(beam_structure_t), intent(in) :: beam_structure
  integer, intent(in) :: lhpdf_member, set
  real(default) :: xmin, xmax, q2min, q2max
  pdf_data%set = set
  if (beam_structure%contains ("lhpdf")) then
    if (LHAPDF6_AVAILABLE) then
      pdf_data%type = STRF_LHAPDF6
    else if (LHAPDF5_AVAILABLE) then
      pdf_data%type = STRF_LHAPDF5
    end if
    write (msg_buffer, "(A,I0)") caller &
      // ": interfacing LHAPDF set #", pdf_data%set
    call msg_message ()
  else if (beam_structure%contains ("pdf_builtin")) then
    pdf_data%type = STRF_PDF_BUILTIN
    write (msg_buffer, "(A,I0)") caller &
      // ": interfacing PDF builtin set #", pdf_data%set
    call msg_message ()
  end if
  select case (pdf_data%type)
  case (STRF_LHAPDF6)
    pdf_data%xmin = pdf_data%pdf%getxmin ()
    pdf_data%xmax = pdf_data%pdf%getxmax ()
    pdf_data%qmin = sqrt(pdf_data%pdf%getq2min ())
    pdf_data%qmax = sqrt(pdf_data%pdf%getq2max ())
  case (STRF_LHAPDF5)
    call GetXminM (1, lhpdf_member, xmin)
    call GetXmaxM (1, lhpdf_member, xmax)
    call GetQ2minM (1, lhpdf_member, q2min)
    call GetQ2maxM (1, lhpdf_member, q2max)
    pdf_data%xmin = xmin
    pdf_data%xmax = xmax
    pdf_data%qmin = sqrt(q2min)
    pdf_data%qmax = sqrt(q2max)
  end select
end subroutine pdf_data_setup

```

This could be overloaded with a version that only asks for a specific flavor as it is supported by LHAPDF6.

<PDF: pdf data: TBP>+≡

```

procedure :: evolve => pdf_data_evolve

```

<PDF: procedures>+≡

```

subroutine pdf_data_evolve (pdf_data, x, q_in, f)
  class(pdf_data_t), intent(inout) :: pdf_data
  real(double), intent(in) :: x, q_in
  real(double), dimension(-6:6), intent(out) :: f
  real(double) :: q
  select case (pdf_data%type)
  case (STRF_PDF_BUILTIN)

```

```

        call pdf_evolve_LHAPDF (pdf_data%set, x, q_in, f)
    case (STRF_LHAPDF6)
        q = min (pdf_data%qmax, q_in)
        q = max (pdf_data%qmin, q)
        call pdf_data%pdf%evolve_pdfm (x, q, f)
    case (STRF_LHAPDF5)
        q = min (pdf_data%qmax, q_in)
        q = max (pdf_data%qmin, q)
        call evolvePDFM (pdf_data%set, x, q, f)
    case default
        call msg_fatal ("PDF function: unknown PDF method.")
    end select
end subroutine pdf_data_evolve

```

16.18 Dispatch

<dispatch_beams.f90>≡
 <File header>

```

module dispatch_beams

  <Use kinds>
  <Use strings>

  use diagnostics
  use os_interface, only: os_data_t
  use variables, only: var_list_t
  use constants, only: PI
  use numeric_utils, only: vanishes
  use physics_defs, only: PHOTON
  use rng_base, only: rng_factory_t
  use pdg_arrays
  use model_data, only: model_data_t
  use dispatch_rng, only: dispatch_rng_factory
  use dispatch_rng, only: update_rng_seed_in_var_list
  use flavors, only: flavor_t
  use sm_qcd, only: qcd_t, alpha_qcd_fixed_t, alpha_qcd_from_scale_t
  use sm_qcd, only: alpha_qcd_from_lambda_t
  use physics_defs, only: MZ_REF, ALPHA_QCD_MZ_REF

  use beam_structures
  use sf_base
  use sf_mappings
  use sf_isr
  use sf_epa
  use sf_ewa
  use sf_escan
  use sf_gaussian
  use sf_beam_events
  use sf_circe1
  use sf_circe2
  use sf_pdf_builtin
  use sf_lhapdf

```

```

    <Standard module head>

    <Dispatch beams: public>

    <Dispatch beams: types>

    <Dispatch beams: variables>

contains

    <Dispatch beams: procedures>

end module dispatch_beams

```

This data type is a container for transferring structure-function specific data from the `dispatch_sf_data` to the `dispatch_sf_channels` subroutine.

```

    <Dispatch beams: public>≡
        public :: sf_prop_t

    <Dispatch beams: types>≡
        type :: sf_prop_t
            real(default), dimension(2) :: isr_eps = 1
        end type sf_prop_t

```

Allocate a structure-function configuration object according to the `sf_method` string.

The `sf_prop` object can be used to transfer structure-function specific data up and to the `dispatch_sf_channels` subroutine below, so they can be used for particular mappings.

The `var_list_global` object is used for the RNG generator seed. It is `intent(inout)` because the RNG generator seed may change during initialization.

The `pdg_in` array is the array of incoming flavors, corresponding to the upstream structure function or the beam array. This will be checked for the structure function in question and replaced by the outgoing flavors. The `pdg_prc` array is the array of incoming flavors (beam index, component index) for the hard process.

```

    <Dispatch beams: public>+≡
        public :: dispatch_sf_data

    <Dispatch beams: procedures>≡
        subroutine dispatch_sf_data (data, sf_method, i_beam, sf_prop, &
            var_list, var_list_global, model, &
            os_data, sqrts, pdg_in, pdg_prc, polarized)
            class(sf_data_t), allocatable, intent(inout) :: data
            type(string_t), intent(in) :: sf_method
            integer, dimension(:), intent(in) :: i_beam
            type(pdg_array_t), dimension(:), intent(inout) :: pdg_in
            type(pdg_array_t), dimension(:, :), intent(in) :: pdg_prc
            type(sf_prop_t), intent(inout) :: sf_prop
            type(var_list_t), intent(in) :: var_list
            type(var_list_t), intent(inout) :: var_list_global
            integer :: next_rng_seed
            class(model_data_t), target, intent(in) :: model
            type(os_data_t), intent(in) :: os_data

```

```

real(default), intent(in) :: sqrts
logical, intent(in) :: polarized
type(pdg_array_t), dimension(:), allocatable :: pdg_out
real(default) :: isr_alpha, isr_q_max, isr_mass
integer :: isr_order
logical :: isr_recoil, isr_keep_energy
real(default) :: epa_alpha, epa_x_min, epa_q_min, epa_q_max, epa_mass
logical :: epa_recoil, epa_keep_energy
integer :: epa_int_mode
type(string_t) :: epa_mode
real(default) :: ewa_x_min, ewa_pt_max, ewa_mass
logical :: ewa_recoil, ewa_keep_energy
type(pdg_array_t), dimension(:), allocatable :: pdg_prc1
integer :: ewa_id
type(string_t) :: pdf_name
type(string_t) :: lhpdf_dir, lhpdf_file
type(string_t), dimension(13) :: lhpdf_photon_sets
integer :: lhpdf_member, lhpdf_photon_scheme
logical :: hoppet_b_matching
class(rng_factory_t), allocatable :: rng_factory
logical :: circe1_photon1, circe1_photon2, circe1_generate, &
    circe1_with_radiation
real(default) :: circe1_sqrts, circe1_eps
integer :: circe1_version, circe1_chattiness, &
    circe1_revision
character(6) :: circe1_accelerator
logical :: circe2_polarized
type(string_t) :: circe2_design, circe2_file
real(default), dimension(2) :: gaussian_spread
logical :: beam_events_warn_eof
type(string_t) :: beam_events_dir, beam_events_file
logical :: escan_normalize
integer :: i
lhpdf_photon_sets = [var_str ("DOG0.LHgrid"), var_str ("DOG1.LHgrid"), &
    var_str ("DGG.LHgrid"), var_str ("LACG.LHgrid"), &
    var_str ("GSG0.LHgrid"), var_str ("GSG1.LHgrid"), &
    var_str ("GSG960.LHgrid"), var_str ("GSG961.LHgrid"), &
    var_str ("GRVG0.LHgrid"), var_str ("GRVG1.LHgrid"), &
    var_str ("ACFGPG.LHgrid"), var_str ("WHITG.LHgrid"), &
    var_str ("SASG.LHgrid")]
select case (char (sf_method))
case ("pdf_builtin")
    allocate (pdf_builtin_data_t :: data)
    select type (data)
    type is (pdf_builtin_data_t)
        pdf_name = &
            var_list%get_sval (var_str ("pdf_builtin_set"))
        hoppet_b_matching = &
            var_list%get_lval (var_str ("hoppet_b_matching"))
        call data%init ( &
            model, pdg_in(i_beam(1)), &
            name = pdf_name, &
            path = os_data%pdf_builtin_datapath, &
            hoppet_b_matching = hoppet_b_matching)

```

```

end select
case ("pdf_builtin_photon")
  call msg_fatal ("Currently, there are no photon PDFs built into WHIZARD,", &
    [var_str ("for the photon content inside a proton or neutron use"), &
      var_str ("the 'lhpdf_photon' structure function.")])
case ("lhpdf")
  allocate (lhpdf_data_t :: data)
  if (pdg_array_get (pdg_in(i_beam(1)), 1) == PHOTON) then
    call msg_fatal ("The 'lhpdf' structure is intended only for protons and", &
      [var_str ("pions, please use 'lhpdf_photon' for photon beams.")])
  end if
  lhpdf_dir = &
    var_list%get_sval (var_str ("lhpdf_dir"))
  lhpdf_file = &
    var_list%get_sval (var_str ("lhpdf_file"))
  lhpdf_member = &
    var_list%get_ival (var_str ("lhpdf_member"))
  lhpdf_photon_scheme = &
    var_list%get_ival (var_str ("lhpdf_photon_scheme"))
  hoppet_b_matching = &
    var_list%get_lval (var_str ("hoppet_b_matching"))
  select type (data)
  type is (lhpdf_data_t)
    call data%init &
      (model, pdg_in(i_beam(1)), &
        lhpdf_dir, lhpdf_file, lhpdf_member, &
        lhpdf_photon_scheme, hoppet_b_matching)
  end select
case ("lhpdf_photon")
  allocate (lhpdf_data_t :: data)
  if (pdg_array_get_length (pdg_in(i_beam(1))) /= 1 .or. &
    pdg_array_get (pdg_in(i_beam(1)), 1) /= PHOTON) then
    call msg_fatal ("The 'lhpdf_photon' structure function is exclusively for", &
      [var_str ("photon PDFs, i.e. for photons as beam particles")])
  end if
  lhpdf_dir = &
    var_list%get_sval (var_str ("lhpdf_dir"))
  lhpdf_file = &
    var_list%get_sval (var_str ("lhpdf_photon_file"))
  lhpdf_member = &
    var_list%get_ival (var_str ("lhpdf_member"))
  lhpdf_photon_scheme = &
    var_list%get_ival (var_str ("lhpdf_photon_scheme"))
  if (.not. any (lhpdf_photon_sets == lhpdf_file)) then
    call msg_fatal ("This PDF set is not supported or not " // &
      "intended for photon beams.")
  end if
  select type (data)
  type is (lhpdf_data_t)
    call data%init &
      (model, pdg_in(i_beam(1)), &
        lhpdf_dir, lhpdf_file, lhpdf_member, &
        lhpdf_photon_scheme)
  end select

```

```

case ("isr")
  allocate (isr_data_t :: data)
  isr_alpha = &
    var_list%get_rval (var_str ("isr_alpha"))
  if (vanishes (isr_alpha)) then
    isr_alpha = (var_list%get_rval (var_str ("ee"))) &
      ** 2 / (4 * PI)
  end if
  isr_q_max = &
    var_list%get_rval (var_str ("isr_q_max"))
  if (vanishes (isr_q_max)) then
    isr_q_max = sqrt(s)
  end if
  isr_mass = var_list%get_rval (var_str ("isr_mass"))
  isr_order = var_list%get_ival (var_str ("isr_order"))
  isr_recoil = var_list%get_lval (var_str ("?isr_recoil"))
  isr_keep_energy = var_list%get_lval (var_str ("?isr_keep_energy"))
  select type (data)
  type is (isr_data_t)
    call data%init &
      (model, pdg_in (i_beam(1)), isr_alpha, isr_q_max, &
        isr_mass, isr_order, recoil = isr_recoil, keep_energy = &
        isr_keep_energy)
    call data%check ()
    sf_prop%isr_eps(i_beam(1)) = data%get_eps ()
  end select
case ("epa")
  allocate (epa_data_t :: data)
  epa_mode = var_list%get_sval (var_str ("$epa_mode"))
  epa_int_mode = 0
  epa_alpha = var_list%get_rval (var_str ("epa_alpha"))
  if (vanishes (epa_alpha)) then
    epa_alpha = (var_list%get_rval (var_str ("ee"))) &
      ** 2 / (4 * PI)
  end if
  epa_x_min = var_list%get_rval (var_str ("epa_x_min"))
  epa_q_min = var_list%get_rval (var_str ("epa_q_min"))
  epa_q_max = var_list%get_rval (var_str ("epa_q_max"))
  if (vanishes (epa_q_max)) then
    epa_q_max = sqrt(s)
  end if
  select case (char (epa_mode))
  case ("default", "Budnev_617")
    epa_int_mode = 0
  case ("Budnev_616e")
    epa_int_mode = 1
  case ("log_power")
    epa_int_mode = 2
    epa_q_max = sqrt(s)
  case ("log_simple")
    epa_int_mode = 3
    epa_q_max = sqrt(s)
  case ("log")
    epa_int_mode = 4

```



```

    epa_q_max = sqrts
case default
    call msg_fatal ("EPA: unsupported EPA mode; please choose " // &
        "'default', 'Budnev_616', 'Budnev_616e', 'log_power', " // &
        "'log_simple', or 'log'")
end select
epa_mass = var_list%get_rval (var_str ("epa_mass"))
epa_recoil = var_list%get_lval (var_str ("?epa_recoil"))
epa_keep_energy = var_list%get_lval (var_str ("?epa_keep_energy"))
select type (data)
type is (epa_data_t)
    call data%init &
        (model, epa_int_mode, pdg_in (i_beam(1)), epa_alpha, &
        epa_x_min, epa_q_min, epa_q_max, epa_mass, &
        recoil = epa_recoil, keep_energy = epa_keep_energy)
    call data%check ()
end select
case ("ewa")
    allocate (ewa_data_t :: data)
    allocate (pdg_prc1 (size (pdg_prc, 2)))
    pdg_prc1 = pdg_prc(i_beam(1),:)
    if (any (pdg_array_get_length (pdg_prc1) /= 1) &
        .or. any (pdg_prc1 /= pdg_prc1(1))) then
        call msg_fatal &
            ("EWA: process incoming particle (W/Z) must be unique")
    end if
    ewa_id = abs (pdg_array_get (pdg_prc1(1), 1))
    ewa_x_min = var_list%get_rval (var_str ("ewa_x_min"))
    ewa_pt_max = var_list%get_rval (var_str ("ewa_pt_max"))
    if (vanishes (ewa_pt_max)) then
        ewa_pt_max = sqrts
    end if
    ewa_mass = var_list%get_rval (var_str ("ewa_mass"))
    ewa_recoil = var_list%get_lval (&
        var_str ("?ewa_recoil"))
    ewa_keep_energy = var_list%get_lval (&
        var_str ("?ewa_keep_energy"))
    select type (data)
    type is (ewa_data_t)
        call data%init &
            (model, pdg_in (i_beam(1)), ewa_x_min, &
            ewa_pt_max, sqrts, ewa_recoil, &
            ewa_keep_energy, ewa_mass)
        call data%set_id (ewa_id)
        call data%check ()
    end select
case ("circe1")
    allocate (circe1_data_t :: data)
    select type (data)
    type is (circe1_data_t)
        circe1_photon1 = &
            var_list%get_lval (var_str ("?circe1_photon1"))
        circe1_photon2 = &
            var_list%get_lval (var_str ("?circe1_photon2"))

```

```

    circe1_sqrts = &
        var_list%get_rval (var_str ("circe1_sqrts"))
    circe1_eps = &
        var_list%get_rval (var_str ("circe1_eps"))
    if (circe1_sqrts <= 0) circe1_sqrts = sqrts
    circe1_generate = &
        var_list%get_lval (var_str ("?circe1_generate"))
    circe1_version = &
        var_list%get_ival (var_str ("circe1_ver"))
    circe1_revision = &
        var_list%get_ival (var_str ("circe1_rev"))
    circe1_accelerator = &
        char (var_list%get_sval (var_str ("$circe1_acc")))
    circe1_chattiness = &
        var_list%get_ival (var_str ("circe1_chat"))
    circe1_with_radiation = &
        var_list%get_lval (var_str ("?circe1_with_radiation"))
    call data%init (model, pdg_in, circe1_sqrts, circe1_eps, &
        [circe1_photon1, circe1_photon2], &
        circe1_version, circe1_revision, circe1_accelerator, &
        circe1_chattiness, circe1_with_radiation)
    if (circe1_generate) then
        call msg_message ("CIRCE1: activating generator mode")
        call dispatch_rng_factory &
            (rng_factory, var_list_global, next_rng_seed)
        call update_rng_seed_in_var_list (var_list_global, next_rng_seed)
        call data%set_generator_mode (rng_factory)
    end if
end select
case ("circe2")
    allocate (circe2_data_t :: data)
    select type (data)
    type is (circe2_data_t)
        circe2_polarized = &
            var_list%get_lval (var_str ("?circe2_polarized"))
        circe2_file = &
            var_list%get_sval (var_str ("$circe2_file"))
        circe2_design = &
            var_list%get_sval (var_str ("$circe2_design"))
        call data%init (os_data, model, pdg_in, sqrts, &
            circe2_polarized, polarized, circe2_file, circe2_design)
        call msg_message ("CIRCE2: activating generator mode")
        call dispatch_rng_factory &
            (rng_factory, var_list_global, next_rng_seed)
        call update_rng_seed_in_var_list (var_list_global, next_rng_seed)
        call data%set_generator_mode (rng_factory)
    end select
case ("gaussian")
    allocate (gaussian_data_t :: data)
    select type (data)
    type is (gaussian_data_t)
        gaussian_spread = &
            [var_list%get_rval (var_str ("gaussian_spread1")), &
            var_list%get_rval (var_str ("gaussian_spread2"))]

```

```

        call dispatch_rng_factory &
            (rng_factory, var_list_global, next_rng_seed)
        call update_rng_seed_in_var_list (var_list_global, next_rng_seed)
        call data%init (model, pdg_in, gaussian_spread, rng_factory)
    end select
case ("beam_events")
    allocate (beam_events_data_t :: data)
    select type (data)
    type is (beam_events_data_t)
        beam_events_dir = os_data%whizard_beamsimpath
        beam_events_file = var_list%get_sval (&
            var_str ("beam_events_file"))
        beam_events_warn_eof = var_list%get_lval (&
            var_str ("beam_events_warn_eof"))
        call data%init (model, pdg_in, &
            beam_events_dir, beam_events_file, beam_events_warn_eof)
    end select
case ("energy_scan")
    escan_normalize = &
        var_list%get_lval (var_str ("energy_scan_normalize"))
    allocate (escan_data_t :: data)
    select type (data)
    type is (escan_data_t)
        if (escan_normalize) then
            call data%init (model, pdg_in)
        else
            call data%init (model, pdg_in, sqrts)
        end if
    end select
case default
    if (associated (dispatch_sf_data_extra)) then
        call dispatch_sf_data_extra (data, sf_method, i_beam, &
            sf_prop, var_list, var_list_global, model, os_data, sqrts, pdg_in, &
            pdg_prc, polarized)
    end if
    if (.not. allocated (data)) then
        call msg_fatal ("Structure function '" &
            // char (sf_method) // "' not implemented")
    end if
end select
if (allocated (data)) then
    allocate (pdg_out (size (pdg_prc, 1)))
    call data%get_pdg_out (pdg_out)
    do i = 1, size (i_beam)
        pdg_in(i_beam(i)) = pdg_out(i)
    end do
end if
end if
end subroutine dispatch_sf_data

```

This is a hook that allows us to inject further handlers for structure-function objects, in particular a test structure function.

```

<Dispatch beams: public>+≡
public :: dispatch_sf_data_extra

```

```

⟨Dispatch beams: variables⟩≡
  procedure (dispatch_sf_data), pointer :: &
    dispatch_sf_data_extra => null ()

```

This is an auxiliary procedure, used by the beam-structure expansion: tell for a given structure function name, whether it corresponds to a pair spectrum ($n = 2$), a single-particle structure function ($n = 1$), or nothing ($n = 0$). Though `energy_scan` can in principle also be a pair spectrum, it always has only one parameter.

```

⟨Dispatch beams: public⟩+≡
  public :: strfun_mode

```

```

⟨Dispatch beams: procedures⟩+≡
  function strfun_mode (name) result (n)
    type(string_t), intent(in) :: name
    integer :: n
    select case (char (name))
    case ("none")
      n = 0
    case ("sf_test_0", "sf_test_1")
      n = 1
    case ("pdf_builtin", "pdf_builtin_photon", &
          "lhpdf", "lhpdf_photon")
      n = 1
    case ("isr", "epa", "ewa")
      n = 1
    case ("circe1", "circe2")
      n = 2
    case ("gaussian")
      n = 2
    case ("beam_events")
      n = 2
    case ("energy_scan")
      n = 2
    case default
      n = -1
      call msg_bug ("Structure function '" // char (name) &
                    // "' not supported yet")
    end select
  end function strfun_mode

```

Dispatch a whole structure-function chain, given beam data and beam structure data.

This could be done generically, but we should look at the specific combination of structure functions in order to select appropriate mappings.

The `beam_structure` argument gets copied because we want to expand it to canonical form (one valid structure-function entry per record) before proceeding further.

The `pdg_prc` argument is the array of incoming flavors. The first index is the beam index, the second one the process component index. Each element is itself a PDG array, notrivial if there is a flavor sum for the incoming state of this component.

The dispatcher is divided in two parts. The first part configures the structure function data themselves. After this, we can configure the phase space for the elementary process.

```

<Dispatch beams: public>+≡
    public :: dispatch_sf_config

<Dispatch beams: procedures>+≡
    subroutine dispatch_sf_config (sf_config, sf_prop, beam_structure, &
        var_list, var_list_global, model, os_data, sqrts, pdg_prc)
        type(sf_config_t), dimension(:), allocatable, intent(out) :: sf_config
        type(sf_prop_t), intent(out) :: sf_prop
        type(beam_structure_t), intent(inout) :: beam_structure
        type(var_list_t), intent(in) :: var_list
        type(var_list_t), intent(inout) :: var_list_global
        class(model_data_t), target, intent(in) :: model
        type(os_data_t), intent(in) :: os_data
        real(default), intent(in) :: sqrts
        class(sf_data_t), allocatable :: sf_data
        type(beam_structure_t) :: beam_structure_tmp
        type(pdg_array_t), dimension(:,:), intent(in) :: pdg_prc
        type(string_t), dimension(:), allocatable :: prt_in
        type(pdg_array_t), dimension(:), allocatable :: pdg_in
        type(flavor_t) :: flv_in
        integer :: n_beam, n_record, i
        beam_structure_tmp = beam_structure
        call beam_structure_tmp%expand (strfun_mode)
        n_record = beam_structure_tmp%get_n_record ()
        allocate (sf_config (n_record))
        n_beam = beam_structure_tmp%get_n_beam ()
        if (n_beam > 0) then
            allocate (prt_in (n_beam), pdg_in (n_beam))
            prt_in = beam_structure_tmp%get_prt ()
            do i = 1, n_beam
                call flv_in%init (prt_in(i), model)
                pdg_in(i) = flv_in%get_pdg ()
            end do
        else
            n_beam = size (pdg_prc, 1)
            allocate (pdg_in (n_beam))
            pdg_in = pdg_prc(:,1)
        end if
        do i = 1, n_record
            call dispatch_sf_data (sf_data, &
                beam_structure_tmp%get_name (i), &
                beam_structure_tmp%get_i_entry (i), &
                sf_prop, var_list, var_list_global, model, os_data, sqrts, &
                pdg_in, pdg_prc, &
                beam_structure_tmp%polarized ())
            call sf_config(i)%init (beam_structure_tmp%get_i_entry (i), sf_data)
            deallocate (sf_data)
        end do
    end subroutine dispatch_sf_config

```

16.18.1 QCD coupling

Allocate the `alpha` (running coupling) component of the `qcd` block with a concrete implementation, depending on the variable settings in the `global` record.

If a fixed α_s is requested, we do not allocate the `qcd%alpha` object. In this case, the matrix element code will just take the model parameter as-is, which implies fixed α_s . If the object is allocated, the α_s value is computed and updated for each matrix-element call.

Also fetch the `alphas_nf` variable from the list and store it in the QCD record. This is not used in the α_s calculation, but the QCD record thus becomes a messenger for this user parameter.

```
(Dispatch beams: public)+≡
    public :: dispatch_qcd

(Dispatch beams: procedures)+≡
    subroutine dispatch_qcd (qcd, var_list, os_data)
        type(qcd_t), intent(inout) :: qcd
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        logical :: fixed, from_mz, from_pdf_builtin, from_lhapdf, from_lambda_qcd
        real(default) :: mz, alpha_val, lambda
        integer :: nf, order, lhpdf_member
        type(string_t) :: pdfset, lhpdf_dir, lhpdf_file
        call unpack_variables ()
        if (allocated (qcd%alpha)) deallocate (qcd%alpha)
        if (from_lhapdf .and. from_pdf_builtin) then
            call msg_fatal (" Mixing alphas evolution", &
                [var_str (" from LHAPDF and builtin PDF is not permitted")])
        end if
        select case (count ([from_mz, from_pdf_builtin, from_lhapdf, from_lambda_qcd]))
        case (0)
            if (fixed) then
                allocate (alpha_qcd_fixed_t :: qcd%alpha)
            else
                call msg_fatal ("QCD alpha: no calculation mode set")
            end if
        case (2:)
            call msg_fatal ("QCD alpha: calculation mode is ambiguous")
        case (1)
            if (fixed) then
                call msg_fatal ("QCD alpha: use '?alphas_is_fixed = false' for " // &
                    "running alphas")
            else if (from_mz) then
                allocate (alpha_qcd_from_scale_t :: qcd%alpha)
            else if (from_pdf_builtin) then
                allocate (alpha_qcd_pdf_builtin_t :: qcd%alpha)
            else if (from_lhapdf) then
                allocate (alpha_qcd_lhapdf_t :: qcd%alpha)
            else if (from_lambda_qcd) then
                allocate (alpha_qcd_from_lambda_t :: qcd%alpha)
            end if
            call msg_message ("QCD alpha: using a running strong coupling")
        end select
        call init_alpha ()
    end subroutine
```

```

    qcd%n_f = var_list%get_ival (var_str ("alphas_nf"))
contains
  <Dispatch qcd: dispatch qcd: procedures>
end subroutine dispatch_qcd

```

```

<Dispatch qcd: dispatch qcd: procedures>≡
subroutine unpack_variables ()
  fixed = var_list%get_lval (var_str ("?alphas_is_fixed"))
  from_mz = var_list%get_lval (var_str ("?alphas_from_mz"))
  from_pdf_builtin = &
    var_list%get_lval (var_str ("?alphas_from_pdf_builtin"))
  from_lhapdf = &
    var_list%get_lval (var_str ("?alphas_from_lhapdf"))
  from_lambda_qcd = &
    var_list%get_lval (var_str ("?alphas_from_lambda_qcd"))
  pdfset = var_list%get_sval (var_str ("pdf_builtin_set"))
  lambda = var_list%get_rval (var_str ("lambda_qcd"))
  nf = var_list%get_ival (var_str ("alphas_nf"))
  order = var_list%get_ival (var_str ("alphas_order"))
  lhpdf_dir = var_list%get_sval (var_str ("lhpdf_dir"))
  lhpdf_file = var_list%get_sval (var_str ("lhpdf_file"))
  lhpdf_member = var_list%get_ival (var_str ("lhpdf_member"))
  if (var_list%contains (var_str ("mZ"))) then
    mz = var_list%get_rval (var_str ("mZ"))
  else
    mz = MZ_REF
  end if
  if (var_list%contains (var_str ("alphas"))) then
    alpha_val = var_list%get_rval (var_str ("alphas"))
  else
    alpha_val = ALPHA_QCD_MZ_REF
  end if
end subroutine unpack_variables

```

```

<Dispatch qcd: dispatch qcd: procedures>+≡
subroutine init_alpha ()
  select type (alpha => qcd%alpha)
  type is (alpha_qcd_fixed_t)
    alpha%val = alpha_val
  type is (alpha_qcd_from_scale_t)
    alpha%mu_ref = mz
    alpha%ref = alpha_val
    alpha%order = order
    alpha%nf = nf
  type is (alpha_qcd_from_lambda_t)
    alpha%lambda = lambda
    alpha%order = order
    alpha%nf = nf
  type is (alpha_qcd_pdf_builtin_t)
    call alpha%init (pdfset, &
      os_data%pdf_builtin_datapath)
  type is (alpha_qcd_lhapdf_t)
    call alpha%init (lhpdf_file, lhpdf_member, lhpdf_dir)

```

```
end select  
end subroutine init_alpha
```


Chapter 17

Interface for Matrix Element Objects

These modules manage internal and, in particular, external matrix-element code.

prc_core We define the abstract `prc_core_t` type which handles all specific features of kinematics matrix-element evaluation that depend on a particular class of processes. This abstract type supplements the `prc_core_def_t` type and related types in another module. Together, they provide a complete set of matrix-element handlers that are implemented in the concrete types below.

These are the implementations:

prc_template_me Implements matrix-element code without actual content (trivial value), but full-fledged interface. This can be used for injecting user-defined matrix-element code.

prc_omega Matrix elements calculated by `O'MEGA` are the default for WHIZARD. Here, we provide all necessary support.

prc_external Matrix elements provided or using external (not `O'MEGA`) code or libraries. This is an abstract type, with concrete extensions below:

prc_external_test Concrete implementation of the external-code type, actually using some pre-defined test matrix elements.

prc_gosam Interface for matrix elements computed using `GoSam`.

prc_openloops Interface for matrix elements computed using `OpenLoops`.

prc_recola Interface for matrix elements computed using `Recola`.

prc_threshold Interface for matrix elements for the top-pair threshold, that use external libraries.

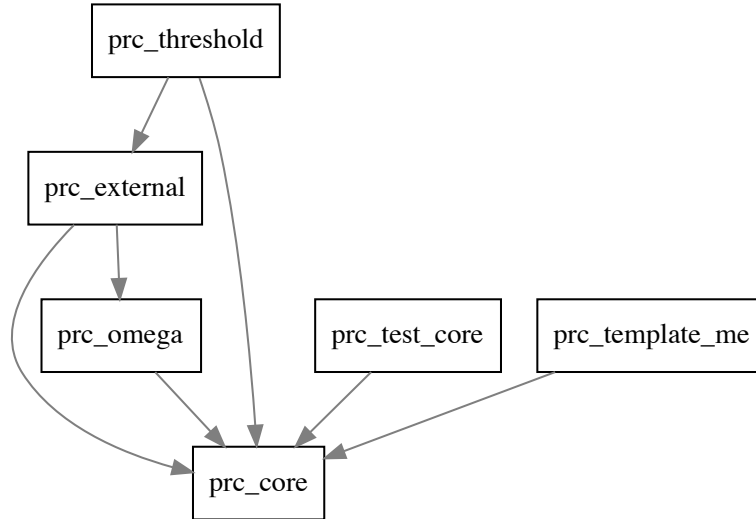


Figure 17.1: Module dependencies in `src/me_methods`.

17.1 Abstract process core

In this module we provide abstract data types for process classes. Each process class represents a set of processes which are handled by a common “method”, e.g., by the O’MEGA matrix-element generator. The process class is also able to select a particular implementation for the phase-space and integration modules.

For a complete implementation of a process class, we have to provide extensions of the following abstract types:

prc_core_def_t process and matrix-element configuration

prc_writer_t (optional) writing external matrix-element code

prc_driver_t accessing the matrix element (internal or external)

prc_core_t evaluating kinematics and matrix element. The process core also selects phase-space and integrator implementations as appropriate for the process class and configuration.

In the actual process-handling data structures, each process component contains an instance of such a process class as its core. This allows us to keep the `processes` module below, which supervises matrix-element evaluation, integration, and event generation, free of any reference to concrete implementations (for the process class, phase space, and integrator).

There are no unit tests, these are deferred to the `processes` module.

`<prc_core.f90>`≡
<File header>

```

module prc_core

  <Use kinds>
  <Use strings>
    use io_units
    use diagnostics
    use os_interface, only: os_data_t
    use lorentz
    use interactions
    use variables, only: var_list_t
    use model_data, only: model_data_t

    use process_constants
    use prc_core_def
    use process_libraries
    use sf_base

  <Standard module head>

  <Prc core: public>

  <Prc core: types>

  <Prc core: interfaces>

  contains

  <Prc core: procedures>

end module prc_core

```

17.1.1 The process core

The process core is of abstract data type. Different types of matrix elements will be represented by different implementations.

```

<Prc core: public>≡
  public :: prc_core_t

<Prc core: types>≡
  type, abstract :: prc_core_t
    class(prc_core_def_t), pointer :: def => null ()
    logical :: data_known = .false.
    type(process_constants_t) :: data
    class(prc_core_driver_t), allocatable :: driver
    logical :: use_color_factors = .false.
    integer :: nc = 3
  contains
    <Prc core: process core: TBP>
  end type prc_core_t

```

In any case there must be an output routine.

```

<Prc core: process core: TBP>≡
  procedure(prc_core_write), deferred :: write

```

```

<Prc core: interfaces>≡
  abstract interface
    subroutine prc_core_write (object, unit)
      import
        class(prc_core_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_core_write
  end interface

```

Just type the name of the actual core method.

```

<Prc core: process core: TBP>+≡
  procedure(prc_core_write_name), deferred :: write_name

<Prc core: interfaces>+≡
  abstract interface
    subroutine prc_core_write_name (object, unit)
      import
        class(prc_core_t), intent(in) :: object
        integer, intent(in), optional :: unit
    end subroutine prc_core_write_name
  end interface

```

For initialization, we assign a pointer to the process entry in the relevant library. This allows us to access all process functions via the implementation of `prc_core_t`.

We declare the object as `intent(inout)`, since just after allocation it may be useful to store some extra data in the object, which we can then use in the actual initialization. This applies to extensions of `prc_core` which override the `init` method.

```

<Prc core: process core: TBP>+≡
  procedure :: init => prc_core_init
  procedure :: base_init => prc_core_init

<Prc core: procedures>≡
  subroutine prc_core_init (object, def, lib, id, i_component)
    class(prc_core_t), intent(inout) :: object
    class(prc_core_def_t), intent(in), target :: def
    type(process_library_t), intent(in), target :: lib
    type(string_t), intent(in) :: id
    integer, intent(in) :: i_component
    object%def => def
    call lib%connect_process (id, i_component, object%data, object%driver)
    object%data_known = .true.
  end subroutine prc_core_init

```

Return true if the matrix element generation was successful. This can be tested by looking at the number of generated flavor states, which should be nonzero.

```

<Prc core: process core: TBP>+≡
  procedure :: has_matrix_element => prc_core_has_matrix_element

<Prc core: procedures>+≡
  function prc_core_has_matrix_element (object) result (flag)
    class(prc_core_t), intent(in) :: object

```

```

    logical :: flag
    flag = object%data%n_flv /= 0
end function prc_core_has_matrix_element

```

Return true if this process-core type needs extra code that has to be compiled and/or linked, beyond the default O'MEGA framework. This depends only on the concrete type, and the default is no.

```

<Prc core: process core: TBP>+≡
    procedure, nopass :: needs_external_code => prc_core_needs_external_code

<Prc core: procedures>+≡
    function prc_core_needs_external_code () result (flag)
        logical :: flag
        flag = .false.
    end function prc_core_needs_external_code

```

The corresponding procedure to create and load extra libraries. The base procedure must not be called but has to be overridden, if extra code is required.

```

<Prc core: process core: TBP>+≡
    procedure :: prepare_external_code => &
        prc_core_prepare_external_code

<Prc core: procedures>+≡
    subroutine prc_core_prepare_external_code &
        (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
        class(prc_core_t), intent(inout) :: core
        integer, intent(in), dimension(:,:), allocatable :: flv_states
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: libname
        type(model_data_t), intent(in), target :: model
        integer, intent(in) :: i_core
        logical, intent(in) :: is_nlo
        call core%write ()
        call msg_bug ("prc_core_prepare_external_code called &
            &but not overridden")
    end subroutine prc_core_prepare_external_code

```

Return true if this process-core type uses the BLHA interface. This depends only on the concrete type, and the default is no.

```

<Prc core: process core: TBP>+≡
    procedure, nopass :: uses_blha => prc_core_uses_blha

<Prc core: procedures>+≡
    function prc_core_uses_blha () result (flag)
        logical :: flag
        flag = .false.
    end function prc_core_uses_blha

```

Tell whether a particular combination of flavor/helicity/color state is allowed for the matrix element.

```

<Prc core: process core: TBP>+≡
    procedure(prc_core_is_allowed), deferred :: is_allowed

```

```

<Prc core: interfaces>+≡
  abstract interface
    function prc_core_is_allowed (object, i_term, f, h, c) result (flag)
      import
      class(prc_core_t), intent(in) :: object
      integer, intent(in) :: i_term, f, h, c
      logical :: flag
    end function prc_core_is_allowed
  end interface

```

Set the constant process data for a specific term. By default, these are the constants stored inside the object, ignoring the term index. Type extensions may override this and provide term-specific data.

```

<Prc core: process core: TBP>+≡
  procedure :: get_constants => prc_core_get_constants

<Prc core: procedures>+≡
  subroutine prc_core_get_constants (object, data, i_term)
    class(prc_core_t), intent(in) :: object
    type(process_constants_t), intent(out) :: data
    integer, intent(in) :: i_term
    data = object%data
  end subroutine prc_core_get_constants

```

The strong coupling is not among the process constants. The default implementation is to return a negative number, which indicates that α_s is not available. This may be overridden by an implementation that provides an (event-specific) value. The value can be stored in the process-specific workspace.

```

<Prc core: process core: TBP>+≡
  procedure :: get_alpha_s => prc_core_get_alpha_s

<Prc core: procedures>+≡
  function prc_core_get_alpha_s (object, core_state) result (alpha_qcd)
    class(prc_core_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qcd
    alpha_qcd = -1
  end function prc_core_get_alpha_s

```

We follow the same strategy for the electromagnetic coupling α_{em} .

```

<Prc core: process core: TBP>+≡
  procedure :: get_alpha_qed => prc_core_get_alpha_qed

<Prc core: procedures>+≡
  function prc_core_get_alpha_qed (object) result (alpha_qed)
    class(prc_core_t), intent(in) :: object
    real(default) :: alpha_qed
    alpha_qed = -1
  end function prc_core_get_alpha_qed

```

Setup an index mapping for flavor structures and helicities that give the same matrix element. The index mapping is according to the order of flavor structures known to the `prc_core` class. This procedure here acts as a fallback in case there is no overridden procedure in the `prc_core` extension.

```

<Prc core: process core: TBP>+≡
  procedure :: set_equivalent_flv_hel_indices => prc_core_set_equivalent_flv_hel_indices

<Prc core: procedures>+≡
  subroutine prc_core_set_equivalent_flv_hel_indices (object)
    class(prc_core_t), intent(inout) :: object
    integer :: i, n_flv, n_hel
    n_flv = object%data%n_flv
    n_hel = object%data%n_hel
    if (.not. allocated (object%data%eqv_flv_index)) &
      allocate (object%data%eqv_flv_index(n_flv))
    if (.not. allocated (object%data%eqv_hel_index)) &
      allocate (object%data%eqv_hel_index(n_hel))
    if (size (object%data%eqv_flv_index) /= n_flv) &
      call msg_bug ("BLHA Core: Size mismatch between eqv_flv_index and number of flavors.")
    if (size (object%data%eqv_hel_index) /= n_hel) &
      call msg_bug ("BLHA Core: Size mismatch between eqv_hel_index and number of helicities.")
    object%data%eqv_flv_index = [(i, i = 1, n_flv)]
    object%data%eqv_hel_index = [(i, i = 1, n_hel)]
  end subroutine prc_core_set_equivalent_flv_hel_indices

```

Get the index mappings for flavor and helicity mappings set up in `prc_core_get_equivalent_flv_index` or any overriding variation.

```

<Prc core: process core: TBP>+≡
  procedure :: get_equivalent_flv_index => prc_core_get_equivalent_flv_index
  procedure :: get_equivalent_hel_index => prc_core_get_equivalent_hel_index

<Prc core: procedures>+≡
  function prc_core_get_equivalent_flv_index (object) result (eqv_flv_index)
    class(prc_core_t), intent(in) :: object
    integer, dimension(:), allocatable :: eqv_flv_index
    eqv_flv_index = object%data%eqv_flv_index
  end function prc_core_get_equivalent_flv_index

  function prc_core_get_equivalent_hel_index (object) result (eqv_hel_index)
    class(prc_core_t), intent(in) :: object
    integer, dimension(:), allocatable :: eqv_hel_index
    eqv_hel_index = object%data%eqv_hel_index
  end function prc_core_get_equivalent_hel_index

```

Allocate the workspace associated to a process component. The default is that there is no workspace, so we do nothing. A type extension may override this and allocate a workspace object of appropriate type, which can be used in further calculations.

In any case, the `intent(out)` attribute deletes any previously allocated workspace.

```

<Prc core: process core: TBP>+≡
  procedure :: allocate_workspace => prc_core_ignore_workspace

```

```

<Prc core: procedures>+≡
  subroutine prc_core_ignore_workspace (object, core_state)
    class(prc_core_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
  end subroutine prc_core_ignore_workspace

```

Compute the momenta in the hard interaction, taking the seed kinematics as input. The `i_term` index tells us which term we want to compute. (The standard method is to just transfer the momenta to the hard interaction.)

```

<Prc core: process core: TBP>+≡
  procedure(prc_core_compute_hard_kinematics), deferred :: &
    compute_hard_kinematics

<Prc core: interfaces>+≡
  abstract interface
    subroutine prc_core_compute_hard_kinematics &
      (object, p_seed, i_term, int_hard, core_state)
    import
    class(prc_core_t), intent(in) :: object
    type(vector4_t), dimension(:), intent(in) :: p_seed
    integer, intent(in) :: i_term
    type(interaction_t), intent(inout) :: int_hard
    class(prc_core_state_t), intent(inout), allocatable :: core_state
  end subroutine prc_core_compute_hard_kinematics
end interface

```

Compute the momenta in the effective interaction, taking the hard kinematics as input. (This is called only if parton recombination is to be applied for the process variant.)

```

<Prc core: process core: TBP>+≡
  procedure(prc_core_compute_eff_kinematics), deferred :: &
    compute_eff_kinematics

<Prc core: interfaces>+≡
  abstract interface
    subroutine prc_core_compute_eff_kinematics &
      (object, i_term, int_hard, int_eff, core_state)
    import
    class(prc_core_t), intent(in) :: object
    integer, intent(in) :: i_term
    type(interaction_t), intent(in) :: int_hard
    type(interaction_t), intent(inout) :: int_eff
    class(prc_core_state_t), intent(inout), allocatable :: core_state
  end subroutine prc_core_compute_eff_kinematics
end interface

```

The process core must implement this function. Here, `j` is the index of the particular term we want to compute. The amplitude may depend on the factorization and renormalization scales.

The `core_state` (workspace) argument may be used if it is provided by the caller. Otherwise, the routine should compute the result directly.

```

<Prc core: process core: TBP>+≡
  procedure(prc_core_compute_amplitude), deferred :: compute_amplitude

```



```

<Prc core: interfaces>+=
  abstract interface
    function prc_core_compute_amplitude &
      (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
       core_state) result (amp)
    import
    complex(default) :: amp
    class(prc_core_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: &
      core_state
    end function prc_core_compute_amplitude
  end interface

```

17.1.2 Storage for intermediate results

The abstract `prc_core_state_t` type allows process cores to set up temporary workspace. The object is an extra argument for each of the individual calculations between kinematics setup and matrix-element evaluation.

```

<Prc core: public>+=
  public :: prc_core_state_t
<Prc core: types>+=
  type, abstract :: prc_core_state_t
  contains
    procedure(workspace_write), deferred :: write
    procedure(workspace_reset_new_kinematics), deferred :: reset_new_kinematics
  end type prc_core_state_t

```

For debugging, we should at least have an output routine.

```

<Prc core: interfaces>+=
  abstract interface
    subroutine workspace_write (object, unit)
    import
    class(prc_core_state_t), intent(in) :: object
    integer, intent(in), optional :: unit
    end subroutine workspace_write
  end interface

```

This is used during the NLO calculation, see there for more information.

```

<Prc core: interfaces>+=
  abstract interface
    subroutine workspace_reset_new_kinematics (object)
    import
    class(prc_core_state_t), intent(inout) :: object
    end subroutine workspace_reset_new_kinematics
  end interface

```

17.1.3 Helicity selection data

This is intended for use with O'MEGA, but may also be made available to other process methods. We set thresholds for counting the times a specific helicity amplitude is zero. When the threshold is reached, we skip this amplitude in subsequent calls.

For initializing the helicity counters, we need an object that holds the two parameters, the threshold (large real number) and the cutoff (integer).

A helicity value suppressed by more than **threshold** (a value which multiplies **epsilon**, to be compared with the average of the current amplitude, default is 10^{10}) is treated as zero. A matrix element is assumed to be zero and not called again if it has been zero **cutoff** times.

```

<Prc core: public>+≡
    public :: helicity_selection_t

<Prc core: types>+≡
    type :: helicity_selection_t
        logical :: active = .false.
        real(default) :: threshold = 0
        integer :: cutoff = 0
    contains
        <Prc core: helicity selection: TBP>
    end type helicity_selection_t

```

Output. If the selection is inactive, print nothing.

```

<Prc core: helicity selection: TBP>≡
    procedure :: write => helicity_selection_write

<Prc core: procedures>+≡
    subroutine helicity_selection_write (object, unit)
        class(helicity_selection_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (object%active) then
            write (u, "(3x,A)") "Helicity selection data:"
            write (u, "(5x,A,ES17.10)") &
                "threshold =", object%threshold
            write (u, "(5x,A,I0)") &
                "cutoff    = ", object%cutoff
        end if
    end subroutine helicity_selection_write

```

17.2 Test process type

For the following tests, we define a simple implementation of the abstract **prc_core_t**, designed such as to complement the **prc_test_t** process definition type.

Note that it is not given that the actual process is defined as **prc_test_t** type. We enforce this by calling **prc_test_create_library**. The driver component in

the process core will then become of type `prc_test_t`.

```

<prc_test_core.f90>≡
  <File header>

  module prc_test_core

    <Use kinds>
    use io_units
    use lorentz
    use interactions
    use prc_test
    use prc_core

    <Standard module head>

    <Prc test core: public>

    <Prc test core: types>

    contains

    <Prc test core: procedures>

    end module prc_test_core

    <Prc test core: public>≡
    public :: test_t

    <Prc test core: types>≡
    type, extends (prc_core_t) :: test_t
    contains
    <Prc test core: test type: TBP>
    end type test_t

    <Prc test core: test type: TBP>≡
    procedure :: write => test_write

    <Prc test core: procedures>≡
    subroutine test_write (object, unit)
      class(test_t), intent(in) :: object
      integer, intent(in), optional :: unit
      integer :: u
      u = given_output_unit (unit)
      write (u, "(3x,A)") "test type implementing prc_test"
    end subroutine test_write

    <Prc test core: test type: TBP>+≡
    procedure :: write_name => test_write_name

    <Prc test core: procedures>+≡
    subroutine test_write_name (object, unit)
      class(test_t), intent(in) :: object
      integer, intent(in), optional :: unit
      integer :: u
      u = given_output_unit (unit)

```

```

        write (u,"(1x,A)") "Core: prc_test"
    end subroutine test_write_name

```

This process type always needs a MC parameter set and a single term. This only state is always allowed.

```

<Prc test core: test type: TBP>+≡
    procedure :: needs_mcset => test_needs_mcset
    procedure :: get_n_terms => test_get_n_terms
    procedure :: is_allowed => test_is_allowed

<Prc test core: procedures>+≡
    function test_needs_mcset (object) result (flag)
        class(test_t), intent(in) :: object
        logical :: flag
        flag = .true.
    end function test_needs_mcset

    function test_get_n_terms (object) result (n)
        class(test_t), intent(in) :: object
        integer :: n
        n = 1
    end function test_get_n_terms

    function test_is_allowed (object, i_term, f, h, c) result (flag)
        class(test_t), intent(in) :: object
        integer, intent(in) :: i_term, f, h, c
        logical :: flag
        flag = .true.
    end function test_is_allowed

```

Transfer the generated momenta directly to the hard interaction in the (only) term. We assume that everything has been set up correctly, so the array fits.

```

<Prc test core: test type: TBP>+≡
    procedure :: compute_hard_kinematics => test_compute_hard_kinematics

<Prc test core: procedures>+≡
    subroutine test_compute_hard_kinematics &
        (object, p_seed, i_term, int_hard, core_state)
        class(test_t), intent(in) :: object
        type(vector4_t), dimension(:), intent(in) :: p_seed
        integer, intent(in) :: i_term
        type(interaction_t), intent(inout) :: int_hard
        class(prc_core_state_t), intent(inout), allocatable :: core_state
        call int_hard%set_momenta (p_seed)
    end subroutine test_compute_hard_kinematics

```

This procedure is not called for test_t, just a placeholder.

```

<Prc test core: test type: TBP>+≡
    procedure :: compute_eff_kinematics => test_compute_eff_kinematics

<Prc test core: procedures>+≡
    subroutine test_compute_eff_kinematics &
        (object, i_term, int_hard, int_eff, core_state)

```

```

class(test_t), intent(in) :: object
integer, intent(in) :: i_term
type(interaction_t), intent(in) :: int_hard
type(interaction_t), intent(inout) :: int_eff
class(prc_core_state_t), intent(inout), allocatable :: core_state
end subroutine test_compute_eff_kinematics

```

Transfer the incoming momenta of `p_seed` directly to the effective interaction, and vice versa for the outgoing momenta.

`int_hard` is left untouched since `int_eff` is an alias (via pointer) to it.

```

<Prc test core: test type: TBP>+≡
  procedure :: recover_kinematics => test_recover_kinematics

<Prc test core: procedures>+≡
  subroutine test_recover_kinematics &
    (object, p_seed, int_hard, int_eff, core_state)
    class(test_t), intent(in) :: object
    type(vector4_t), dimension(:), intent(inout) :: p_seed
    type(interaction_t), intent(inout) :: int_hard
    type(interaction_t), intent(inout) :: int_eff
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    integer :: n_in
    n_in = int_eff%get_n_in ()
    call int_eff%set_momenta (p_seed(1:n_in), outgoing = .false.)
    p_seed(n_in+1:) = int_eff%get_momenta (outgoing = .true.)
  end subroutine test_recover_kinematics

```

Compute the amplitude. The driver ignores all quantum numbers and, in fact, returns a constant. Nevertheless, we properly transfer the momentum vectors.

```

<Prc test core: test type: TBP>+≡
  procedure :: compute_amplitude => test_compute_amplitude

<Prc test core: procedures>+≡
  function test_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, core_state) &
    result (amp)
    class(test_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
    complex(default) :: amp
    real(default), dimension(:,:), allocatable :: parray
    integer :: i, n_tot
    select type (driver => object%driver)
    type is (prc_test_t)
      if (driver%scattering) then
        n_tot = 4
      else
        n_tot = 3
      end if
      allocate (parray (0:3,n_tot))

```

```

        forall (i = 1:n_tot) parray(:,i) = vector4_get_components (p(i))
        amp = driver%get_amplitude (parray)
    end select
end function test_compute_amplitude

```

17.3 Template matrix elements

Here, we provide template matrix elements that are in structure very similar to O'MEGA matrix elements, but do not need its infrastructure. Per default, the matrix elements are flat, i.e. they have the constant value one. Analogous to the O'MEGA implementation, this section implements the interface to the templates (via the makefile) and the driver.

```

<prc_template_me.f90>≡
  <File header>

  module prc_template_me

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use io_units
    use system_defs, only: TAB
    use diagnostics
    use os_interface
    use lorentz
    use flavors
    use interactions
    use model_data

    use particle_specifiers, only: new_prt_spec
    use process_constants
    use prclib_interfaces
    use prc_core_def
    use process_libraries
    use prc_core

    <Standard module head>

    <Template matrix elements: public>

    <Template matrix elements: types>

    <Template matrix elements: interfaces>

    contains

    <Template matrix elements: procedures>

  end module prc_template_me

```

17.3.1 Process definition

For the process definition we implement an extension of the `prc_core_def_t` abstract type.

```
<Template matrix elements: public>≡
    public :: template_me_def_t

<Template matrix elements: types>≡
    type, extends (prc_core_def_t) :: template_me_def_t
    contains
    <Template matrix elements: template ME def: TBP>
    end type template_me_def_t

<Template matrix elements: template ME def: TBP>≡
    procedure, nopass :: type_string => template_me_def_type_string

<Template matrix elements: procedures>≡
    function template_me_def_type_string () result (string)
        type(string_t) :: string
        string = "template"
    end function template_me_def_type_string
```

Initialization: allocate the writer for the template matrix element. Also set any data for this process that the writer needs.

```
<Template matrix elements: template ME def: TBP>+≡
    procedure :: init => template_me_def_init

<Template matrix elements: procedures>+≡
    subroutine template_me_def_init &
        (object, model, prt_in, prt_out, unity)
        class(template_me_def_t), intent(out) :: object
        class(model_data_t), intent(in), target :: model
        type(string_t), dimension(:), intent(in) :: prt_in
        type(string_t), dimension(:), intent(in) :: prt_out
        logical, intent(in) :: unity
        allocate (template_me_writer_t :: object%writer)
        select type (writer => object%writer)
        type is (template_me_writer_t)
            call writer%init (model, prt_in, prt_out, unity)
        end select
    end subroutine template_me_def_init
```

Write/read process- and method-specific data.

```
<Template matrix elements: template ME def: TBP>+≡
    procedure :: write => template_me_def_write

<Template matrix elements: procedures>+≡
    subroutine template_me_def_write (object, unit)
        class(template_me_def_t), intent(in) :: object
        integer, intent(in) :: unit
        select type (writer => object%writer)
        type is (template_me_writer_t)
            call writer%write (unit)
        end select
```

```
end subroutine template_me_def_write
```

```
<Template matrix elements: template ME def: TBP>+≡
  procedure :: read => template_me_def_read
```

```
<Template matrix elements: procedures>+≡
  subroutine template_me_def_read (object, unit)
    class(template_me_def_t), intent(out) :: object
    integer, intent(in) :: unit
    call msg_bug &
      ("WHIZARD template process definition: input not supported (yet)")
  end subroutine template_me_def_read
```

Allocate the driver for template matrix elements.

```
<Template matrix elements: template ME def: TBP>+≡
  procedure :: allocate_driver => template_me_def_allocate_driver

<Template matrix elements: procedures>+≡
  subroutine template_me_def_allocate_driver (object, driver, basename)
    class(template_me_def_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    allocate (template_me_driver_t :: driver)
  end subroutine template_me_def_allocate_driver
```

We need code:

```
<Template matrix elements: template ME def: TBP>+≡
  procedure, nopass :: needs_code => template_me_def_needs_code

<Template matrix elements: procedures>+≡
  function template_me_def_needs_code () result (flag)
    logical :: flag
    flag = .true.
  end function template_me_def_needs_code
```

These are the features that a template matrix element provides.

```
<Template matrix elements: template ME def: TBP>+≡
  procedure, nopass :: get_features => template_me_def_get_features

<Template matrix elements: procedures>+≡
  subroutine template_me_def_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (5))
    features = [ &
      var_str ("init"), &
      var_str ("update_alpha_s"), &
      var_str ("is_allowed"), &
      var_str ("new_event"), &
      var_str ("get_amplitude")]
  end subroutine template_me_def_get_features
```


The interface of the specific features.

<Template matrix elements: interfaces>≡

```

abstract interface
  subroutine init_t (par, scheme) bind(C)
  import
    real(c_default_float), dimension(*), intent(in) :: par
    integer(c_int), intent(in) :: scheme
  end subroutine init_t
end interface

abstract interface
  subroutine update_alpha_s_t (alpha_s) bind(C)
  import
    real(c_default_float), intent(in) :: alpha_s
  end subroutine update_alpha_s_t
end interface

abstract interface
  subroutine is_allowed_t (flv, hel, col, flag) bind(C)
  import
    integer(c_int), intent(in) :: flv, hel, col
    logical(c_bool), intent(out) :: flag
  end subroutine is_allowed_t
end interface

abstract interface
  subroutine new_event_t (p) bind(C)
  import
    real(c_default_float), dimension(0:3,*), intent(in) :: p
  end subroutine new_event_t
end interface

abstract interface
  subroutine get_amplitude_t (flv, hel, col, amp) bind(C)
  import
    integer(c_int), intent(in) :: flv, hel, col
    complex(c_default_complex), intent(out) :: amp
  end subroutine get_amplitude_t
end interface

```

Connect the template matrix element features with the process driver.

<Template matrix elements: template ME def: TBP>+≡

```

procedure :: connect => template_me_def_connect

```

<Template matrix elements: procedures>+≡

```

subroutine template_me_def_connect (def, lib_driver, i, proc_driver)
  class(template_me_def_t), intent(in) :: def
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
  integer(c_int) :: pid, fid
  type(c_funptr) :: fptr
  select type (proc_driver)
  type is (template_me_driver_t)

```

```

pid = i
fid = 1
call lib_driver%get_fptr (pid, fid, fptr)
call c_f_procpointer (fptr, proc_driver%init)
fid = 2
call lib_driver%get_fptr (pid, fid, fptr)
call c_f_procpointer (fptr, proc_driver%update_alpha_s)
fid = 3
call lib_driver%get_fptr (pid, fid, fptr)
call c_f_procpointer (fptr, proc_driver%is_allowed)
fid = 4
call lib_driver%get_fptr (pid, fid, fptr)
call c_f_procpointer (fptr, proc_driver%new_event)
fid = 5
call lib_driver%get_fptr (pid, fid, fptr)
call c_f_procpointer (fptr, proc_driver%get_amplitude)
end select
end subroutine template_me_def_connect

```

17.3.2 The Template Matrix element writer

Unlike O'MEGA, the template matrix element is directly written by the main WHIZARD program, so there will be no entry in the makefile for calling an external program. The template matrix element writer is responsible for writing interfaces and wrappers.

```

<Template matrix elements: types>+≡
type, extends (prc_writer_f_module_t) :: template_me_writer_t
class(model_data_t), pointer :: model => null ()
type(string_t) :: model_name
logical :: unity
type(string_t), dimension(:), allocatable :: prt_in
type(string_t), dimension(:), allocatable :: prt_out
integer :: n_in
integer :: n_out
integer :: n_tot
contains
<Template matrix elements: template ME writer: TBP>
end type template_me_writer_t

```

The reported type is the same as for the `template_me_def.t` type.

```

<Template matrix elements: template ME writer: TBP>≡
procedure, nopass :: type_name => template_me_writer_type_name
<Template matrix elements: procedures>+≡
function template_me_writer_type_name () result (string)
type(string_t) :: string
string = "template"
end function template_me_writer_type_name

```

Taking into account the prefix for template ME module names.

```

<Template matrix elements: template ME writer: TBP>+≡
procedure, nopass :: get_module_name => template_me_writer_get_module_name

```

```

<Template matrix elements: procedures>+≡
function template_me_writer_get_module_name (id) result (name)
  type(string_t) :: name
  type(string_t), intent(in) :: id
  name = "tpr_" // id
end function template_me_writer_get_module_name

```

Output. This is called by `template_me_def.write`.

```

<Template matrix elements: template ME writer: TBP>+≡
procedure :: write => template_me_writer_write

<Template matrix elements: procedures>+≡
subroutine template_me_writer_write (object, unit)
  class(template_me_writer_t), intent(in) :: object
  integer, intent(in) :: unit
  integer :: i, j
  write (unit, "(5x,A,I0)") "# incoming part. = ", object%n_in
  write (unit, "(7x,A)", advance="no") &
    "      Initial state: "
  do i = 1, object%n_in - 1
    write (unit, "(1x,A)", advance="no") char (object%prt_in(i))
  end do
  write (unit, "(1x,A)") char (object%prt_in(object%n_in))
  write (unit, "(5x,A,I0)") "# outgoing part. = ", object%n_out
  write (unit, "(7x,A)", advance="no") &
    "      Final state:  "
  do j = 1, object%n_out - 1
    write (unit, "(1x,A)", advance="no") char (object%prt_out(j))
  end do
  write (unit, "(1x,A)") char (object%prt_out(object%n_out))
  write (unit, "(5x,A,I0)") "# part. (total) = ", object%n_tot
end subroutine template_me_writer_write

```

Initialize with process data.

```

<Template matrix elements: template ME writer: TBP>+≡
procedure :: init => template_me_writer_init

<Template matrix elements: procedures>+≡
subroutine template_me_writer_init (writer, model, &
  prt_in, prt_out, unity)
  class(template_me_writer_t), intent(out) :: writer
  class(model_data_t), intent(in), target :: model
  type(string_t), dimension(:), intent(in) :: prt_in
  type(string_t), dimension(:), intent(in) :: prt_out
  logical, intent(in) :: unity
  writer%model => model
  writer%model_name = model%get_name ()
  writer%n_in = size (prt_in)
  writer%n_out = size (prt_out)
  writer%n_tot = size (prt_in) + size (prt_out)
  allocate (writer%prt_in (size (prt_in)), source = prt_in)
  allocate (writer%prt_out (size (prt_out)), source = prt_out)
  writer%unity = unity
end subroutine template_me_writer_init

```

The makefile is the driver file for the test matrix elements.

```

<Template matrix elements: template ME writer: TBP>+≡
    procedure :: write_makefile_code => template_me_write_makefile_code

<Template matrix elements: procedures>+≡
    subroutine template_me_write_makefile_code &
        (writer, unit, id, os_data, verbose, testflag)
        class(template_me_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: testflag
        write (unit, "(5A)") "SOURCES += ", char (id), ".f90"
        write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
        write (unit, "(5A)") "clean-", char (id), ":"
        if (verbose) then
            write (unit, "(5A)") TAB, "rm -f tpr-", char (id), ".mod"
            write (unit, "(5A)") TAB, "rm -f ", char (id), ".lo"
        else
            write (unit, "(5A)") TAB // '@echo " RM          ', &
                trim (char (id)), '.mod"'
            write (unit, "(5A)") TAB, "@rm -f tpr-", char (id), ".mod"
            write (unit, "(5A)") TAB // '@echo " RM          ', &
                trim (char (id)), '.lo"'
            write (unit, "(5A)") TAB, "@rm -f ", char (id), ".lo"
        end if
        write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".f90"
        write (unit, "(5A)") "CLEAN_OBJECTS += tpr-", char (id), ".mod"
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), ".lo"
        write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
        if (.not. verbose) then
            write (unit, "(5A)") TAB // '@echo " FC          " $@"
        end if
        write (unit, "(5A)") TAB, "$ (LTF_COMPILE) $<"
    end subroutine template_me_write_makefile_code

```

The source is written by this routine.

```

<Template matrix elements: template ME writer: TBP>+≡
    procedure :: write_source_code => template_me_write_source_code

<Template matrix elements: procedures>+≡
    subroutine template_me_write_source_code (writer, id)
        class(template_me_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
        integer, dimension(writer%n_in) :: prt_in, mult_in, col_in
        type(flavor_t), dimension(1:writer%n_in) :: flv_in
        integer, dimension(writer%n_out) :: prt_out, mult_out
        integer, dimension(writer%n_tot) :: prt, mult
        integer, dimension(:, :), allocatable :: sxxx
        integer :: dummy, status
        type(flavor_t), dimension(1:writer%n_out) :: flv_out
        type(string_t) :: proc_str, comment_str, col_str
    end subroutine template_me_write_source_code

```

```

integer :: u, i, j
integer :: hel, hel_in, hel_out, fac, factor, col_fac
type(string_t) :: filename
comment_str = ""
do i = 1, writer%n_in
    comment_str = comment_str // writer%prt_in(i) // " "
end do
do j = 1, writer%n_out
    comment_str = comment_str // writer%prt_out(j) // " "
end do
do i = 1, writer%n_in
    prt_in(i) = writer%model%get_pdg (writer%prt_in(i))
    call flv_in(i)%init (prt_in(i), writer%model)
    mult_in(i) = flv_in(i)%get_multiplicity ()
    col_in(i) = abs (flv_in(i)%get_color_type ())
    mult(i) = mult_in(i)
end do
do j = 1, writer%n_out
    prt_out(j) = writer%model%get_pdg (writer%prt_out(j))
    call flv_out(j)%init (prt_out(j), writer%model)
    mult_out(j) = flv_out(j)%get_multiplicity ()
    mult(writer%n_in + j) = mult_out(j)
end do
prt(1:writer%n_in) = prt_in(1:writer%n_in)
prt(writer%n_in+1:writer%n_tot) = prt_out(1:writer%n_out)
proc_str = converter (prt)
hel_in = product (mult_in)
hel_out = product (mult_out)
col_fac = product (col_in)
hel = hel_in * hel_out
fac = hel
dummy = 1
factor = 1
if (writer%n_out >= 3) then
    do i = 3, writer%n_out
        factor = factor * (i - 2) * (i - 1)
    end do
end if
factor = factor * col_fac
allocate (sxxx(1:hel,1:writer%n_tot))
call create_spin_table (dummy,hel,fac,mult,sxxx)
call msg_message ("Writing test matrix element for process '" &
    // char (id) // "'")
filename = id // ".f90"
u = free_unit ()
open (unit=u, file=char(filename), action="write")
write (u, "(A)") "! File generated automatically by WHIZARD"
write (u, "(A)") "! "
write (u, "(A)") "! Note that irresp. of what you demanded WHIZARD"
write (u, "(A)") "! treats this as colorless process "
write (u, "(A)") "! "
write (u, "(A)") "module tpr_" // char(id)
write (u, "(A)") " "
write (u, "(A)") " use kinds"

```

```

write (u, "(A)") " use omega_color, OCF => omega_color_factor"
write (u, "(A)") "
write (u, "(A)") " implicit none"
write (u, "(A)") " private"
write (u, "(A)") "
write (u, "(A)") " public :: md5sum"
write (u, "(A)") " public :: number_particles_in, number_particles_out"
write (u, "(A)") " public :: number_spin_states, spin_states"
write (u, "(A)") " public :: number_flavor_states, flavor_states"
write (u, "(A)") " public :: number_color_flows, color_flows"
write (u, "(A)") " public :: number_color_indices, number_color_factors, &"
write (u, "(A)") " color_factors, color_sum, openmp_supported"
write (u, "(A)") " public :: init, final, update_alpha_s"
write (u, "(A)") "
write (u, "(A)") " public :: new_event, is_allowed, get_amplitude"
write (u, "(A)") "
write (u, "(A)") " real(default), parameter :: &"
write (u, "(A)") " & conv = 0.38937966e12_default"
write (u, "(A)") "
write (u, "(A)") " real(default), parameter :: &"
write (u, "(A)") " & pi = 3.1415926535897932384626433832795028841972_default"
write (u, "(A)") "
write (u, "(A)") " real(default), parameter :: &"
if (writer%unity) then
write (u, "(A)") " & const = 1"
else
write (u, "(A,1x,I0,A)") " & const = (16 * pi / conv) * " &
// "(16 * pi**2)**(", writer%n_out, "-2) "
end if
write (u, "(A)") "
write (u, "(A,1x,I0)") " integer, parameter, private :: n_prt = ", &
writer%n_tot
write (u, "(A,1x,I0)") " integer, parameter, private :: n_in = ", &
writer%n_in
write (u, "(A,1x,I0)") " integer, parameter, private :: n_out = ", &
writer%n_out
write (u, "(A)") " integer, parameter, private :: n_cflow = 1"
write (u, "(A)") " integer, parameter, private :: n_cindex = 2"
write (u, "(A)") " !!! We ignore tensor products and take only one flavor state."
write (u, "(A)") " integer, parameter, private :: n_flg = 1"
write (u, "(A,1x,I0)") " integer, parameter, private :: n_hel = ", hel
write (u, "(A)") "
write (u, "(A)") " logical, parameter, private :: T = .true."
write (u, "(A)") " logical, parameter, private :: F = .false."
write (u, "(A)") "
do i = 1, hel
write (u, "(A)") " integer, dimension(n_prt), parameter, private :: &"
write (u, "(A)") " " // s_conv(i) // " = [ " // &
char(converter(sxxx(i,1:writer%n_tot))) // " ]"
end do
write (u, "(A)") " integer, dimension(n_prt,n_hel), parameter, private :: table_spin_states =
write (u, "(A)") " reshape ( [ & "
do i = 1, hel-1
write (u, "(A)") " " // s_conv(i) // ", & "

```

```

end do
write (u, "(A)") " " // s_conv(hel) // " & "
write (u, "(A)") " ], [ n_prt, n_hel ] )"
write (u, "(A)") " "
write (u, "(A)") " integer, dimension(n_prt), parameter, private :: &"
write (u, "(A)") " f0001 = [ " // char(proc_str) // " ] ! " // char(comment_str)
write (u, "(A)") " integer, dimension(n_prt,n_flv), parameter, private :: table_flavor_states
write (u, "(A)") " reshape ( [ f0001 ], [ n_prt, n_flv ] )"
write (u, "(A)") " "
write (u, "(A)") " integer, dimension(n_cindex, n_prt), parameter, private :: &"
!!! This produces non-matching color flows, better keep it completely colorless
! write (u, "(A)") " c0001 = reshape ( [ " // char (dummy_colorizer (flv_in)) // &
! " " // &
select case (writer%n_in)
case (1)
col_str = "0,0,"
case (2)
col_str = "0,0,0,0,"
end select
write (u, "(A)") " c0001 = reshape ( [ " // char (col_str) // &
(repeat ("0,0, ", writer%n_out-1)) // "0,0 ], " // " [ n_cindex, n_prt ] )"
write (u, "(A)") " integer, dimension(n_cindex, n_prt, n_cflow), parameter, private :: &"
write (u, "(A)") " table_color_flows = reshape ( [ c0001 ], [ n_cindex, n_prt, n_cflow ] )"
write (u, "(A)") " "
write (u, "(A)") " logical, dimension(n_prt), parameter, private :: & "
write (u, "(A)") " g0001 = [ " // (repeat ("F, ", writer%n_tot-1)) // "F ] "
write (u, "(A)") " logical, dimension(n_prt, n_cflow), parameter, private " &
// ":: table_ghost_flags = &"
write (u, "(A)") " reshape ( [ g0001 ], [ n_prt, n_cflow ] )"
write (u, "(A)") " "
write (u, "(A)") " integer, parameter, private :: n_cfactors = 1"
write (u, "(A)") " type(OCF), dimension(n_cfactors), parameter, private :: &"
write (u, "(A)") " table_color_factors = [ OCF(1,1,+1._default) ]"
write (u, "(A)") " "
write (u, "(A)") " logical, dimension(n_flv), parameter, private :: a0001 = [ T ]"
write (u, "(A)") " logical, dimension(n_flv, n_cflow), parameter, private :: &"
write (u, "(A)") " flv_col_is_allowed = reshape ( [ a0001 ], [ n_flv, n_cflow ] )"
write (u, "(A)") " "
write (u, "(A)") " complex(default), dimension (n_flv, n_hel, n_cflow), private, save :: amp"
write (u, "(A)") " "
write (u, "(A)") " logical, dimension(n_hel), private, save :: hel_is_allowed = T"
write (u, "(A)") " "
write (u, "(A)") "contains"
write (u, "(A)") " "
write (u, "(A)") " pure function md5sum ()"
write (u, "(A)") " character(len=32) :: md5sum"
write (u, "(A)") " ! DON'T EVEN THINK of modifying the following line!"
write (u, "(A)") " md5sum = "" // writer%md5sum // ""
write (u, "(A)") " end function md5sum"
write (u, "(A)") " "
write (u, "(A)") " subroutine init (par, scheme)"
write (u, "(A)") " real(default), dimension(*), intent(in) :: par"
write (u, "(A)") " integer, intent(in) :: scheme"
write (u, "(A)") " end subroutine init"

```

```

write (u, "(A)") "
write (u, "(A)") " subroutine final ()
write (u, "(A)") " end subroutine final
write (u, "(A)") "
write (u, "(A)") " subroutine update_alpha_s (alpha_s)
write (u, "(A)") "   real(default), intent(in) :: alpha_s
write (u, "(A)") " end subroutine update_alpha_s
write (u, "(A)") "
write (u, "(A)") " pure function number_particles_in () result (n)
write (u, "(A)") "   integer :: n
write (u, "(A)") "   n = n_in
write (u, "(A)") " end function number_particles_in
write (u, "(A)") "
write (u, "(A)") " pure function number_particles_out () result (n)
write (u, "(A)") "   integer :: n
write (u, "(A)") "   n = n_out
write (u, "(A)") " end function number_particles_out
write (u, "(A)") "
write (u, "(A)") " pure function number_spin_states () result (n)
write (u, "(A)") "   integer :: n
write (u, "(A)") "   n = size (table_spin_states, dim=2)
write (u, "(A)") " end function number_spin_states
write (u, "(A)") "
write (u, "(A)") " pure subroutine spin_states (a)
write (u, "(A)") "   integer, dimension(:,,:), intent(out) :: a
write (u, "(A)") "   a = table_spin_states
write (u, "(A)") " end subroutine spin_states
write (u, "(A)") "
write (u, "(A)") " pure function number_flavor_states () result (n)
write (u, "(A)") "   integer :: n
write (u, "(A)") "   n = 1
write (u, "(A)") " end function number_flavor_states
write (u, "(A)") "
write (u, "(A)") " pure subroutine flavor_states (a)
write (u, "(A)") "   integer, dimension(:,,:), intent(out) :: a
write (u, "(A)") "   a = table_flavor_states
write (u, "(A)") " end subroutine flavor_states
write (u, "(A)") "
write (u, "(A)") " pure function number_color_indices () result (n)
write (u, "(A)") "   integer :: n
write (u, "(A)") "   n = size(table_color_flows, dim=1)
write (u, "(A)") " end function number_color_indices
write (u, "(A)") "
write (u, "(A)") " pure subroutine color_factors (cf)
write (u, "(A)") "   type(OCF), dimension(:,), intent(out) :: cf
write (u, "(A)") "   cf = table_color_factors
write (u, "(A)") " end subroutine color_factors
write (u, "(A)") "
!pure unless OpenMP
!write (u, "(A)") " pure function color_sum (flv, hel) result (amp2)
write (u, "(A)") " function color_sum (flv, hel) result (amp2)
write (u, "(A)") "   integer, intent(in) :: flv, hel
write (u, "(A)") "   real(kind=default) :: amp2
write (u, "(A)") "   amp2 = real (omega_color_sum (flv, hel, amp, table_color_factors))

```



```

write (u, "(A)") " end function color_sum"
write (u, "(A)") "
write (u, "(A)") " pure function number_color_flows () result (n)"
write (u, "(A)") " integer :: n"
write (u, "(A)") " n = size (table_color_flows, dim=3)"
write (u, "(A)") " end function number_color_flows"
write (u, "(A)") "
write (u, "(A)") " pure subroutine color_flows (a, g)"
write (u, "(A)") " integer, dimension(:,:,:), intent(out) :: a"
write (u, "(A)") " logical, dimension(:,:), intent(out) :: g"
write (u, "(A)") " a = table_color_flows"
write (u, "(A)") " g = table_ghost_flags"
write (u, "(A)") " end subroutine color_flows"
write (u, "(A)") "
write (u, "(A)") " pure function number_color_factors () result (n)"
write (u, "(A)") " integer :: n"
write (u, "(A)") " n = size (table_color_factors)"
write (u, "(A)") " end function number_color_factors"
write (u, "(A)") "
write (u, "(A)") " pure function openmp_supported () result (status)"
write (u, "(A)") " logical :: status"
write (u, "(A)") " status = .false."
write (u, "(A)") " end function openmp_supported"
write (u, "(A)") "
write (u, "(A)") " subroutine new_event (p)"
write (u, "(A)") " real(default), dimension(0:3,*), intent(in) :: p"
write (u, "(A)") " call calculate_amplitudes (amp, p)"
write (u, "(A)") " end subroutine new_event"
write (u, "(A)") "
write (u, "(A)") " pure function is_allowed (flv, hel, col) result (yorn)"
write (u, "(A)") " logical :: yorn"
write (u, "(A)") " integer, intent(in) :: flv, hel, col"
write (u, "(A)") " yorn = hel_is_allowed(hel) .and. flv_col_is_allowed(fl, col)"
write (u, "(A)") " end function is_allowed"
write (u, "(A)") "
write (u, "(A)") " pure function get_amplitude (flv, hel, col) result (amp_result)"
write (u, "(A)") " complex(default) :: amp_result"
write (u, "(A)") " integer, intent(in) :: flv, hel, col"
write (u, "(A)") " amp_result = amp (flv, hel, col)"
write (u, "(A)") " end function get_amplitude"
write (u, "(A)") "
write (u, "(A)") " pure subroutine calculate_amplitudes (amp, k)"
write (u, "(A)") " complex(default), dimension(:,:,:), intent(out) :: amp"
write (u, "(A)") " real(default), dimension(0:3,*), intent(in) :: k"
write (u, "(A)") " real(default) :: fac"
write (u, "(A)") " integer :: i"
write (u, "(A)") " ! We give all helicities the same weight!"
if (writer%unity) then
  write (u, "(A,1x,I0,1x,A)") " fac = ", col_fac
  write (u, "(A)") " amp = const * sqrt(fac)"
else
  write (u, "(A,1x,I0,1x,A)") " fac = ", factor
  write (u, "(A)") " amp = sqrt((2 * (k(0,1)*k(0,2) &
  write (u, "(A,1x,I0,A)") " - dot_product (k(1:,1), k(1:,2)))) ** (3-, &

```

```

writer%n_out, ")) * sqrt(const * fac)"
end if
write (u, "(A,1x,I0,A)") "    amp = amp / sqrt(", hel_out, "._default)"
write (u, "(A)") "    end subroutine calculate_amplitudes"
write (u, "(A)") "
write (u, "(A)") "end module tpr_" // char(id)
close (u, iostat=status)
deallocate (sxxx)
contains
function s_conv (num) result (chrt)
    integer, intent(in) :: num
    character(len=10) :: chrt
    write (chrt, "(I10)") num
    chrt = trim(adjustl(chrt))
    if (num < 10) then
        chrt = "s000" // chrt
    else if (num < 100) then
        chrt = "s00" // chrt
    else if (num < 1000) then
        chrt = "s0" // chrt
    else
        chrt = "s" // chrt
    end if
end function s_conv
function converter (flv) result (str)
    integer, dimension(:), intent(in) :: flv
    type(string_t) :: str
    character(len=150), dimension(size(flv)) :: chrt
    integer :: i
    str = ""
    do i = 1, size(flv) - 1
        write (chrt(i), "(I10)") flv(i)
        str = str // var_str(trim(adjustl(chrt(i)))) // ", "
    end do
    write (chrt(size(flv)), "(I10)") flv(size(flv))
    str = str // trim(adjustl(chrt(size(flv))))
end function converter
integer function sj (j,m)
    integer, intent(in) :: j, m
    if (((j == 1) .and. (m == 1)) .or. &
        ((j == 2) .and. (m == 2)) .or. &
        ((j == 3) .and. (m == 3)) .or. &
        ((j == 4) .and. (m == 3)) .or. &
        ((j == 5) .and. (m == 4))) then
        sj = 1
    else if (((j == 2) .and. (m == 1)) .or. &
        ((j == 3) .and. (m == 1)) .or. &
        ((j == 4) .and. (m == 2)) .or. &
        ((j == 5) .and. (m == 2))) then
        sj = -1
    else if (((j == 3) .and. (m == 2)) .or. &
        ((j == 5) .and. (m == 3))) then
        sj = 0
    else if (((j == 4) .and. (m == 1)) .or. &

```

```

        ((j == 5) .and. (m == 1))) then
            sj = -2
        else if (((j == 4) .and. (m == 4)) .or. &
            ((j == 5) .and. (m == 5))) then
            sj = 2
        else
            call msg_fatal ("template_me_write_source_code: Wrong spin type")
        end if
    end function sj
    recursive subroutine create_spin_table (index, nhel, fac, mult, inta)
        integer, intent(inout) :: index, fac
        integer, intent(in) :: nhel
        integer, dimension(:), intent(in) :: mult
        integer, dimension(nhel,size(mult)), intent(out) :: inta
        integer :: j
        if (index > size(mult)) return
        fac = fac / mult(index)
        do j = 1, nhel
            inta(j,index) = sj (mult(index),mod(((j-1)/fac),mult(index))+1)
        end do
        index = index + 1
        call create_spin_table (index, nhel, fac, mult, inta)
    end subroutine create_spin_table
    function dummy_colorizer (flv) result (str)
        type(flavor_t), dimension(:), intent(in) :: flv
        type(string_t) :: str
        integer :: i, k
        str = ""
        k = 0
        do i = 1, size(flvr)
            k = k + 1
            select case (flvr(i)%get_color_type ())
            case (1,-1)
                str = str // "0,0, "
            case (3)
                str = str // int2string(k) // ",0, "
            case (-3)
                str = str // "0," // int2string(-k) // ", "
            case (8)
                str = str // int2string(k) // "," // int2string(-k-1) // ", "
                k = k + 1
            case default
                call msg_error ("Color type not supported.")
            end select
        end do
        str = adjustl(trim(str))
    end function dummy_colorizer
end subroutine template_me_write_source_code

```

Nothing to be done here.

```

<Template matrix elements: template ME writer: TBP>+≡
    procedure :: before_compile => template_me_before_compile
    procedure :: after_compile => template_me_after_compile

```

```

<Template matrix elements: procedures>+≡
  subroutine template_me_before_compile (writer, id)
    class(template_me_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
  end subroutine template_me_before_compile

  subroutine template_me_after_compile (writer, id)
    class(template_me_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
  end subroutine template_me_after_compile

```

Return the name of a procedure that implements a given feature, as it is provided by the template matrix-element code. Template ME names are chosen completely in analogy to the O'MEGA matrix element conventions.

```

<Template matrix elements: template ME writer: TBP>+≡
  procedure, nopass :: get_procname => template_me_writer_get_procname

```

```

<Template matrix elements: procedures>+≡
  function template_me_writer_get_procname (feature) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: feature
    select case (char (feature))
      case ("n_in");   name = "number_particles_in"
      case ("n_out");  name = "number_particles_out"
      case ("n_flv");  name = "number_flavor_states"
      case ("n_hel");  name = "number_spin_states"
      case ("n_col");  name = "number_color_flows"
      case ("n_cin");  name = "number_color_indices"
      case ("n_cf");   name = "number_color_factors"
      case ("flv_state"); name = "flavor_states"
      case ("hel_state"); name = "spin_states"
      case ("col_state"); name = "color_flows"
      case default
        name = feature
      end select
  end function template_me_writer_get_procname

```

The interfaces for the template-specific features.

```

<Template matrix elements: template ME writer: TBP>+≡
  procedure :: write_interface => template_me_write_interface

<Template matrix elements: procedures>+≡
  subroutine template_me_write_interface (writer, unit, id, feature)
    class(template_me_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(string_t), intent(in) :: feature
    type(string_t) :: name
    name = writer%get_c_procname (id, feature)
    write (unit, "(2x,9A)") "interface"
    select case (char (feature))
      case ("init")
        write (unit, "(5x,9A)") "subroutine ", char (name), &
          " (par, scheme) bind(C)"

```

```

        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "real(c_default_float), dimension(*), &
            &intent(in) :: par"
        write (unit, "(7x,9A)") "integer(c_int), intent(in) :: scheme"
        write (unit, "(5x,9A)") "end subroutine ", char (name)
    case ("update_alpha_s")
        write (unit, "(5x,9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: alpha_s"
        write (unit, "(5x,9A)") "end subroutine ", char (name)
    case ("is_allowed")
        write (unit, "(5x,9A)") "subroutine ", char (name), " &
            &(flv, hel, col, flag) bind(C)"
        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
        write (unit, "(7x,9A)") "logical(c_bool), intent(out) :: flag"
        write (unit, "(5x,9A)") "end subroutine ", char (name)
    case ("new_event")
        write (unit, "(5x,9A)") "subroutine ", char (name), " (p) bind(C)"
        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "real(c_default_float), dimension(0:3,*), &
            &intent(in) :: p"
        write (unit, "(5x,9A)") "end subroutine ", char (name)
    case ("get_amplitude")
        write (unit, "(5x,9A)") "subroutine ", char (name), " &
            &(flv, hel, col, amp) bind(C)"
        write (unit, "(7x,9A)") "import"
        write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
        write (unit, "(7x,9A)") "complex(c_default_complex), intent(out) &
            &:: amp"
        write (unit, "(5x,9A)") "end subroutine ", char (name)
    end select
    write (unit, "(2x,9A)") "end interface"
end subroutine template_me_write_interface

```

The wrappers have to take into account conversion between C and Fortran data types.

NOTE: The case `c_default_float` \neq `default` is not yet covered.

<Template matrix elements: template ME writer: TBP>+≡

```

    procedure :: write_wrapper => template_me_write_wrapper

```

<Template matrix elements: procedures>+≡

```

    subroutine template_me_write_wrapper (writer, unit, id, feature)
        class(template_me_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id, feature
        type(string_t) :: name
        name = writer%get_c_procname (id, feature)
        write (unit, *)
        select case (char (feature))
        case ("init")
            write (unit, "(9A)") "subroutine ", char (name), &
                " (par, scheme) bind(C)"
            write (unit, "(2x,9A)") "use iso_c_binding"

```

```

write (unit, "(2x,9A)") "use kinds"
write (unit, "(2x,9A)") "use tpr_", char (id)
write (unit, "(2x,9A)") "real(c_default_float), dimension(*), &
    &intent(in) :: par"
write (unit, "(2x,9A)") "integer(c_int), intent(in) :: scheme"
if (c_default_float == default .and. c_int == kind(1)) then
    write (unit, "(2x,9A)") "call ", char (feature), " (par, scheme)"
end if
write (unit, "(9A)") "end subroutine ", char (name)
case ("update_alpha_s")
write (unit, "(9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
write (unit, "(2x,9A)") "use iso_c_binding"
write (unit, "(2x,9A)") "use kinds"
write (unit, "(2x,9A)") "use tpr_", char (id)
if (c_default_float == default) then
    write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
        &:: alpha_s"
    write (unit, "(2x,9A)") "call ", char (feature), " (alpha_s)"
end if
write (unit, "(9A)") "end subroutine ", char (name)
case ("is_allowed")
write (unit, "(9A)") "subroutine ", char (name), &
    " (flv, hel, col, flag) bind(C)"
write (unit, "(2x,9A)") "use iso_c_binding"
write (unit, "(2x,9A)") "use kinds"
write (unit, "(2x,9A)") "use tpr_", char (id)
write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
write (unit, "(2x,9A)") "logical(c_bool), intent(out) :: flag"
write (unit, "(2x,9A)") "flag = ", char (feature), &
    " (int (flv), int (hel), int (col))"
write (unit, "(9A)") "end subroutine ", char (name)
case ("new_event")
write (unit, "(9A)") "subroutine ", char (name), " (p) bind(C)"
write (unit, "(2x,9A)") "use iso_c_binding"
write (unit, "(2x,9A)") "use kinds"
write (unit, "(2x,9A)") "use tpr_", char (id)
if (c_default_float == default) then
    write (unit, "(2x,9A)") "real(c_default_float), dimension(0:3,*), &
        &intent(in) :: p"
    write (unit, "(2x,9A)") "call ", char (feature), " (p)"
end if
write (unit, "(9A)") "end subroutine ", char (name)
case ("get_amplitude")
write (unit, "(9A)") "subroutine ", char (name), &
    " (flv, hel, col, amp) bind(C)"
write (unit, "(2x,9A)") "use iso_c_binding"
write (unit, "(2x,9A)") "use kinds"
write (unit, "(2x,9A)") "use tpr_", char (id)
write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
write (unit, "(2x,9A)") "complex(c_default_complex), intent(out) &
    &:: amp"
write (unit, "(2x,9A)") "amp = ", char (feature), &
    " (int (flv), int (hel), int (col))"
write (unit, "(9A)") "end subroutine ", char (name)

```

```

end select
end subroutine template_me_write_wrapper

```

17.3.3 Driver

```

<Template matrix elements: public>+≡
public :: template_me_driver_t

<Template matrix elements: types>+≡
type, extends (prc_core_driver_t) :: template_me_driver_t
  procedure(init_t), nopass, pointer :: &
    init => null ()
  procedure(update_alpha_s_t), nopass, pointer :: &
    update_alpha_s => null ()
  procedure(is_allowed_t), nopass, pointer :: &
    is_allowed => null ()
  procedure(new_event_t), nopass, pointer :: &
    new_event => null ()
  procedure(get_amplitude_t), nopass, pointer :: &
    get_amplitude => null ()
contains
  <Template matrix elements: template ME driver: TBP>
end type template_me_driver_t

```

The reported type is the same as for the `template_me_def_t` type.

```

<Template matrix elements: template ME driver: TBP>≡
  procedure, nopass :: type_name => template_me_driver_type_name

<Template matrix elements: procedures>+≡
function template_me_driver_type_name () result (string)
  type(string_t) :: string
  string = "template"
end function template_me_driver_type_name

```

17.3.4 High-level process definition

This procedure wraps the details filling a process-component definition entry as appropriate for an template matrix element.

```

<Template matrix elements: public>+≡
public :: template_me_make_process_component

<Template matrix elements: procedures>+≡
subroutine template_me_make_process_component (entry, component_index, &
  model, model_name, prt_in, prt_out, unity)
  class(process_def_entry_t), intent(inout) :: entry
  integer, intent(in) :: component_index
  type(string_t), intent(in) :: model_name
  class(model_data_t), intent(in), target :: model
  type(string_t), dimension(:), intent(in) :: prt_in
  type(string_t), dimension(:), intent(in) :: prt_out
  logical, intent(in) :: unity
  class(prc_core_def_t), allocatable :: def

```

```

allocate (template_me_def_t :: def)
select type (def)
type is (template_me_def_t)
    call def%init (model, prt_in, prt_out, unity)
end select
call entry%import_component (component_index, &
    n_out = size (prt_out), &
    prt_in  = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("template"), &
    variant = def)
end subroutine template_me_make_process_component

```

17.3.5 The prc_template_me_t wrapper

This is an instance of the generic prc_core_t object. It contains a pointer to the process definition (template_me_def_t), a data component (process_constants_t), and the matrix-element driver (template_me_driver_t).

```

<Template matrix elements: public>+≡
public :: prc_template_me_t

<Template matrix elements: types>+≡
type, extends (prc_core_t) :: prc_template_me_t
    real(default), dimension(:), allocatable :: par
    integer :: scheme = 0
contains
    <Template matrix elements: prc template ME: TBP>
end type prc_template_me_t

```

The workspace associated to a prc_template_me_t object contains a single flag. The flag is used to suppress re-evaluating the matrix element for each quantum-number combination, after the first amplitude belonging to a given kinematics has been computed.

We can also store the value of a running coupling once it has been calculated for an event. The default value is negative, which indicates an undefined value in this context.

```

<Template matrix elements: types>+≡
type, extends (prc_core_state_t) :: template_me_state_t
    logical :: new_kinematics = .true.
    real(default) :: alpha_qcd = -1
contains
    procedure :: write => template_me_state_write
    procedure :: reset_new_kinematics => template_me_state_reset_new_kinematics
end type template_me_state_t

<Template matrix elements: procedures>+≡
subroutine template_me_state_write (object, unit)
    class(template_me_state_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)

```



```

        write (u, "(3x,A,L1)") "Template ME state: new kinematics = ", &
            object%new_kinematics
    end subroutine template_me_state_write

```

```

<Template matrix elements: procedures>+≡
    subroutine template_me_state_reset_new_kinematics (object)
        class(template_me_state_t), intent(inout) :: object
    end subroutine template_me_state_reset_new_kinematics

```

Allocate the workspace with the above specific type.

```

<Template matrix elements: prc template ME: TBP>≡
    procedure :: allocate_workspace => prc_template_me_allocate_workspace

<Template matrix elements: procedures>+≡
    subroutine prc_template_me_allocate_workspace (object, core_state)
        class(prc_template_me_t), intent(in) :: object
        class(prc_core_state_t), intent(inout), allocatable :: core_state
        allocate (template_me_state_t :: core_state)
    end subroutine prc_template_me_allocate_workspace

```

The following procedures are inherited from the base type as deferred, thus must be implemented. The corresponding unit tests are skipped here; the procedures are tested when called from the `processes` module.

Output: print just the ID of the associated matrix element. Then display any stored parameters.

```

<Template matrix elements: prc template ME: TBP>+≡
    procedure :: write => prc_template_me_write

<Template matrix elements: procedures>+≡
    subroutine prc_template_me_write (object, unit)
        class(prc_template_me_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(3x,A)", advance="no") "Template process core:"
        if (object%data_known) then
            write (u, "(1x,A)") char (object%data%id)
        else
            write (u, "(1x,A)") "[undefined]"
        end if
        if (allocated (object%par)) then
            write (u, "(3x,A)") "Parameter array:"
            do i = 1, size (object%par)
                write (u, "(5x,I0,1x,ES17.10)") i, object%par(i)
            end do
        end if
    end subroutine prc_template_me_write

```

```

<Template matrix elements: prc template ME: TBP>+≡
    procedure :: write_name => prc_template_me_write_name

```

```

<Template matrix elements: procedures>+=
subroutine prc_template_me_write_name (object, unit)
  class(prc_template_me_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u,"(1x,A)") "Core: template"
end subroutine prc_template_me_write_name

```

Temporarily store the parameter array inside the `prc_template_me` object, so we can use it later during the actual initialization.

```

<Template matrix elements: prc template ME: TBP>+=
procedure :: set_parameters => prc_template_me_set_parameters

<Template matrix elements: procedures>+=
subroutine prc_template_me_set_parameters (prc_template_me, model)
  class(prc_template_me_t), intent(inout) :: prc_template_me
  class(model_data_t), intent(in), target, optional :: model
  if (present (model)) then
    if (.not. allocated (prc_template_me%par)) &
      allocate (prc_template_me%par (model%get_n_real ()))
    call model%real_parameters_to_array (prc_template_me%par)
    prc_template_me%scheme = model%get_scheme_num ()
  end if
end subroutine prc_template_me_set_parameters

```

To fully initialize the process core, we perform base initialization, then initialize the external matrix element code.

This procedure overrides the `init` method of the base type, which we nevertheless can access via its binding `base_init`. When done, we have an allocated driver. The driver will call the `init` procedure for the external matrix element, and thus transfer the parameter set to where it finally belongs.

```

<Template matrix elements: prc template ME: TBP>+=
procedure :: init => prc_template_me_init

<Template matrix elements: procedures>+=
subroutine prc_template_me_init (object, def, lib, id, i_component)
  class(prc_template_me_t), intent(inout) :: object
  class(prc_core_def_t), intent(in), target :: def
  type(process_library_t), intent(in), target :: lib
  type(string_t), intent(in) :: id
  integer, intent(in) :: i_component
  call object%base_init (def, lib, id, i_component)
  call object%activate_parameters ()
end subroutine prc_template_me_init

```

Activate the stored parameters by transferring them to the external matrix element.

```

<Template matrix elements: prc template ME: TBP>+=
procedure :: activate_parameters => prc_template_me_activate_parameters

```

```

<Template matrix elements: procedures>+≡
subroutine prc_template_me_activate_parameters (object)
class (prc_template_me_t), intent(inout) :: object
if (allocated (object%driver)) then
  if (allocated (object%par)) then
    select type (driver => object%driver)
    type is (template_me_driver_t)
      if (associated (driver%init)) then
        call driver%init (object%par, object%scheme)
      end if
    end select
  else
    call msg_bug ("prc_template_me_activate: parameter set is not allocated")
  end if
else
  call msg_bug ("prc_template_me_activate: driver is not allocated")
end if
end subroutine prc_template_me_activate_parameters

```

Tell whether a particular combination of flavor, helicity, color is allowed. Here we have to consult the matrix-element driver.

```

<Template matrix elements: prc template ME: TBP>+≡
procedure :: is_allowed => prc_template_me_is_allowed

<Template matrix elements: procedures>+≡
function prc_template_me_is_allowed (object, i_term, f, h, c) result (flag)
class(prc_template_me_t), intent(in) :: object
integer, intent(in) :: i_term, f, h, c
logical :: flag
logical(c_bool) :: cflag
select type (driver => object%driver)
type is (template_me_driver_t)
  call driver%is_allowed (f, h, c, cflag)
  flag = cflag
end select
end function prc_template_me_is_allowed

```

Transfer the generated momenta directly to the hard interaction in the (only) term. We assume that everything has been set up correctly, so the array fits.

```

<Template matrix elements: prc template ME: TBP>+≡
procedure :: compute_hard_kinematics => &
  prc_template_me_compute_hard_kinematics

<Template matrix elements: procedures>+≡
subroutine prc_template_me_compute_hard_kinematics &
  (object, p_seed, i_term, int_hard, core_state)
class(prc_template_me_t), intent(in) :: object
type(vector4_t), dimension(:), intent(in) :: p_seed
integer, intent(in) :: i_term
type(interaction_t), intent(inout) :: int_hard
class(prc_core_state_t), intent(inout), allocatable :: core_state
call int_hard%set_momenta (p_seed)
end subroutine prc_template_me_compute_hard_kinematics

```

This procedure is not called for `prc_template_me_t`, just a placeholder.

<Template matrix elements: prc template ME: TBP>+≡

```
procedure :: compute_eff_kinematics => &
    prc_template_me_compute_eff_kinematics
```

<Template matrix elements: procedures>+≡

```
subroutine prc_template_me_compute_eff_kinematics &
    (object, i_term, int_hard, int_eff, core_state)
class(prc_template_me_t), intent(in) :: object
integer, intent(in) :: i_term
type(interaction_t), intent(in) :: int_hard
type(interaction_t), intent(inout) :: int_eff
class(prc_core_state_t), intent(inout), allocatable :: core_state
end subroutine prc_template_me_compute_eff_kinematics
```

Compute the amplitude. For the tree-level process, we can ignore the scale settings. The term index j is also irrelevant.

We first call `new_event` for the given momenta (which we must unpack), then retrieve the amplitude value for the given quantum numbers.

If the `core_state` status flag is present, we can make sure that we call `new_event` only once for a given kinematics. After the first call, we unset the `new_kinematics` flag.

<Template matrix elements: prc template ME: TBP>+≡

```
procedure :: compute_amplitude => prc_template_me_compute_amplitude
```

<Template matrix elements: procedures>+≡

```
function prc_template_me_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
    core_state) result (amp)
class(prc_template_me_t), intent(in) :: object
integer, intent(in) :: j
type(vector4_t), dimension(:), intent(in) :: p
integer, intent(in) :: f, h, c
real(default), intent(in) :: fac_scale, ren_scale
real(default), intent(in), allocatable :: alpha_qcd_forced
class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
complex(default) :: amp
integer :: n_tot, i
real(c_default_float), dimension(:,:), allocatable :: parray
complex(c_default_complex) :: camp
logical :: new_event
select type (driver => object%driver)
type is (template_me_driver_t)
    new_event = .true.
    if (present (core_state)) then
        if (allocated (core_state)) then
            select type (core_state)
            type is (template_me_state_t)
                new_event = core_state%new_kinematics
                core_state%new_kinematics = .false.
            end select
        end if
    end if
    if (new_event) then
```

```

        n_tot = object%data%n_in + object%data%n_out
        allocate (parray (0:3, n_tot))
        forall (i = 1:n_tot) parray(:,i) = vector4_get_components (p(i))
        call driver%new_event (parray)
    end if
    if (object%is_allowed (1, f, h, c)) then
        call driver%get_amplitude &
            (int (f, c_int), int (h, c_int), int (c, c_int), camp)
        amp = camp
    else
        amp = 0
    end if
end select
end function prc_template_me_compute_amplitude

```

We do not overwrite the `prc_core_t` routine for α_s .

17.3.6 Unit Test

Test module, followed by the corresponding implementation module.

```

<prc_template_me_ut.f90>≡
  <File header>

  module prc_template_me_ut
    use unit_tests
    use prc_template_me_util

    <Standard module head>

    <Template matrix elements: public test>

    contains

    <Template matrix elements: test driver>

  end module prc_template_me_ut
<prc_template_me_util.f90>≡
  <File header>

  module prc_template_me_util

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use os_interface
    use particle_specifiers, only: new_prt_spec
    use model_data
    use prc_core_def
    use process_constants
    use process_libraries
    use model_testbed, only: prepare_model, cleanup_model

```

```

        use prc_template_me

        <Standard module head>

        <Template matrix elements: test declarations>

contains

        <Template matrix elements: tests>

    end module prc_template_me_util
API: driver for the unit tests below.
    <Template matrix elements: public test>≡
        public :: prc_template_me_test
    <Template matrix elements: test driver>≡
        subroutine prc_template_me_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <Template matrix elements: execute tests>
    end subroutine prc_template_me_test

```

Generate, compile and load a simple process matrix element

The process is $e^+e^- \rightarrow \mu^+\mu^-$ for vanishing masses and $e = 0.3$. We initialize the process, build the library, and compute a particular matrix element for momenta of unit energy and right-angle scattering. The matrix element, as it happens, is equal to e^2 . (Note that are no conversion factors applied, so this result is exact.)

For GNU make, makeflags is set to -j1. This eliminates a potential clash with a -j<n> flag if this test is called from a parallel make.

```

    <Template matrix elements: execute tests>≡
        call test (prc_template_me_1, "prc_template_me_1", &
            "build and load simple template process", &
            u, results)

    <Template matrix elements: test declarations>≡
        public :: prc_template_me_1

    <Template matrix elements: tests>≡
        subroutine prc_template_me_1 (u)
            integer, intent(in) :: u
            type(process_library_t) :: lib
            class(prc_core_def_t), allocatable :: def
            type(process_def_entry_t), pointer :: entry
            type(os_data_t) :: os_data
            class(model_data_t), pointer :: model
            type(string_t) :: model_name
            type(string_t), dimension(:), allocatable :: prt_in, prt_out
            type(process_constants_t) :: data
            class(prc_core_driver_t), allocatable :: driver
            integer, parameter :: cdf = c_default_float
            integer, parameter :: ci = c_int

```

```

real(cdf), dimension(4) :: par
real(cdf), dimension(0:3,4) :: p
logical(c_bool) :: flag
complex(c_default_complex) :: amp
integer :: i

write (u, "(A)")  "* Test output: prc_template_me_1"
write (u, "(A)")  "* Purpose: create a template matrix element,"
write (u, "(A)")  "*           normalized to give unit integral,"
write (u, "(A)")  "*           build a library, link, load, and &
           &access the matrix element"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("template_me1"))
call os_data%init ()

model_name = "QED"
model => null ()
call prepare_model (model, model_name)

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e+"), var_str ("e-")]
prt_out = [var_str ("m+"), var_str ("m-")]

allocate (template_me_def_t :: def)
select type (def)
type is (template_me_def_t)
    call def%init (model, prt_in, prt_out, unity = .false.)
end select
allocate (entry)
call entry%init (var_str ("template_me1_a"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("template"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Clean any left-over files"
write (u, "(A)")
call lib%clean (os_data, distclean = .false.)

write (u, "(A)")  "* Write driver"

```

```

write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code, compile, link, load"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u, libpath = .false.)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active          = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes        = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of template_me1_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("template_me1_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID      = ", char (data%id)
write (u, "(1x,A,A)")  "model name        = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum          = '", data%md5sum, "'"
write (u, "(1x,A,I0)")  "n_in = ", data%n_in
write (u, "(1x,A,I0)")  "n_out = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I2))")  "hel state =", data%hel_state(:,1)
do i = 2, 16
    write (u, "(12x,4(1x,I2))")  data%hel_state(:,i)
end do
write (u, "(1x,A,10(1x,I0))")  "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))")  "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))")  "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))")  "cf index =", data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set parameters for template_me1_a and initialize:"
write (u, "(A)")

par = [0.3_cdf, 0.0_cdf, 0.0_cdf, 0.0_cdf]
write (u, "(2x,A,F6.4)")  "ee = ", par(1)
write (u, "(2x,A,F6.4)")  "me = ", par(2)
write (u, "(2x,A,F6.4)")  "mmu = ", par(3)
write (u, "(2x,A,F6.4)")  "mtau = ", par(4)

```



```

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
    1.0_cdf, 0.0_cdf, 0.0_cdf,-1.0_cdf, &
    1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
    1.0_cdf,-1.0_cdf, 0.0_cdf, 0.0_cdf &
    ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))")  "p", i, " =", p(:,i)
end do

select type (driver)
type is (template_me_driver_t)
    call driver%init (par, 0)

    call driver%new_event (p)

    write (u, "(A)")
    write (u, "(A)")  "* Compute matrix element:"
    write (u, "(A)")

    call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
    write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()
call cleanup_model (model)
deallocate (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_template_me_1"

end subroutine prc_template_me_1

<Template matrix elements: execute tests>+≡
call test (prc_template_me_2, "prc_template_me_2", &
    "build and load simple template_unity process", &
    u, results)

<Template matrix elements: test declarations>+≡
public :: prc_template_me_2

<Template matrix elements: tests>+≡
subroutine prc_template_me_2 (u)
    integer, intent(in) :: u
    type(process_library_t) :: lib
    class(prc_core_def_t), allocatable :: def
    type(process_def_entry_t), pointer :: entry
    type(os_data_t) :: os_data

```

```

class(model_data_t), pointer :: model
type(string_t) :: model_name
type(string_t), dimension(:), allocatable :: prt_in, prt_out
type(process_constants_t) :: data
class(prc_core_driver_t), allocatable :: driver
integer, parameter :: cdf = c_default_float
integer, parameter :: ci = c_int
real(cdf), dimension(4) :: par
real(cdf), dimension(0:3,4) :: p
logical(c_bool) :: flag
complex(c_default_complex) :: amp
integer :: i

write (u, "(A)")  "* Test output: prc_template_me_1"
write (u, "(A)")  "*   Purpose: create a template matrix element,"
write (u, "(A)")  "*               being identical to unity,"
write (u, "(A)")  "*               build a library, link, load, and &
               &access the matrix element"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("template_me2"))
call os_data%init ()

model_name = "QED"
model => null ()
call prepare_model (model, model_name)

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e+"), var_str ("e-")]
prt_out = [var_str ("m+"), var_str ("m-")]

allocate (template_me_def_t :: def)
select type (def)
type is (template_me_def_t)
    call def%init (model, prt_in, prt_out, unity = .true.)
end select
allocate (entry)
call entry%init (var_str ("template_me2_a"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("template_unity"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure library"
write (u, "(A)")
call lib%configure (os_data)

write (u, "(A)")  "* Write makefile"
write (u, "(A)")

```

```

call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Clean any left-over files"
write (u, "(A)")
call lib%clean (os_data, distclean = .false.)

write (u, "(A)")  "* Write driver"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code, compile, link, load"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u, libpath = .false.)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active" = ", &
lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes" = ", &
lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of template_me2_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("template_me2_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID" = ", char (data%id)
write (u, "(1x,A,A)")  "model name" = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum" = "'", data%md5sum, "'"
write (u, "(1x,A,I0)")  "n_in" = ", data%n_in
write (u, "(1x,A,I0)")  "n_out" = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv" = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel" = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col" = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin" = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf" = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =" , data%flv_state
write (u, "(1x,A,10(1x,I2))")  "hel state =" , data%hel_state(:,1)
do i = 2, 16
  write (u, "(12x,4(1x,I2))")  data%hel_state(:,i)
end do
write (u, "(1x,A,10(1x,I0))")  "col state =" , data%col_state
write (u, "(1x,A,10(1x,L1))")  "ghost flag =" , data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))")  "color factors =" , data%color_factors
write (u, "(1x,A,10(1x,I0))")  "cf index =" , data%cf_index

write (u, "(A)")
write (u, "(A)")  "* Set parameters for template_me2_a and initialize:"
write (u, "(A)")

```

```

par = [0.3_cdf, 0.0_cdf, 0.0_cdf, 0.0_cdf]
write (u, "(2x,A,F6.4)") "ee  = ", par(1)
write (u, "(2x,A,F6.4)") "me  = ", par(2)
write (u, "(2x,A,F6.4)") "mmu = ", par(3)
write (u, "(2x,A,F6.4)") "mtau = ", par(4)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
    1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
    1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
    1.0_cdf, -1.0_cdf, 0.0_cdf, 0.0_cdf &
], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

select type (driver)
type is (template_me_driver_t)
    call driver%init (par, 0)

    call driver%new_event (p)

    write (u, "(A)")
    write (u, "(A)")  "* Compute matrix element:"
    write (u, "(A)")

    call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
    write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()
call cleanup_model (model)
deallocate (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_template_me_2"

end subroutine prc_template_me_2

```

17.4 O'MEGA Interface

The standard method for process computation with WHIZARD is the O'MEGA matrix element generator.

This section implements the interface to the code generator (via the makefile) and the driver for the features provided by the **O’MEGA** matrix element.

There are actually two different methods steered by this interface, the traditional one which delivers compiled Fortran code, while the **O’MEGA** virtual machine (OVM) produces bytecode with look-up tables.

```

<prc_omega.f90>≡
  <File header>

  module prc_omega

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use io_units
    use system_defs, only: TAB
    use constants, only: one
    use diagnostics
    use os_interface
    use lorentz
    use sm_qcd
    use sm_qed
    use interactions
    use model_data

    use particle_specifiers, only: new_prt_spec
    use process_constants
    use prclib_interfaces
    use prc_core_def
    use process_libraries
    use prc_core

    <Standard module head>

    <Omega interface: public>

    <Omega interface: types>

    <Omega interface: interfaces>

    contains

    <Omega interface: procedures>

  end module prc_omega

```

17.4.1 Process definition

For the process definition we implement an extension of the `prc_core_def_t` abstract type.

```

<Omega interface: public>≡
  public :: omega_def_t

```

```

<Omega interface: types>≡
  type, extends (prc_core_def_t) :: omega_def_t
    logical :: ufo = .false.
    logical :: ovm = .false.
  contains
    <Omega interface: omega def: TBP>
  end type omega_def_t

<Omega interface: omega def: TBP>≡
  procedure, nopass :: type_string => omega_def_type_string

<Omega interface: procedures>≡
  function omega_def_type_string () result (string)
    type(string_t) :: string
    string = "omega"
  end function omega_def_type_string

```

Initialization: allocate the writer for the O'MEGA matrix element. The writer type depends on the settings of the ufo and ovm flags. Also set any data for this process that the writer needs.

```

<Omega interface: omega def: TBP>+≡
  procedure :: init => omega_def_init

<Omega interface: procedures>+≡
  subroutine omega_def_init (object, &
    model_name, prt_in, prt_out, &
    ovm, ufo, ufo_path, &
    restrictions, cms_scheme, &
    openmp_support, report_progress, write_phs_output, extra_options, diags, diags_color)
    class(omega_def_t), intent(out) :: object
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
    logical, intent(in) :: ovm
    logical, intent(in) :: ufo
    type(string_t), intent(in), optional :: ufo_path
    type(string_t), intent(in), optional :: restrictions
    logical, intent(in), optional :: cms_scheme
    logical, intent(in), optional :: openmp_support
    logical, intent(in), optional :: report_progress
    logical, intent(in), optional :: write_phs_output
    type(string_t), intent(in), optional :: extra_options
    logical, intent(in), optional :: diags, diags_color
    object%ufo = ufo
    object%ovm = ovm
    if (object%ufo) then
      if (object%ovm) then
        call msg_fatal ("Omega process: OVM method does not support UFO model")
      else
        allocate (omega_ufo_writer_t :: object%writer)
      end if
    else
      if (object%ovm) then
        allocate (omega_ovm_writer_t :: object%writer)
      end if
    end if
  end subroutine omega_def_init

```

```

        else
            allocate (omega_omega_writer_t :: object%writer)
        end if
    end if
    select type (writer => object%writer)
    class is (omega_writer_t)
        call writer%init (model_name, prt_in, prt_out, &
            ufo_path, restrictions, cms_scheme, &
            openmp_support, report_progress, write_phs_output, extra_options, diags, diags_color)
    end select
end subroutine omega_def_init

```

Write/read process- and method-specific data.

<Omega interface: omega def: TBP>+≡

```

    procedure :: write => omega_def_write

```

<Omega interface: procedures>+≡

```

    subroutine omega_def_write (object, unit)
        class(omega_def_t), intent(in) :: object
        integer, intent(in) :: unit
        select type (writer => object%writer)
        class is (omega_writer_t)
            call writer%write (unit)
        end select
    end subroutine omega_def_write

```

<Omega interface: omega def: TBP>+≡

```

    procedure :: read => omega_def_read

```

<Omega interface: procedures>+≡

```

    subroutine omega_def_read (object, unit)
        class(omega_def_t), intent(out) :: object
        integer, intent(in) :: unit
        call msg_bug ("O'Mega process definition: input not supported yet")
    end subroutine omega_def_read

```

Allocate the driver for O'MEGAmatrix elements.

<Omega interface: omega def: TBP>+≡

```

    procedure :: allocate_driver => omega_def_allocate_driver

```

<Omega interface: procedures>+≡

```

    subroutine omega_def_allocate_driver (object, driver, basename)
        class(omega_def_t), intent(in) :: object
        class(prc_core_driver_t), intent(out), allocatable :: driver
        type(string_t), intent(in) :: basename
        allocate (omega_driver_t :: driver)
    end subroutine omega_def_allocate_driver

```

We need code:

<Omega interface: omega def: TBP>+≡

```

    procedure, nopass :: needs_code => omega_def_needs_code

```

```

<Omega interface: procedures>+≡
  function omega_def_needs_code () result (flag)
    logical :: flag
    flag = .true.
  end function omega_def_needs_code

```

These are the features that an O'MEGA matrix element provides.

```

<Omega interface: omega def: TBP>+≡
  procedure, nopass :: get_features => omega_def_get_features

<Omega interface: procedures>+≡
  subroutine omega_def_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (6))
    features = [ &
      var_str ("init"), &
      var_str ("update_alpha_s"), &
      var_str ("reset_helicity_selection"), &
      var_str ("is_allowed"), &
      var_str ("new_event"), &
      var_str ("get_amplitude")]
  end subroutine omega_def_get_features

```

The interface of the specific features.

```

<Omega interface: interfaces>≡
  abstract interface
    subroutine init_t (par, scheme) bind(C)
      import
      real(c_default_float), dimension(*), intent(in) :: par
      integer(c_int), intent(in) :: scheme
    end subroutine init_t
  end interface

  abstract interface
    subroutine update_alpha_s_t (alpha_s) bind(C)
      import
      real(c_default_float), intent(in) :: alpha_s
    end subroutine update_alpha_s_t
  end interface

  abstract interface
    subroutine reset_helicity_selection_t (threshold, cutoff) bind(C)
      import
      real(c_default_float), intent(in) :: threshold
      integer(c_int), intent(in) :: cutoff
    end subroutine reset_helicity_selection_t
  end interface

  abstract interface
    subroutine is_allowed_t (flv, hel, col, flag) bind(C)
      import
      integer(c_int), intent(in) :: flv, hel, col
      logical(c_bool), intent(out) :: flag
    end subroutine is_allowed_t
  end interface

```



```

        end subroutine is_allowed_t
    end interface

    abstract interface
        subroutine new_event_t (p) bind(C)
            import
            real(c_default_float), dimension(0:3,*), intent(in) :: p
        end subroutine new_event_t
    end interface

    abstract interface
        subroutine get_amplitude_t (flv, hel, col, amp) bind(C)
            import
            integer(c_int), intent(in) :: flv, hel, col
            complex(c_default_complex), intent(out):: amp
        end subroutine get_amplitude_t
    end interface

```

Connect the O'MEGA features with the process driver.

(Omega interface: omega def: TBP)+≡

```

    procedure :: connect => omega_def_connect

```

(Omega interface: procedures)+≡

```

    subroutine omega_def_connect (def, lib_driver, i, proc_driver)
        class(omega_def_t), intent(in) :: def
        class(prclib_driver_t), intent(in) :: lib_driver
        integer, intent(in) :: i
        class(proc_core_driver_t), intent(inout) :: proc_driver
        integer(c_int) :: pid, fid
        type(c_funptr) :: fptr
        select type (proc_driver)
        type is (omega_driver_t)
            pid = i
            fid = 1
            call lib_driver%get_fptr (pid, fid, fptr)
            call c_f_procpointer (fptr, proc_driver%init)
            fid = 2
            call lib_driver%get_fptr (pid, fid, fptr)
            call c_f_procpointer (fptr, proc_driver%update_alpha_s)
            fid = 3
            call lib_driver%get_fptr (pid, fid, fptr)
            call c_f_procpointer (fptr, proc_driver%reset_helicity_selection)
            fid = 4
            call lib_driver%get_fptr (pid, fid, fptr)
            call c_f_procpointer (fptr, proc_driver%is_allowed)
            fid = 5
            call lib_driver%get_fptr (pid, fid, fptr)
            call c_f_procpointer (fptr, proc_driver%new_event)
            fid = 6
            call lib_driver%get_fptr (pid, fid, fptr)
            call c_f_procpointer (fptr, proc_driver%get_amplitude)
        end select
    end subroutine omega_def_connect

```

17.4.2 The O'MEGA writer

The O'MEGA writer is responsible for inserting the appropriate lines in the make-file that call O'MEGA, and for writing interfaces and wrappers.

```
<Omega interface: types>+≡
  type, extends (prc_writer_f_module_t), abstract :: omega_writer_t
    type(string_t) :: model_name
    type(string_t) :: process_mode
    type(string_t) :: process_string
    type(string_t) :: restrictions
    logical :: openmp_support = .false.
    logical :: report_progress = .false.
    logical :: diags = .false.
    logical :: diags_color = .false.
    logical :: complex_mass_scheme = .false.
    logical :: write_phs_output = .false.
    type(string_t) :: extra_options
  contains
    <Omega interface: omega writer: TBP>
  end type omega_writer_t

<Omega interface: types>+≡
  type, extends (omega_writer_t) :: omega_omega_writer_t
  contains
    <Omega interface: omega omega writer: TBP>
  end type omega_omega_writer_t

<Omega interface: types>+≡
  type, extends (omega_omega_writer_t) :: omega_ufo_writer_t
    type(string_t) :: ufo_path
  contains
    <Omega interface: omega ufo writer: TBP>
  end type omega_ufo_writer_t

<Omega interface: types>+≡
  type, extends (omega_writer_t) :: omega_ovm_writer_t
  contains
    <Omega interface: omega ovm writer: TBP>
  end type omega_ovm_writer_t

<Omega interface: omega omega writer: TBP>≡
  procedure, nopass :: type_name => omega_omega_writer_type_name

<Omega interface: procedures>+≡
  function omega_omega_writer_type_name () result (string)
    type(string_t) :: string
    string = "omega"
  end function omega_omega_writer_type_name

<Omega interface: omega ufo writer: TBP>≡
  procedure, nopass :: type_name => omega_ufo_writer_type_name
```

```

<Omega interface: procedures>+≡
  function omega_ufo_writer_type_name () result (string)
    type(string_t) :: string
    string = "omega/UFO"
  end function omega_ufo_writer_type_name

<Omega interface: omega ovm writer: TBP>≡
  procedure, nopass :: type_name => omega_ovm_writer_type_name

<Omega interface: procedures>+≡
  function omega_ovm_writer_type_name () result (string)
    type(string_t) :: string
    string = "ovm"
  end function omega_ovm_writer_type_name

```

Taking into account the prefix for O'MEGA module names.

```

<Omega interface: omega writer: TBP>≡
  procedure, nopass :: get_module_name => omega_writer_get_module_name

<Omega interface: procedures>+≡
  function omega_writer_get_module_name (id) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: id
    name = "opr_" // id
  end function omega_writer_get_module_name

```

Output. This is called by omega_def.write.

```

<Omega interface: omega writer: TBP>+≡
  procedure :: write => omega_writer_write

<Omega interface: procedures>+≡
  subroutine omega_writer_write (object, unit)
    class(omega_writer_t), intent(in) :: object
    integer, intent(in) :: unit
    write (unit, "(5x,A,A)") "Model name      = ", &
      ''' // char (object%model_name) // '''
    write (unit, "(5x,A,A)") "Mode string    = ", &
      ''' // char (object%process_mode) // '''
    write (unit, "(5x,A,A)") "Process string = ", &
      ''' // char (object%process_string) // '''
    write (unit, "(5x,A,A)") "Restrictions   = ", &
      ''' // char (object%restrictions) // '''
    write (unit, "(5x,A,L1)") "OpenMP support = ", object%openmp_support
    write (unit, "(5x,A,L1)") "Report progress = ", object%report_progress
    ! write (unit, "(5x,A,L1)") "Write phs output = ", object%write_phs_output
    write (unit, "(5x,A,A)") "Extra options  = ", &
      ''' // char (object%extra_options) // '''
    write (unit, "(5x,A,L1)") "Write diagrams  = ", object%diags
    write (unit, "(5x,A,L1)") "Write color diag. = ", object%diags_color
    write (unit, "(5x,A,L1)") "Complex Mass S. = ", &
      object%complex_mass_scheme
  end subroutine omega_writer_write

```

Initialize with process data.

```

(Omega interface: omega writer: TBP)+≡
  procedure :: init => omega_writer_init
(Omega interface: procedures)+≡
  subroutine omega_writer_init (writer, model_name, prt_in, prt_out, &
    ufo_path, restrictions, cms_scheme, openmp_support, &
    report_progress, write_phs_output, extra_options, diags, diags_color)
    class(omega_writer_t), intent(out) :: writer
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
    type(string_t), intent(in), optional :: ufo_path
    type(string_t), intent(in), optional :: restrictions
    logical, intent(in), optional :: cms_scheme
    logical, intent(in), optional :: openmp_support
    logical, intent(in), optional :: report_progress
    logical, intent(in), optional :: write_phs_output
    type(string_t), intent(in), optional :: extra_options
    logical, intent(in), optional :: diags, diags_color
    integer :: i
    writer%model_name = model_name
    select type (writer)
    type is (omega_ufo_writer_t)
      if (present (ufo_path)) then
        writer%ufo_path = ufo_path
      else
        call msg_fatal ("O'Mega: UFO model option is selected, but UFO model path is unset")
      end if
    end select
    if (present (restrictions)) then
      writer%restrictions = restrictions
    else
      writer%restrictions = ""
    end if
    if (present (cms_scheme)) writer%complex_mass_scheme = cms_scheme
    if (present (openmp_support)) writer%openmp_support = openmp_support
    if (present (report_progress)) writer%report_progress = report_progress
    if (present (write_phs_output)) writer%write_phs_output = write_phs_output
    if (present (extra_options)) then
      writer%extra_options = " " // extra_options
    else
      writer%extra_options = ""
    end if
    if (present (diags)) writer%diags = diags
    if (present (diags_color)) writer%diags_color = diags_color
    select case (size (prt_in))
    case (1); writer%process_mode = " -decay"
    case (2); writer%process_mode = " -scatter"
    end select
    associate (s => writer%process_string)
      s = " '"
      do i = 1, size (prt_in)
        if (i > 1) s = s // " "
        s = s // prt_in(i)
      end do
    end associate
  end subroutine

```

```

end do
s = s // " ->"
do i = 1, size (prt_out)
    s = s // " " // prt_out(i)
end do
s = s // ""
end associate
end subroutine omega_writer_init

```

The makefile implements the actual O'MEGA call. For old L^AT_EX distributions, we filter out the hyperref options for O'MEGA diagrams, at least in the testsuite.

```

<Omega interface: omega writer: TBP>+≡
    procedure :: write_makefile_code => omega_write_makefile_code

<Omega interface: procedures>+≡
    subroutine omega_write_makefile_code &
        (writer, unit, id, os_data, verbose, testflag)
        class(omega_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: testflag
        type(string_t) :: omega_binary, omega_path
        type(string_t) :: restrictions_string
        type(string_t) :: openmp_string
        type(string_t) :: kmatrix_string
        type(string_t) :: progress_string
        type(string_t) :: diagrams_string
        type(string_t) :: cms_string
        type(string_t) :: write_phs_output_string
        type(string_t) :: parameter_module
        logical :: escape_hyperref
        escape_hyperref = .false.
        if (present (testflag)) escape_hyperref = testflag
        select type (writer)
        type is (omega_omega_writer_t)
            omega_binary = "omega-" // writer%model_name // ".opt"
        type is (omega_ufo_writer_t)
            omega_binary = "omega_UFO.opt"
        type is (omega_ovm_writer_t)
            select case (char (writer%model_name))
            case ("SM", "SM_CKM", "SM_Higgs", "THDM", "THDM_CKM", &
                "HSExt", "QED", "QCD", "Zprime")
            case default
                call msg_fatal ("The model " // char (writer%model_name) &
                    // " is not available for the O'Mega VM.")
            end select
            omega_binary = "omega-" // writer%model_name // "_VM.opt"
        end select
        omega_path = os_data%whizard_omega_binpath // "/" // omega_binary
        if (.not. verbose) omega_path = "@" // omega_path
        if (writer%restrictions /= "") then
            restrictions_string = " -cascade '" // writer%restrictions // "'

```

```

else
    restrictions_string = ""
end if
if (writer%openmp_support) then
    openmp_string = " -target:openmp"
else
    openmp_string = ""
end if
if (writer%report_progress) then
    progress_string = " -fusion:progress"
else
    progress_string = ""
end if
if (writer%diags) then
    if (writer%diags_color) then
        diagrams_string = " -diagrams:C " // char(id) // &
            "_diags -diagrams_LaTeX"
    else
        diagrams_string = " -diagrams " // char(id) // &
            "_diags -diagrams_LaTeX"
    end if
else
    if (writer%diags_color) then
        diagrams_string = " -diagrams:c " // char(id) // &
            "_diags -diagrams_LaTeX"
    else
        diagrams_string = ""
    end if
end if
if (writer%complex_mass_scheme) then
    cms_string = " -model:cms_width"
else
    cms_string = ""
end if
if (writer%write_phs_output) then
    write_phs_output_string = " -phase_space " // char (id) // ".fds"
else
    write_phs_output_string = ""
endif
select case (char (writer%model_name))
case ("SM_rx", "SSC", "NoH_rx", "AltH")
    kmatrix_string = " -target:kmatrix_2_write"
case ("SSC_2", "SSC_AltT", "SM_ul")
    kmatrix_string = " -target:kmatrix_write"
case default
    kmatrix_string = ""
end select
write (unit, "(5A)") "SOURCES += ", char (id), ".f90"
select type (writer)
type is (omega_ovm_writer_t)
    write (unit, "(5A)") "SOURCES += ", char (id), ".hbc"
end select
if (writer%diags .or. writer%diags_color) then
    write (unit, "(5A)") "TEX_SOURCES += ", char (id), "_diags.tex"

```

```

        if (os_data%event_analysis_pdf) then
            write (unit, "(5A)") "TEX_OBJECTS += ", char (id), "_diags.pdf"
        else
            write (unit, "(5A)") "TEX_OBJECTS += ", char (id), "_diags.ps"
        end if
    end if
write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
select type (writer)
type is (omega_omega_writer_t)
    write (unit, "(5A)") char (id), ".f90:"
    if (.not. verbose) then
        write (unit, "(5A)") TAB // '@echo " OMEGA      ', trim (char (id)), '.f90"'
    end if
    write (unit, "(99A)") TAB, char (omega_path), &
        " -o ", char (id), ".f90", &
        " -target:whizard", &
        " -target:parameter_module parameters_", char (writer%model_name), &
        " -target:module opr_", char (id), &
        " -target:md5sum '", writer%md5sum, "'", &
        char (cms_string), &
        char (openmp_string), &
        char (progress_string), &
        char (kmatrix_string), &
        char (writer%process_mode), char (writer%process_string), &
        char (restrictions_string), char (diagrams_string), &
        char (writer%extra_options), char (write_phs_output_string)
type is (omega_ufo_writer_t)
    parameter_module = char (id) // "_par_" // replace (char (writer%model_name), &
        "-", "_", every=.true.)
    write (unit, "(5A)") char (id), ".f90: ", char (parameter_module), ".lo"
    if (.not. verbose) then
        write (unit, "(5A)") TAB // '@echo " OMEGA[UFO]', trim (char (id)), '.f90"'
    end if
    write (unit, "(99A)") TAB, char (omega_path), &
        " -o ", char (id), ".f90", &
        " -model:UFO_dir ", &
        char (writer%ufo_path), "/", char (writer%model_name), &
        " -model:exec", &
        " -target:whizard", &
        " -target:parameter_module ", char (parameter_module), &
        " -target:module opr_", char (id), &
        " -target:md5sum '", writer%md5sum, "'", &
        char (cms_string), &
        char (openmp_string), &
        char (progress_string), &
        char (kmatrix_string), &
        char (writer%process_mode), char (writer%process_string), &
        char (restrictions_string), char (diagrams_string), &
        char (writer%extra_options), char (write_phs_output_string)
    write (unit, "(5A)") "SOURCES += ", char (parameter_module), ".f90"
    write (unit, "(5A)") "OBJECTS += ", char (parameter_module), ".lo"
    write (unit, "(5A)") char (parameter_module), ".f90:"
    write (unit, "(99A)") TAB, char (omega_path), &
        " -model:UFO_dir ", &

```

```

        char (writer%ufo_path), "/", char (writer%model_name), &
        " -model:exec", &
        " -target:parameter_module ", char (parameter_module), &
        " -params", &
        " -o $"
    write (unit, "(5A)") char (parameter_module), ".lo: ", char (parameter_module), ".f90"
    if (.not. verbose) then
        write (unit, "(5A)") TAB // '@echo " FC          "$@'
    end if
    write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"
type is (omega_ovm_writer_t)
    write (unit, "(5A)") char (id), ".hbc:"
    write (unit, "(99A)") TAB, char (omega_path), &
        " -o ", char (id), ".hbc", &
        char (progress_string), &
        char (cms_string), &
        char (writer%process_mode), char (writer%process_string), &
        char (restrictions_string), char (diagrams_string), &
        char (writer%extra_options), char (write_phs_output_string)
    write (unit, "(5A)") char (id), ".f90:"
    if (.not. verbose) then
        write (unit, "(5A)") TAB // '@echo " OVM          ', trim (char (id)), '.f90"'
    end if
    write (unit, "(99A)") TAB, char (omega_path), &
        " -o ", char (id), ".f90 -params", &
        " -target:whizard ", &
        " -target:bytecode_file ", char (id), ".hbc", &
        " -target:wrapper_module opr_", char (id), &
        " -target:parameter_module_external parameters-", &
        char (writer%model_name), &
        " -target:md5sum '", writer%md5sum, "'", &
        char (openmp_string)
end select
if (writer%diags .or. writer%diags_color) &
    write (unit, "(5A)") char (id), "_diags.tex: ", char (id), ".f90"
write (unit, "(5A)") "clean-", char (id), ":"
if (verbose) then
    write (unit, "(5A)") TAB, "rm -f ", char (id), ".f90"
    write (unit, "(5A)") TAB, "rm -f opr_", char (id), ".mod"
    write (unit, "(5A)") TAB, "rm -f ", char (id), ".lo"
else
    write (unit, "(5A)") TAB // '@echo " RM          ', &
        trim (char (id)), '.f90,.mod,.lo"'
    write (unit, "(5A)") TAB, "@rm -f ", char (id), ".f90"
    write (unit, "(5A)") TAB, "@rm -f opr_", char (id), ".mod"
    write (unit, "(5A)") TAB, "@rm -f ", char (id), ".lo"
end if
write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".f90"
select type (writer)
type is (omega_ufo_writer_t)
    write (unit, "(5A)") "CLEAN_SOURCES += ", char (writer%model_name), ".mdl"
    write (unit, "(5A)") "CLEAN_SOURCES += ", char (parameter_module), ".f90"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (parameter_module), ".mod"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (parameter_module), ".lo"

```



```

type is (omega_ovm_writer_t)
    write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".hbc"
end select
if (writer%diags .or. writer%diags_color) then
    write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), "_diags.tex"
end if
write (unit, "(5A)") "CLEAN_OBJECTS += opr_", char (id), ".mod"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), ".lo"
if (writer%diags .or. writer%diags_color) then
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.aux"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.log"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.dvi"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.toc"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.out"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.[1-9]"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.[1-9][0-9]"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.[1-9][0-9][0-9]"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.t[1-9]"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.t[1-9][0-9]"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.t[1-9][0-9][0-9]"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.mp"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags-fmf.log"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.dvi"
    write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.ps"
    if (os_data%event_analysis_pdf) &
        write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_diags.pdf"
end if
write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
write (unit, "(5A)") TAB, "$(LTF_COMPILE) $<"
if (writer%diags .or. writer%diags_color) then
    if (os_data%event_analysis_ps) then
        if (os_data%event_analysis_pdf) then
            write (unit, "(5A)") char (id), "_diags.pdf: ", char (id), "_diags.tex"
        else
            write (unit, "(5A)") char (id), "_diags.ps: ", char (id), "_diags.tex"
        end if
    end if
    if (escape_hyperref) then
        if (verbose) then
            write (unit, "(5A)") TAB, "-cat ", char (id), "_diags.tex | \"
        else
            write (unit, "(5A)") TAB // '@echo " HYPERREF ', &
                trim (char (id)) // '_diags.tex"'
            write (unit, "(5A)") TAB, "@cat ", char (id), "_diags.tex | \"
        end if
    end if
    write (unit, "(5A)") TAB, " sed -e" // &
        "'s/\\usepackage\\[colorlinks\\]{hyperref}.*/%\\usepackage" // &
        "\\[colorlinks\\]{hyperref}/' > \"
    write (unit, "(5A)") TAB, " ", char (id), "_diags.tex.tmp"
    if (verbose) then
        write (unit, "(5A)") TAB, "mv -f ", char (id), "_diags.tex.tmp \"
    else
        write (unit, "(5A)") TAB, "@mv -f ", char (id), "_diags.tex.tmp \"
    end if
    write (unit, "(5A)") TAB, " ", char (id), "_diags.tex"
end if

```

```

end if
if (verbose) then
  write (unit, "(5A)") TAB, "-TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
    char (id) // "_diags.tex"
  write (unit, "(5A)") TAB, "MPINPUTS=$(MP_FLAGS) $(MPOST) " // &
    char (id) // "_diags-fmf.mp"
  write (unit, "(5A)") TAB, "TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
    char (id) // "_diags.tex"
  write (unit, "(5A)") TAB, "$$(DVIPS) -o " // char (id) // "_diags.ps " // &
    char (id) // "_diags.dvi"
else
  write (unit, "(5A)") TAB // '@echo " LATEX      ', &
    trim (char (id)) // '_diags.tex"'
  write (unit, "(5A)") TAB, "@TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
    char (id) // "_diags.tex > /dev/null"
  write (unit, "(5A)") TAB // '@echo " METAPOST    ', &
    trim (char (id)) // '_diags-fmf.mp"'
  write (unit, "(5A)") TAB, "@MPINPUTS=$(MP_FLAGS) $(MPOST) " // &
    char (id) // "_diags-fmf.mp > /dev/null"
  write (unit, "(5A)") TAB // '@echo " LATEX      ', &
    trim (char (id)) // '_diags.tex"'
  write (unit, "(5A)") TAB, "@TEXINPUTS=$(TEX_FLAGS) $(LATEX) " // &
    char (id) // "_diags.tex > /dev/null"
  write (unit, "(5A)") TAB // '@echo " DVIPS      ', &
    trim (char (id)) // '_diags.dvi"'
  write (unit, "(5A)") TAB, "@$(DVIPS) -q -o " // char (id) &
    // "_diags.ps " // char (id) // "_diags.dvi"
end if
if (os_data%event_analysis_pdf) then
  if (verbose) then
    write (unit, "(5A)") TAB, "$$(PS2PDF) " // char (id) // "_diags.ps"
  else
    write (unit, "(5A)") TAB // '@echo " PS2PDF      ', &
      trim (char (id)) // '_diags.ps"'
    write (unit, "(5A)") TAB, "@$(PS2PDF) " // char (id) // "_diags.ps"
  end if
end if
end if
end if
end subroutine omega_write_makefile_code

```

The source is written by the makefile, so nothing to do here.

```

<Omega interface: omega writer: TBP>+≡
  procedure :: write_source_code => omega_write_source_code

<Omega interface: procedures>+≡
  subroutine omega_write_source_code (writer, id)
    class(omega_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
  end subroutine omega_write_source_code

```

Nothing to be done here.

```

<Omega interface: omega writer: TBP>+≡

```

```

    procedure :: before_compile => omega_before_compile
    procedure :: after_compile => omega_after_compile

    <Omega interface: procedures>+≡
    subroutine omega_before_compile (writer, id)
        class(omega_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine omega_before_compile

    subroutine omega_after_compile (writer, id)
        class(omega_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
    end subroutine omega_after_compile

```

Return the name of a procedure that implements a given feature, as it is provided by the external matrix-element code. O'MEGA names some procedures differently, therefore we translate here and override the binding of the base type.

```

    <Omega interface: omega writer: TBP>+≡
    procedure, nopass :: get_procname => omega_writer_get_procname

    <Omega interface: procedures>+≡
    function omega_writer_get_procname (feature) result (name)
        type(string_t) :: name
        type(string_t), intent(in) :: feature
        select case (char (feature))
        case ("n_in");   name = "number_particles_in"
        case ("n_out");  name = "number_particles_out"
        case ("n_flv");  name = "number_flavor_states"
        case ("n_hel");  name = "number_spin_states"
        case ("n_col");  name = "number_color_flows"
        case ("n_cin");  name = "number_color_indices"
        case ("n_cf");   name = "number_color_factors"
        case ("flv_state"); name = "flavor_states"
        case ("hel_state"); name = "spin_states"
        case ("col_state"); name = "color_flows"
        case default
            name = feature
        end select
    end function omega_writer_get_procname

```

The interfaces for the O'MEGA-specific features.

```

    <Omega interface: omega writer: TBP>+≡
    procedure :: write_interface => omega_write_interface

    <Omega interface: procedures>+≡
    subroutine omega_write_interface (writer, unit, id, feature)
        class(omega_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        type(string_t), intent(in) :: feature
        type(string_t) :: name
        name = writer%get_c_procname (id, feature)
        write (unit, "(2x,9A)") "interface"
        select case (char (feature))

```

```

case ("init")
  write (unit, "(5x,9A)") "subroutine ", char (name), &
    " (par, scheme) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "real(c_default_float), dimension(*), &
    &intent(in) :: par"
  write (unit, "(7x,9A)") "integer(c_int), intent(in) :: scheme"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("update_alpha_s")
  write (unit, "(5x,9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: alpha_s"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("reset_helicity_selection")
  write (unit, "(5x,9A)") "subroutine ", char (name), " &
    &(threshold, cutoff) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: threshold"
  write (unit, "(7x,9A)") "integer(c_int), intent(in) :: cutoff"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("is_allowed")
  write (unit, "(5x,9A)") "subroutine ", char (name), " &
    &(flv, hel, col, flag) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
  write (unit, "(7x,9A)") "logical(c_bool), intent(out) :: flag"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("new_event")
  write (unit, "(5x,9A)") "subroutine ", char (name), " (p) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "real(c_default_float), dimension(0:3,*), &
    &intent(in) :: p"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("get_amplitude")
  write (unit, "(5x,9A)") "subroutine ", char (name), " &
    &(flv, hel, col, amp) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
  write (unit, "(7x,9A)") "complex(c_default_complex), intent(out) &
    &:: amp"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
end select
write (unit, "(2x,9A)") "end interface"
end subroutine omega_write_interface

```

The wrappers have to take into account conversion between C and Fortran data types.

NOTE: The case `c_default_float` \neq default is not yet covered.

(Omega interface: omega writer: TBP)+ \equiv

```
procedure :: write_wrapper => omega_write_wrapper
```

(Omega interface: procedures)+ \equiv

```
subroutine omega_write_wrapper (writer, unit, id, feature)
  class(omega_writer_t), intent(in) :: writer

```

```

integer, intent(in) :: unit
type(string_t), intent(in) :: id, feature
type(string_t) :: name
name = writer%get_c_procname (id, feature)
write (unit, *)
select case (char (feature))
case ("init")
  write (unit, "(9A)") "subroutine ", char (name), &
    " (par, scheme) bind(C)"
  write (unit, "(2x,9A)") "use iso_c_binding"
  write (unit, "(2x,9A)") "use kinds"
  write (unit, "(2x,9A)") "use opr_", char (id)
  write (unit, "(2x,9A)") "real(c_default_float), dimension(*), &
    &intent(in) :: par"
  write (unit, "(2x,9A)") "integer(c_int), intent(in) :: scheme"
  if (c_default_float == default .and. c_int == kind(1)) then
    write (unit, "(2x,9A)") "call ", char (feature), " (par, scheme)"
  end if
  write (unit, "(9A)") "end subroutine ", char (name)
case ("update_alpha_s")
  write (unit, "(9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
  write (unit, "(2x,9A)") "use iso_c_binding"
  write (unit, "(2x,9A)") "use kinds"
  write (unit, "(2x,9A)") "use opr_", char (id)
  if (c_default_float == default) then
    write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
      &:: alpha_s"
    write (unit, "(2x,9A)") "call ", char (feature), " (alpha_s)"
  end if
  write (unit, "(9A)") "end subroutine ", char (name)
case ("reset_helicity_selection")
  write (unit, "(9A)") "subroutine ", char (name), &
    " (threshold, cutoff) bind(C)"
  write (unit, "(2x,9A)") "use iso_c_binding"
  write (unit, "(2x,9A)") "use kinds"
  write (unit, "(2x,9A)") "use opr_", char (id)
  if (c_default_float == default) then
    write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
      &:: threshold"
    write (unit, "(2x,9A)") "integer(c_int), intent(in) :: cutoff"
    write (unit, "(2x,9A)") "call ", char (feature), &
      " (threshold, int (cutoff))"
  end if
  write (unit, "(9A)") "end subroutine ", char (name)
case ("is_allowed")
  write (unit, "(9A)") "subroutine ", char (name), &
    " (flv, hel, col, flag) bind(C)"
  write (unit, "(2x,9A)") "use iso_c_binding"
  write (unit, "(2x,9A)") "use kinds"
  write (unit, "(2x,9A)") "use opr_", char (id)
  write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
  write (unit, "(2x,9A)") "logical(c_bool), intent(out) :: flag"
  write (unit, "(2x,9A)") "flag = ", char (feature), &
    " (int (flv), int (hel), int (col))"

```

```

        write (unit, "(9A)") "end subroutine ", char (name)
    case ("new_event")
        write (unit, "(9A)") "subroutine ", char (name), " (p) bind(C)"
        write (unit, "(2x,9A)") "use iso_c_binding"
        write (unit, "(2x,9A)") "use kinds"
        write (unit, "(2x,9A)") "use opr_", char (id)
        if (c_default_float == default) then
            write (unit, "(2x,9A)") "real(c_default_float), dimension(0:3,*), &
                &intent(in) :: p"
            write (unit, "(2x,9A)") "call ", char (feature), " (p)"
        end if
        write (unit, "(9A)") "end subroutine ", char (name)
    case ("get_amplitude")
        write (unit, "(9A)") "subroutine ", char (name), &
            " (flv, hel, col, amp) bind(C)"
        write (unit, "(2x,9A)") "use iso_c_binding"
        write (unit, "(2x,9A)") "use kinds"
        write (unit, "(2x,9A)") "use opr_", char (id)
        write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
        write (unit, "(2x,9A)") "complex(c_default_complex), intent(out) &
            &:: amp"
        write (unit, "(2x,9A)") "amp = ", char (feature), &
            " (int (flv), int (hel), int (col))"
        write (unit, "(9A)") "end subroutine ", char (name)
    end select
end subroutine omega_write_wrapper

```

17.4.3 Driver

```

<Omega interface: public>+≡
    public :: omega_driver_t

<Omega interface: types>+≡
    type, extends (prc_core_driver_t) :: omega_driver_t
        procedure(init_t), nopass, pointer :: &
            init => null ()
        procedure(update_alpha_s_t), nopass, pointer :: &
            update_alpha_s => null ()
        procedure(reset_helicity_selection_t), nopass, pointer :: &
            reset_helicity_selection => null ()
        procedure(is_allowed_t), nopass, pointer :: &
            is_allowed => null ()
        procedure(new_event_t), nopass, pointer :: &
            new_event => null ()
        procedure(get_amplitude_t), nopass, pointer :: &
            get_amplitude => null ()
    contains
        <Omega interface: omega driver: TBP>
    end type omega_driver_t

```

The reported type is the same as for the `omega_def_t` type.

```

<Omega interface: omega driver: TBP>≡
    procedure, nopass :: type_name => omega_driver_type_name

```

```

<Omega interface: procedures>+≡
  function omega_driver_type_name () result (string)
    type(string_t) :: string
    string = "omega"
  end function omega_driver_type_name

```

17.4.4 High-level process definition

This procedure wraps the details filling a process-component definition entry as appropriate for an O'MEGA matrix element.

```

<Omega interface: public>+≡
  public :: omega_make_process_component

<Omega interface: procedures>+≡
  subroutine omega_make_process_component (entry, component_index, &
    model_name, prt_in, prt_out, &
    ufo, ufo_path, restrictions, cms_scheme, &
    openmp_support, report_progress, write_omega_output, extra_options, diags, diags_color)
    class(process_def_entry_t), intent(inout) :: entry
    integer, intent(in) :: component_index
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in
    type(string_t), dimension(:), intent(in) :: prt_out
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path
    type(string_t), intent(in), optional :: restrictions
    logical, intent(in), optional :: cms_scheme
    logical, intent(in), optional :: openmp_support
    logical, intent(in), optional :: report_progress
    logical, intent(in), optional :: write_omega_output
    type(string_t), intent(in), optional :: extra_options
    logical, intent(in), optional :: diags, diags_color
    logical :: ufo_model
    class(prc_core_def_t), allocatable :: def
    ufo_model = .false.; if (present (ufo)) ufo_model = ufo
    allocate (omega_def_t :: def)
    select type (def)
    class is (omega_def_t)
      call def%init (model_name, prt_in, prt_out, &
        .false., ufo_model, ufo_path, &
        restrictions, cms_scheme, &
        openmp_support, report_progress, write_omega_output, extra_options, diags, diags_color)
    end select
    call entry%import_component (component_index, &
      n_out = size (prt_out), &
      prt_in = new_prt_spec (prt_in), &
      prt_out = new_prt_spec (prt_out), &
      method = var_str ("omega"), &
      variant = def)
  end subroutine omega_make_process_component

```

17.4.5 The prc_omega_t wrapper

This is an instance of the generic prc_core_t object. It contains a pointer to the process definition (omega_def_t), a data component (process_constants_t), and the matrix-element driver (omega_driver_t).

```

<Omega interface: public>+≡
    public :: prc_omega_t

<Omega interface: types>+≡
    type, extends (prc_core_t) :: prc_omega_t
        real(default), dimension(:), allocatable :: par
        integer :: scheme = 0
        type(helicity_selection_t) :: helicity_selection
        type(qcd_t) :: qcd
        type(qed_t) :: qed
    contains
        <Omega interface: prc omega: TBP>
    end type prc_omega_t

```

The workspace associated to a prc_omega_t object contains a single flag. The flag is used to suppress re-evaluating the matrix element for each quantum-number combination, after the first amplitude belonging to a given kinematics has been computed.

We can also store the value of a running coupling once it has been calculated for an event. The default value is negative, which indicates an undefined value in this context.

```

<Omega interface: public>+≡
    public :: omega_state_t

<Omega interface: types>+≡
    type, extends (prc_core_state_t) :: omega_state_t
        logical :: new_kinematics = .true.
        real(default) :: alpha_qcd = -1
    contains
        <Omega interface: omega state: TBP>
    end type omega_state_t

<Omega interface: omega state: TBP>≡
    procedure :: write => omega_state_write

<Omega interface: procedures>+≡
    subroutine omega_state_write (object, unit)
        class(omega_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A,L1)") "0'Mega state: new kinematics = ", &
            object%new_kinematics
    end subroutine omega_state_write

<Omega interface: omega state: TBP>+≡
    procedure :: reset_new_kinematics => omega_state_reset_new_kinematics

```



```

<Omega interface: procedures>+≡
  subroutine omega_state_reset_new_kinematics (object)
    class(omega_state_t), intent(inout) :: object
    object%new_kinematics = .true.
  end subroutine omega_state_reset_new_kinematics

```

Allocate the workspace with the above specific type.

```

<Omega interface: prc omega: TBP>≡
  procedure :: allocate_workspace => prc_omega_allocate_workspace

<Omega interface: procedures>+≡
  subroutine prc_omega_allocate_workspace (object, core_state)
    class(prc_omega_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    allocate (omega_state_t :: core_state)
  end subroutine prc_omega_allocate_workspace

```

The following procedures are inherited from the base type as deferred, thus must be implemented. The corresponding unit tests are skipped here; the procedures are tested when called from the `processes` module.

Output: print just the ID of the associated matrix element. Then display any stored parameters and the helicity selection data. (The latter are printed only if active.)

```

<Omega interface: prc omega: TBP>+≡
  procedure :: write => prc_omega_write

<Omega interface: procedures>+≡
  subroutine prc_omega_write (object, unit)
    class(prc_omega_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(3x,A)", advance="no") "0'Mega process core:"
    if (object%data_known) then
      write (u, "(1x,A)") char (object%data%id)
    else
      write (u, "(1x,A)") "[undefined]"
    end if
    if (allocated (object%par)) then
      write (u, "(3x,A)") "Parameter array:"
      do i = 1, size (object%par)
        write (u, "(5x,I0,1x,ES17.10)") i, object%par(i)
      end do
    end if
    call object%helicity_selection%write (u)
    call object%qcd%write (u)
    call object%qed%write (u)
  end subroutine prc_omega_write

```

```

<Omega interface: prc omega: TBP>+≡
  procedure :: write_name => prc_omega_write_name

```

```

<Omega interface: procedures>+=
  subroutine prc_omega_write_name (object, unit)
    class(prc_omega_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u,"(1x,A)") "Core: 0'Mega"
  end subroutine prc_omega_write_name

```

Temporarily store the parameter array inside the `prc_omega` object, so we can use it later during the actual initialization. Also store threshold and cutoff for helicity selection.

```

<Omega interface: prc omega: TBP>+=
  procedure :: set_parameters => prc_omega_set_parameters

<Omega interface: procedures>+=
  subroutine prc_omega_set_parameters (prc_omega, model, &
    helicity_selection, qcd, use_color_factors)
    class(prc_omega_t), intent(inout) :: prc_omega
    class(model_data_t), intent(in), target, optional :: model
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    type(qcd_t), intent(in), optional :: qcd
    type(qed_t) :: qed
    logical, intent(in), optional :: use_color_factors
    if (present (model)) then
      if (.not. allocated (prc_omega%par)) &
        allocate (prc_omega%par (model%get_n_real ()))
      call model%real_parameters_to_array (prc_omega%par)
      prc_omega%scheme = model%get_scheme_num ()
      if (associated (model%get_par_data_ptr (var_str ('alpha_em_i')))) then
        call qed%set_alpha_qed (one / model%get_real (var_str ('alpha_em_i')))
      end if
      prc_omega%qed = qed
    end if
    if (present (helicity_selection)) then
      prc_omega%helicity_selection = helicity_selection
    end if
    if (present (qcd)) then
      prc_omega%qcd = qcd
    end if
    if (present (use_color_factors)) then
      prc_omega%use_color_factors = use_color_factors
    end if
  end subroutine prc_omega_set_parameters

```

To fully initialize the process core, we perform base initialization, then initialize the external matrix element code.

This procedure overrides the `init` method of the base type, which we nevertheless can access via its binding `base_init`. When done, we have an allocated driver. The driver will call the `init` procedure for the external matrix element, and thus transfer the parameter set to where it finally belongs.

If requested, we initialize the helicity selection counter.

```

<Omega interface: prc omega: TBP>+=

```

```

    procedure :: init => prc_omega_init
<Omega interface: procedures>+≡
    subroutine prc_omega_init (object, def, lib, id, i_component)
        class(prc_omega_t), intent(inout) :: object
        class(prc_core_def_t), intent(in), target :: def
        type(process_library_t), intent(in), target :: lib
        type(string_t), intent(in) :: id
        integer, intent(in) :: i_component
        call object%base_init (def, lib, id, i_component)
        call object%activate_parameters ()
    end subroutine prc_omega_init

```

Activate the stored parameters by transferring them to the external matrix element. Also reset the helicity selection, if requested.

```

<Omega interface: prc omega: TBP>+≡
    procedure :: activate_parameters => prc_omega_activate_parameters
<Omega interface: procedures>+≡
    subroutine prc_omega_activate_parameters (object)
        class (prc_omega_t), intent(inout) :: object
        if (allocated (object%driver)) then
            if (allocated (object%par)) then
                select type (driver => object%driver)
                    type is (omega_driver_t)
                        if (associated (driver%init)) then
                            call driver%init (object%par, object%scheme)
                        end if
                    end select
            else
                call msg_bug ("prc_omega_activate: parameter set is not allocated")
            end if
            call object%reset_helicity_selection ()
        else
            call msg_bug ("prc_omega_activate: driver is not allocated")
        end if
    end subroutine prc_omega_activate_parameters

```

Tell whether a particular combination of flavor, helicity, color is allowed. Here we have to consult the matrix-element driver.

```

<Omega interface: prc omega: TBP>+≡
    procedure :: is_allowed => prc_omega_is_allowed
<Omega interface: procedures>+≡
    function prc_omega_is_allowed (object, i_term, f, h, c) result (flag)
        class(prc_omega_t), intent(in) :: object
        integer, intent(in) :: i_term, f, h, c
        logical :: flag
        logical(c_bool) :: cflag
        select type (driver => object%driver)
            type is (omega_driver_t)
                call driver%is_allowed (f, h, c, cflag)
                flag = cflag
            end select
    end function

```

```
end function prc_omega_is_allowed
```

Transfer the generated momenta directly to the hard interaction in the (only) term. We assume that everything has been set up correctly, so the array fits.

We don't reset the `new_kinematics` flag here. This has to be done explicitly by the caller (`reset_new_kinematics`) when a new kinematics configuration is to be considered.

```
<Omega interface: prc omega: TBP>+≡
  procedure :: compute_hard_kinematics => prc_omega_compute_hard_kinematics

<Omega interface: procedures>+≡
  subroutine prc_omega_compute_hard_kinematics &
    (object, p_seed, i_term, int_hard, core_state)
    class(prc_omega_t), intent(in) :: object
    type(vector4_t), dimension(:), intent(in) :: p_seed
    integer, intent(in) :: i_term
    type(interaction_t), intent(inout) :: int_hard
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    call int_hard%set_momenta (p_seed)
  end subroutine prc_omega_compute_hard_kinematics
```

This procedure is not called for `prc_omega_t`, just a placeholder.

```
<Omega interface: prc omega: TBP>+≡
  procedure :: compute_eff_kinematics => prc_omega_compute_eff_kinematics

<Omega interface: procedures>+≡
  subroutine prc_omega_compute_eff_kinematics &
    (object, i_term, int_hard, int_eff, core_state)
    class(prc_omega_t), intent(in) :: object
    integer, intent(in) :: i_term
    type(interaction_t), intent(in) :: int_hard
    type(interaction_t), intent(inout) :: int_eff
    class(prc_core_state_t), intent(inout), allocatable :: core_state
  end subroutine prc_omega_compute_eff_kinematics
```

Reset the helicity selection counters and start counting zero helicities. We assume that the `helicity_selection` object is allocated. Otherwise, reset and switch off helicity counting.

In the test routine, the driver is allocated but the driver methods are not. Therefore, guard against a disassociated method.

```
<Omega interface: prc omega: TBP>+≡
  procedure :: reset_helicity_selection => prc_omega_reset_helicity_selection

<Omega interface: procedures>+≡
  subroutine prc_omega_reset_helicity_selection (object)
    class(prc_omega_t), intent(inout) :: object
    select type (driver => object%driver)
    type is (omega_driver_t)
      if (associated (driver%reset_helicity_selection)) then
        if (object%helicity_selection%active) then
          call driver%reset_helicity_selection &
            (real (object%helicity_selection%threshold, &
              c_default_float), &
```

```

        int (object%helicity_selection%cutoff, c_int))
    else
        call driver%reset_helicity_selection &
            (0._c_default_float, 0_c_int)
    end if
end if
end select
end subroutine prc_omega_reset_helicity_selection

```

Compute the amplitude. For the tree-level process, we can ignore the scale settings. The term index j is also irrelevant.

We first call `new_event` for the given momenta (which we must unpack), then retrieve the amplitude value for the given quantum numbers.

If the `core_state` status flag is present, we can make sure that we call `new_event` only once for a given kinematics. After the first call, we unset the `new_kinematics` flag.

The core objects computes the appropriate α_s value via the `qcd` subobject, taking into account the provided `fac_scale` value. However, if the extra parameter `alpha_qcd_forced` is allocated, it overrides this setting.

The `is_allowed` query is not redundant, since the status may change during the run if helicities are switched off.

(Omega interface: prc omega: TBP)+≡

```

procedure :: compute_amplitude => prc_omega_compute_amplitude

```

(Omega interface: procedures)+≡

```

function prc_omega_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
    core_state) result (amp)
    class(prc_omega_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
    real(default) :: alpha_qcd
    complex(default) :: amp
    integer :: n_tot, i
    real(c_default_float), dimension(:, :), allocatable :: parray
    complex(c_default_complex) :: camp
    logical :: new_event
    select type (driver => object%driver)
    type is (omega_driver_t)
        new_event = .true.
    if (present (core_state)) then
        if (allocated (core_state)) then
            select type (core_state)
            type is (omega_state_t)
                new_event = core_state%new_kinematics
                core_state%new_kinematics = .false.
            end select
        end if
    end if
end if

```

```

if (new_event) then
  if (allocated (object%qcd%alpha)) then
    if (allocated (alpha_qcd_forced)) then
      alpha_qcd = alpha_qcd_forced
    else
      alpha_qcd = object%qcd%alpha%get (fac_scale)
    end if
    call driver%update_alpha_s (alpha_qcd)
    if (present (core_state)) then
      if (allocated (core_state)) then
        select type (core_state)
        type is (omega_state_t)
          core_state%alpha_qcd = alpha_qcd
        end select
      end if
    end if
  end if
  n_tot = object%data%get_n_tot ()
  allocate (parray (0:3, n_tot))
  do i = 1, n_tot
    parray(:,i) = vector4_get_components (p(i))
  end do
  call driver%new_event (parray)
end if
if (object%is_allowed (1, f, h, c)) then
  call driver%get_amplitude &
    (int (f, c_int), int (h, c_int), int (c, c_int), camp)
  amp = camp
else
  amp = 0
end if
end select
end function prc_omega_compute_amplitude

```

After the amplitude has been computed, we may read off the current value of α_s . This works only if α_s varies, and if the workspace `core_state` is present which stores this value.

(Omega interface: prc omega: TBP)+≡

```

procedure :: get_alpha_s => prc_omega_get_alpha_s

```

(Omega interface: procedures)+≡

```

function prc_omega_get_alpha_s (object, core_state) result (alpha_qcd)
  class(prc_omega_t), intent(in) :: object
  class(prc_core_state_t), intent(in), allocatable :: core_state
  real(default) :: alpha_qcd
  alpha_qcd = -1
  if (allocated (object%qcd%alpha) .and. allocated (core_state)) then
    select type (core_state)
    type is (omega_state_t)
      alpha_qcd = core_state%alpha_qcd
    end select
  end if
end function prc_omega_get_alpha_s

```

α_{em} is not updated after computing the amplitude because we currently only support a fixed α_{em} but we still need a routine to get the value of `alpha_qed`.

```

<Omega interface: prc omega: TBP>+≡
  procedure :: get_alpha_qed => prc_omega_get_alpha_qed

<Omega interface: procedures>+≡
  function prc_omega_get_alpha_qed (object) result (alpha_qed)
    class(prc_omega_t), intent(in) :: object
    real(default) :: alpha_qed
    alpha_qed = object%qed%get_alpha_qed ()
  end function prc_omega_get_alpha_qed

```

17.4.6 Unit Test

Test module, followed by the corresponding implementation module. There is a separate test for testing O'MEGA diagram generation as this depends on a working analysis setup.

```

<prc_omega_ut.f90>≡
  <File header>

  module prc_omega_ut
    use unit_tests
    use prc_omega_util

    <Standard module head>

    <Omega interface: public test>

    contains

    <Omega interface: test driver>

  end module prc_omega_ut

<prc_omega_util.f90>≡
  <File header>

  module prc_omega_util

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    <Use strings>
    use io_units
    use file_utils, only: delete_file
    use os_interface
    use sm_qcd
    use lorentz
    use model_data
    use var_base
    use particle_specifiers, only: new_prt_spec
    use prc_core_def
    use process_constants

```

```

    use process_libraries
    use prc_core
    use model_testbed, only: prepare_model, cleanup_model

    use prc_omega

    <Standard module head>

    <Omega interface: test declarations>

contains

    <Omega interface: tests>

    end module prc_omega_util

API: driver for the unit tests below.
<Omega interface: public test>≡
    public :: prc_omega_test

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

<Omega interface: public test>+≡
    public :: prc_omega_diags_test

<Omega interface: test driver>+≡
    subroutine prc_omega_diags_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Omega interface: execute diags tests>
    end subroutine prc_omega_diags_test

```

Generate, compile and load a simple process matrix element

The process is $e^+e^- \rightarrow \mu^+\mu^-$ for vanishing masses and $e = 0.3$. We initialize the process, build the library, and compute a particular matrix element for momenta of unit energy and right-angle scattering. The matrix element, as it happens, is equal to e^2 . (Note that are no conversion factors applied, so this result is exact.)

For GNU make, `makeflags` is set to `-j1`. This eliminates a potential clash with a `-j<n>` flag if this test is called from a parallel make.

```

<Omega interface: execute tests>≡
    call test (prc_omega_1, "prc_omega_1", &
        "build and load simple OMega process", &
        u, results)

<Omega interface: test declarations>≡
    public :: prc_omega_1

```



```

(Omega interface: tests)≡
subroutine prc_omega_1 (u)
  integer, intent(in) :: u
  type(process_library_t) :: lib
  class(prc_core_def_t), allocatable :: def
  type(process_def_entry_t), pointer :: entry
  type(os_data_t) :: os_data
  type(string_t) :: model_name
  type(string_t), dimension(:), allocatable :: prt_in, prt_out
  type(process_constants_t) :: data
  class(prc_core_driver_t), allocatable :: driver
  integer, parameter :: cdf = c_default_float
  integer, parameter :: ci = c_int
  real(cdf), dimension(4) :: par
  real(cdf), dimension(0:3,4) :: p
  logical(c_bool) :: flag
  complex(c_default_complex) :: amp
  integer :: i

  write (u, "(A)")  "* Test output: prc_omega_1"
  write (u, "(A)")  "* Purpose: create a simple process with OMega"
  write (u, "(A)")  "* build a library, link, load, and &
    &access the matrix element"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize a process library with one entry"
  write (u, "(A)")
  call lib%init (var_str ("omega1"))
  call os_data%init ()

  model_name = "QED"
  allocate (prt_in (2), prt_out (2))
  prt_in = [var_str ("e+"), var_str ("e-")]
  prt_out = [var_str ("m+"), var_str ("m-")]

  allocate (omega_def_t :: def)
  select type (def)
  type is (omega_def_t)
    call def%init (model_name, prt_in, prt_out, &
      ufo = .false., ovm = .false.)
  end select
  allocate (entry)
  call entry%init (var_str ("omega1_a"), model_name = model_name, &
    n_in = 2, n_components = 1)
  call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
  call lib%append (entry)

  write (u, "(A)")  "* Configure library"
  write (u, "(A)")
  call lib%configure (os_data)

```

```

write (u, "(A)")  "* Write makefile"
write (u, "(A)")
call lib%write_makefile (os_data, force = .true., verbose = .false.)

write (u, "(A)")  "* Clean any left-over files"
write (u, "(A)")
call lib%clean (os_data, distclean = .false.)

write (u, "(A)")  "* Write driver"
write (u, "(A)")
call lib%write_driver (force = .true.)

write (u, "(A)")  "* Write process source code, compile, link, load"
write (u, "(A)")
call lib%load (os_data)

call lib%write (u, libpath = .false.)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active" = ", &
lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes" = ", &
lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Constants of omega1_a_i1:"
write (u, "(A)")

call lib%connect_process (var_str ("omega1_a"), 1, data, driver)

write (u, "(1x,A,A)")  "component ID" = ", char (data%id)
write (u, "(1x,A,A)")  "model name" = ", char (data%model_name)
write (u, "(1x,A,A,A)")  "md5sum" = ', ', data%md5sum, "'
write (u, "(1x,A,L1)")  "openmp supported = ", data%openmp_supported
write (u, "(1x,A,I0)")  "n_in = ", data%n_in
write (u, "(1x,A,I0)")  "n_out = ", data%n_out
write (u, "(1x,A,I0)")  "n_flv = ", data%n_flv
write (u, "(1x,A,I0)")  "n_hel = ", data%n_hel
write (u, "(1x,A,I0)")  "n_col = ", data%n_col
write (u, "(1x,A,I0)")  "n_cin = ", data%n_cin
write (u, "(1x,A,I0)")  "n_cf = ", data%n_cf
write (u, "(1x,A,10(1x,I0))")  "flv state =", data%flv_state
write (u, "(1x,A,10(1x,I2))")  "hel state =", data%hel_state(:,1)
do i = 2, 16
  write (u, "(12x,4(1x,I2))")  data%hel_state(:,i)
end do
write (u, "(1x,A,10(1x,I0))")  "col state =", data%col_state
write (u, "(1x,A,10(1x,L1))")  "ghost flag =", data%ghost_flag
write (u, "(1x,A,10(1x,F5.3))")  "color factors =", data%color_factors
write (u, "(1x,A,10(1x,I0))")  "cf index =", data%cf_index

```

```

write (u, "(A)")
write (u, "(A)")  "* Set parameters for omega1_a and initialize:"
write (u, "(A)")

par = [0.3_cdf, 0.0_cdf, 0.0_cdf, 0.0_cdf]
write (u, "(2x,A,F6.4)") "ee  = ", par(1)
write (u, "(2x,A,F6.4)") "me  = ", par(2)
write (u, "(2x,A,F6.4)") "mmu = ", par(3)
write (u, "(2x,A,F6.4)") "mtau = ", par(4)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
    1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
    1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
    1.0_cdf, -1.0_cdf, 0.0_cdf, 0.0_cdf &
    ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

select type (driver)
type is (omega_driver_t)
    call driver%init (par, 0)

    call driver%new_event (p)

    write (u, "(A)")
    write (u, "(A)")  "* Compute matrix element:"
    write (u, "(A)")

    call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
    write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_1"

end subroutine prc_omega_1

```

Check prc_omega_t wrapper and options

The process is $e^-e^+ \rightarrow e^-e^+$ for vanishing masses and $e = 0.3$. We build the library using the high-level procedure `omega.make_process_component` and

the “black box” `prc_omega_t` object. Two variants with different settings for restrictions and OpenMP.

For GNU make, `makeflags` is set to `-j1`. This eliminates a potential clash with a `-j<n>` flag if this test is called from a parallel make.

```

<Omega interface: execute tests>+≡
    call test (prc_omega_2, "prc_omega_2", &
               "OMega option passing", &
               u, results)

<Omega interface: test declarations>+≡
    public :: prc_omega_2

<Omega interface: tests>+≡
    subroutine prc_omega_2 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(process_def_entry_t), pointer :: entry
        type(os_data_t) :: os_data
        type(string_t) :: model_name
        class(model_data_t), pointer :: model
        class(vars_t), pointer :: vars
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        type(string_t) :: restrictions
        type(process_component_def_t), pointer :: config
        type(prc_omega_t) :: prc1, prc2
        type(process_constants_t) :: data
        integer, parameter :: cdf = c_default_float
        integer, parameter :: ci = c_int
        real(cdf), dimension(:), allocatable :: par
        real(cdf), dimension(0:3,4) :: p
        complex(c_default_complex) :: amp
        integer :: i
        logical :: exist

        write (u, "(A)")  "* Test output: prc_omega_2"
        write (u, "(A)")  "* Purpose: create simple processes with OMega"
        write (u, "(A)")  "*           use the prc_omega wrapper for this"
        write (u, "(A)")  "*           and check OMega options"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize a process library with two entries, &
                           &different options."
        write (u, "(A)")  "* (1) e- e+ -> e- e+  &
                           &(all diagrams, no OpenMP, report progress)"
        write (u, "(A)")  "* (2) e- e+ -> e- e+  &
                           &(s-channel only, with OpenMP, report progress to file)"

        call lib%init (var_str ("omega2"))
        call os_data%init ()

        model_name = "QED"
        model => null ()
        call prepare_model (model, model_name, vars)

        allocate (prt_in (2), prt_out (2))

```

```

prt_in = [var_str ("e-"), var_str ("e+")]
prt_out = prt_in
restrictions = "3+4~A"

allocate (entry)
call entry%init (var_str ("omega2_a"), &
    model, n_in = 2, n_components = 2)

call omega_make_process_component (entry, 1, &
    model_name, prt_in, prt_out, &
    report_progress=.true.)
call omega_make_process_component (entry, 2, &
    model_name, prt_in, prt_out, &
    restrictions=restrictions, openmp_support=.true., &
    extra_options=var_str ("-fusion:progress_file omega2.log"))

call lib%append (entry)

write (u, "(A)")
write (u, "(A)")  "* Remove left-over file"
write (u, "(A)")

call delete_file ("omega2.log")
inquire (file="omega2.log", exist=exist)
write (u, "(1x,A,L1)") "omega2.log exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Build and load library"

call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")
write (u, "(A)")  "* Check extra output of OMega"
write (u, "(A)")

inquire (file="omega2.log", exist=exist)
write (u, "(1x,A,L1)") "omega2.log exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)") "is active                = ", &
    lib%is_active ()
write (u, "(1x,A,I0)") "n_processes            = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Set parameters for omega2_a and initialize:"
write (u, "(A)")

```

```

call vars%set_rval (var_str ("ee"), 0.3_default)
call vars%set_rval (var_str ("me"), 0._default)
call vars%set_rval (var_str ("mmu"), 0._default)
call vars%set_rval (var_str ("mtau"), 0._default)
allocate (par (model%get_n_real ()))
call model%real_parameters_to_c_array (par)

write (u, "(2x,A,F6.4)") "ee = ", par(1)
write (u, "(2x,A,F6.4)") "me = ", par(2)
write (u, "(2x,A,F6.4)") "mmu = ", par(3)
write (u, "(2x,A,F6.4)") "mtau = ", par(4)

call prc1%set_parameters (model)
call prc2%set_parameters (model)

write (u, "(A)")
write (u, "(A)")  "* Constants of omega2_a_i1:"
write (u, "(A)")

entry => lib%get_process_def_ptr (var_str ("omega2_a"))
config => entry%get_component_def_ptr (1)
call prc1%init (config%get_core_def_ptr (), &
lib, var_str ("omega2_a"), 1)
call prc1%get_constants (data, 1)

write (u, "(1x,A,A)") "component ID = ", &
char (data%id)
write (u, "(1x,A,L1)") "openmp supported = ", &
data%openmp_supported
write (u, "(1x,A,A,A)") "model name = ', &
char (data%model_name), "'"

write (u, "(A)")
write (u, "(A)")  "* Constants of omega2_a_i2:"
write (u, "(A)")

config => entry%get_component_def_ptr (2)
call prc2%init (config%get_core_def_ptr (), &
lib, var_str ("omega2_a"), 2)
call prc2%get_constants (data, 1)

write (u, "(1x,A,A)") "component ID = ", &
char (data%id)
write (u, "(1x,A,L1)") "openmp supported = ", &
data%openmp_supported
write (u, "(1x,A,A,A)") "model name = ', &
char (data%model_name), "'"

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &

```

```

        1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
        1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
        1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
        1.0_cdf, -1.0_cdf, 0.0_cdf, 0.0_cdf &
    ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver => prc1%driver)
type is (omega_driver_t)
    call driver%new_event (p)
    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(2x,A,1x,E11.4)") "(1) |amp (1, 6, 1)| =", abs (amp)
end select

select type (driver => prc2%driver)
type is (omega_driver_t)
    call driver%new_event (p)
    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(2x,A,1x,E11.4)") "(2) |amp (1, 6, 1)| =", abs (amp)
end select

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &
    1.0_cdf, 0.0_cdf, 0.0_cdf, -1.0_cdf, &
    1.0_cdf, sqrt(0.5_cdf), 0.0_cdf, sqrt(0.5_cdf), &
    1.0_cdf, -sqrt(0.5_cdf), 0.0_cdf, -sqrt(0.5_cdf) &
], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute matrix element:"
write (u, "(A)")

select type (driver => prc1%driver)
type is (omega_driver_t)
    call driver%new_event (p)
    call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
    write (u, "(2x,A,1x,E11.4)") "(1) |amp (1, 6, 1)| =", abs (amp)
end select

select type (driver => prc2%driver)
type is (omega_driver_t)

```

```

        call driver%new_event (p)
        call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
        write (u, "(2x,A,1x,E11.4)") "(2) |amp (1, 6, 1)| =", abs (amp)
    end select

    call lib%final ()
    call cleanup_model (model)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: prc_omega_2"

end subroutine prc_omega_2

```

Check helicity selection

The process is $e^-e^+ \rightarrow e^-e^+$ for vanishing masses. We call the matrix element several times to verify the switching off of irrelevant helicities.

```

<Omega interface: execute tests>+=
    call test (prc_omega_3, "prc_omega_3", &
        "helicity selection", &
        u, results)

<Omega interface: test declarations>+=
    public :: prc_omega_3

<Omega interface: tests>+=
    subroutine prc_omega_3 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(process_def_entry_t), pointer :: entry
        type(os_data_t) :: os_data
        type(string_t) :: model_name
        class(model_data_t), pointer :: model
        class(vars_t), pointer :: vars => null ()
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        type(process_component_def_t), pointer :: config
        type(prc_omega_t) :: prc1
        type(process_constants_t) :: data
        integer, parameter :: cdf = c_default_float
        real(cdf), dimension(:), allocatable :: par
        real(cdf), dimension(0:3,4) :: p
        type(helicity_selection_t) :: helicity_selection
        integer :: i, h

        write (u, "(A)")  "* Test output: prc_omega_3"
        write (u, "(A)")  "*   Purpose: create simple process with OMega"
        write (u, "(A)")  "*               and check helicity selection"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize a process library."
        write (u, "(A)")  "* (1) e- e+ -> e- e+   (all diagrams, no OpenMP)"

        call lib%init (var_str ("omega3"))
    end subroutine prc_omega_3

```



```

call os_data%init ()

model_name = "QED"
model => null ()
call prepare_model (model, model_name, vars)

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e-"), var_str ("e+")]
prt_out = prt_in

allocate (entry)
call entry%init (var_str ("omega3_a"), &
    model, n_in = 2, n_components = 1)

call omega_make_process_component (entry, 1, &
    model_name, prt_in, prt_out)
call lib%append (entry)

write (u, "(A)")
write (u, "(A)")  "* Build and load library"

call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active" = ", &
    lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes" = ", &
    lib%get_n_processes ()

write (u, "(A)")
write (u, "(A)")  "* Set parameters for omega3_a and initialize:"
write (u, "(A)")

call vars%set_rval (var_str ("ee"), 0.3_default)
call vars%set_rval (var_str ("me"), 0._default)
call vars%set_rval (var_str ("mmu"), 0._default)
call vars%set_rval (var_str ("mtau"), 0._default)
allocate (par (model%get_n_real ()))
call model%real_parameters_to_c_array (par)

write (u, "(2x,A,F6.4)")  "ee  = ", par(1)
write (u, "(2x,A,F6.4)")  "me  = ", par(2)
write (u, "(2x,A,F6.4)")  "mmu = ", par(3)
write (u, "(2x,A,F6.4)")  "mtau = ", par(4)

call prc1%set_parameters (model, helicity_selection=helicity_selection)

```

```

write (u, "(A)")
write (u, "(A)")  "* Helicity states of omega3_a_i1:"
write (u, "(A)")

entry => lib%get_process_def_ptr (var_str ("omega3_a"))
config => entry%get_component_def_ptr (1)
call prc1%init (config%get_core_def_ptr (), &
               lib, var_str ("omega3_a"), 1)
call prc1%get_constants (data, 1)

do i = 1, data%n_hel
  write (u, "(3x,I2,':',4(1x,I2))") i, data%hel_state(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Initially allowed helicities:"
write (u, "(A)")

write (u, "(4x,16(1x,I2))") [(h, h = 1, data%n_hel)]
write (u, "(4x)", advance = "no")
do h = 1, data%n_hel
  write (u, "(2x,L1)", advance = "no") prc1%is_allowed (1, 1, h, 1)
end do
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Reset helicity selection (cutoff = 4)"
write (u, "(A)")

helicity_selection%active = .true.
helicity_selection%threshold = 1e10_default
helicity_selection%cutoff = 4
call helicity_selection%write (u)

call prc1%set_parameters (model, helicity_selection=helicity_selection)
call prc1%reset_helicity_selection ()

write (u, "(A)")
write (u, "(A)")  "* Allowed helicities:"
write (u, "(A)")

write (u, "(4x,16(1x,I2))") [(h, h = 1, data%n_hel)]
write (u, "(4x)", advance = "no")
do h = 1, data%n_hel
  write (u, "(2x,L1)", advance = "no") prc1%is_allowed (1, 1, h, 1)
end do
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
              1.0_cdf, 0.0_cdf, 0.0_cdf, 1.0_cdf, &

```

```

        1.0_cdf, 0.0_cdf, 0.0_cdf,-1.0_cdf, &
        1.0_cdf, 1.0_cdf, 0.0_cdf, 0.0_cdf, &
        1.0_cdf,-1.0_cdf, 0.0_cdf, 0.0_cdf &
        ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.4))") "p", i, " =", p(:,i)
end do

write (u, "(A)")
write (u, "(A)")  "* Compute scattering matrix 5 times"
write (u, "(A)")

write (u, "(4x,16(1x,I2))") [(h, h = 1, data%n_hel)]

select type (driver => prc1%driver)
type is (omega_driver_t)
    do i = 1, 5
        call driver%new_event (p)
        write (u, "(2x,I2)", advance = "no") i
        do h = 1, data%n_hel
            write (u, "(2x,L1)", advance = "no") prc1%is_allowed (1, 1, h, 1)
        end do
        write (u, "(A)")
    end do
end select

write (u, "(A)")
write (u, "(A)")  "* Reset helicity selection again"
write (u, "(A)")

call prc1%activate_parameters ()

write (u, "(A)")  "* Allowed helicities:"
write (u, "(A)")

write (u, "(4x,16(1x,I2))") [(h, h = 1, data%n_hel)]
write (u, "(4x)", advance = "no")
do h = 1, data%n_hel
    write (u, "(2x,L1)", advance = "no") prc1%is_allowed (1, 1, h, 1)
end do
write (u, "(A)")

call lib%final ()
call cleanup_model (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_3"

end subroutine prc_omega_3

```

QCD coupling

The process is $u\bar{u} \rightarrow d\bar{d}$ for vanishing masses. We compute the amplitude for a fixed configuration once, then reset α_s , then compute again.

For GNU make, makeflags is set to -j1. This eliminates a potential clash with a -j<n> flag if this test is called from a parallel make.

```
<Omega interface: execute tests>+≡
    call test (prc_omega_4, "prc_omega_4", &
               "update QCD alpha", &
               u, results)

<Omega interface: test declarations>+≡
    public :: prc_omega_4

<Omega interface: tests>+≡
    subroutine prc_omega_4 (u)
        integer, intent(in) :: u
        type(process_library_t) :: lib
        class(prc_core_def_t), allocatable :: def
        type(process_def_entry_t), pointer :: entry
        type(os_data_t) :: os_data
        type(string_t) :: model_name
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        type(process_constants_t) :: data
        class(prc_core_driver_t), allocatable :: driver
        integer, parameter :: cdf = c_default_float
        integer, parameter :: ci = c_int
        real(cdf), dimension(8) :: par
        real(cdf), dimension(0:3,4) :: p
        logical(c_bool) :: flag
        complex(c_default_complex) :: amp
        integer :: i
        real(cdf) :: alpha_s

        write (u, "(A)")  "* Test output: prc_omega_4"
        write (u, "(A)")  "*   Purpose: create a QCD process with OMega"
        write (u, "(A)")  "*               and check alpha_s dependence"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize a process library with one entry"
        write (u, "(A)")
        call lib%init (var_str ("prc_omega_4_lib"))
        call os_data%init ()

        model_name = "QCD"
        allocate (prt_in (2), prt_out (2))
        prt_in = [var_str ("u"), var_str ("ubar")]
        prt_out = [var_str ("d"), var_str ("dbar")]

        allocate (omega_def_t :: def)
        select type (def)
        type is (omega_def_t)
            call def%init (model_name, prt_in, prt_out, &
                          ufo = .false., ovm = .false.)
        end select
```

```

allocate (entry)
call entry%init (var_str ("prc_omega_4_p"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure and compile process"
write (u, "(A)")
call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active = ", lib%is_active ()

write (u, "(A)")
write (u, "(A)")  "* Set parameters:"
write (u, "(A)")

alpha_s = 0.1178_cdf

par = [alpha_s, &
    0._cdf, 0._cdf, 0._cdf, 0._cdf, 0._cdf, 173.1_cdf, 1.523_cdf]
write (u, "(2x,A,F8.4)")  "alpha_s = ", par(1)
write (u, "(2x,A,F8.4)")  "md      = ", par(2)
write (u, "(2x,A,F8.4)")  "mu      = ", par(3)
write (u, "(2x,A,F8.4)")  "ms      = ", par(4)
write (u, "(2x,A,F8.4)")  "mc      = ", par(5)
write (u, "(2x,A,F8.4)")  "mb      = ", par(6)
write (u, "(2x,A,F8.4)")  "mtop    = ", par(7)
write (u, "(2x,A,F8.4)")  "wtop    = ", par(8)

write (u, "(A)")
write (u, "(A)")  "* Set kinematics:"
write (u, "(A)")

p = reshape ([ &
    100.0_cdf, 0.0_cdf, 0.0_cdf, 100.0_cdf, &
    100.0_cdf, 0.0_cdf, 0.0_cdf, -100.0_cdf, &
    100.0_cdf, 100.0_cdf, 0.0_cdf, 0.0_cdf, &
    100.0_cdf, -100.0_cdf, 0.0_cdf, 0.0_cdf &
    ], [4,4])
do i = 1, 4
    write (u, "(2x,A,I0,A,4(1x,F7.1))")  "p", i, " =", p(:,i)
end do

```

```

call lib%connect_process (var_str ("prc_omega_4_p"), 1, data, driver)

select type (driver)
type is (omega_driver_t)
  call driver%init (par, 0)

  write (u, "(A)")
  write (u, "(A)")  "* Compute matrix element:"
  write (u, "(A)")

  call driver%new_event (p)

  call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
  write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

  call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
  write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)

  write (u, "(A)")
  write (u, "(A)")  "* Double alpha_s and compute matrix element again:"
  write (u, "(A)")

  call driver%update_alpha_s (2 * alpha_s)
  call driver%new_event (p)

  call driver%is_allowed (1_ci, 6_ci, 1_ci, flag)
  write (u, "(1x,A,L1)") "is_allowed (1, 6, 1) = ", flag

  call driver%get_amplitude (1_ci, 6_ci, 1_ci, amp)
  write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)
end select

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_4"

end subroutine prc_omega_4

```

Amplitude and QCD coupling

The same process as before. Here, we initialize with a running α_s coupling and compute twice with different scales. We use the high-level method `compute_amplitude`.

```

<Omega interface: execute tests>+≡
  call test (prc_omega_5, "prc_omega_5", &
    "running QCD alpha", &
    u, results)

<Omega interface: test declarations>+≡
  public :: prc_omega_5

<Omega interface: tests>+≡
  subroutine prc_omega_5 (u)

```

```

integer, intent(in) :: u
type(process_library_t) :: lib
class(prc_core_def_t), allocatable :: def
type(process_component_def_t), pointer :: cdef_ptr
class(prc_core_def_t), pointer :: def_ptr
type(process_def_entry_t), pointer :: entry
type(os_data_t) :: os_data
class(model_data_t), pointer :: model
type(string_t) :: model_name
type(string_t), dimension(:), allocatable :: prt_in, prt_out
type(qcd_t) :: qcd
class(prc_core_t), allocatable :: core
class(prc_core_state_t), allocatable :: core_state
type(vector4_t), dimension(4) :: p
complex(default) :: amp
real(default) :: fac_scale
real(default), allocatable :: alpha_qcd_forced
integer :: i

write (u, "(A)")  "* Test output: prc_omega_5"
write (u, "(A)")  "*   Purpose: create a QCD process with OMega"
write (u, "(A)")  "*               and check alpha_s dependence"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("prc_omega_5_lib"))
call os_data%init ()

model_name = "QCD"
model => null ()
call prepare_model (model, model_name)

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("u"), var_str ("ubar")]
prt_out = [var_str ("d"), var_str ("dbar")]

allocate (omega_def_t :: def)
select type (def)
type is (omega_def_t)
    call def%init (model_name, prt_in, prt_out, &
        ufo = .false., ovm = .false.)
end select
allocate (entry)
call entry%init (var_str ("prc_omega_5_p"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure and compile process"

```

```

write (u, "(A)")
call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")  "* Probe library API"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active = ", lib%is_active ()

write (u, "(A)")
write (u, "(A)")  "* Set kinematics"
write (u, "(A)")

p(1) = vector4_moving (100._default, 100._default, 3)
p(2) = vector4_moving (100._default,-100._default, 3)
p(3) = vector4_moving (100._default, 100._default, 1)
p(4) = vector4_moving (100._default,-100._default, 1)
do i = 1, 4
  call vector4_write (p(i), u)
end do

write (u, "(A)")
write (u, "(A)")  "* Setup QCD data"
write (u, "(A)")

allocate (alpha_qcd_from_scale_t :: qcd%alpha)

write (u, "(A)")  "* Setup process core"
write (u, "(A)")

allocate (prc_omega_t :: core)
entry => lib%get_process_def_ptr (var_str ("prc_omega_5_p"))
cdef_ptr => entry%get_component_def_ptr (1)
def_ptr => cdef_ptr%get_core_def_ptr ()

select type (core)
type is (prc_omega_t)
  call core%allocate_workspace (core_state)
  call core%set_parameters (model, qcd = qcd)
  call core%init (def_ptr, lib, var_str ("prc_omega_5_p"), 1)
  call core%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Compute matrix element"
  write (u, "(A)")

  fac_scale = 100
  write (u, "(1x,A,F4.0)")  "factorization scale = ", fac_scale

  amp = core%compute_amplitude &
    (1, p, 1, 6, 1, fac_scale, 100._default, alpha_qcd_forced)

```



```

write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)

write (u, "(A)")
write (u, "(A)")  "* Modify factorization scale and &
                   &compute matrix element again"
write (u, "(A)")

fac_scale = 200
write (u, "(1x,A,F4.0)") "factorization scale = ", fac_scale

amp = core%compute_amplitude &
      (1, p, 1, 6, 1, fac_scale, 100._default, alpha_qcd_forced)

write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)

write (u, "(A)")
write (u, "(A)")  "* Set alpha(QCD) directly and &
                   &compute matrix element again"
write (u, "(A)")

allocate (alpha_qcd_forced, source = 0.1_default)
write (u, "(1x,A,F6.4)") "alpha_qcd = ", alpha_qcd_forced

amp = core%compute_amplitude &
      (1, p, 1, 6, 1, fac_scale, 100._default, alpha_qcd_forced)

write (u, "(1x,A,1x,E11.4)") "|amp (1, 6, 1)| =", abs (amp)

end select

call lib%final ()
call cleanup_model (model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_5"

end subroutine prc_omega_5

```

UFO model file support

Again, the process is $e^-e^+ \rightarrow e^-e^+$ for vanishing masses and $e = 0.3$. We build the library using the high-level procedure `omega_make_process_component` and the “black box” `prc_omega_t` object. OMega must be able to digest the specified UFO file and provide use with a fresh model file that can be read after producing the process code.

For GNU make, `makeflags` is set to `-j1`. This eliminates a potential clash with a `-j<n>` flag if this test is called from a parallel make.

```

<Omega interface: execute tests>+≡
call test (prc_omega_6, "prc_omega_6", &
          "OMega UFO support", &
          u, results)

```

```

<Omega interface: test declarations>+≡
    public :: prc_omega_6

<Omega interface: tests>+≡
    subroutine prc_omega_6 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(process_def_entry_t), pointer :: entry
        type(os_data_t) :: os_data
        type(string_t) :: model_name
        class(model_data_t), pointer :: model
        class(vars_t), pointer :: vars
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        type(string_t) :: restrictions
        type(process_component_def_t), pointer :: config
        type(prc_omega_t) :: prc1, prc2
        type(process_constants_t) :: data
        integer, parameter :: cdf = c_default_float
        integer, parameter :: ci = c_int
        real(cdf), dimension(:), allocatable :: par
        real(cdf), dimension(0:3,4) :: p
        complex(c_default_complex) :: amp
        integer :: i
        logical :: exist

        write (u, "(A)")  "* Test output: prc_omega_6"
        write (u, "(A)")  "* Purpose: create simple process with OMega / UFO file"
        write (u, "(A)")

        call os_data%init ()

        model_name = "SM"
        model => null ()

        os_data%whizard_modelpath_ufo = "../models/UFO"

        write (u, "(A)")  "* Create process library entry"
        write (u, "(A)")

        allocate (prt_in (2), prt_out (2))
        prt_in = [var_str ("e-"), var_str ("e+")]
        prt_out = prt_in
        restrictions = "3+4~A"

        allocate (entry)
        call entry%init (var_str ("omega_6_a"), &
            model_name = model_name, n_in = 2, n_components = 1)

        call omega_make_process_component (entry, 1, &
            model_name, prt_in, prt_out, &
            ufo=.true., ufo_path=os_data%whizard_modelpath_ufo, &
            report_progress=.true.)

        call entry%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Build and load library"

call lib%init (var_str ("omega_6"))
call lib%append (entry)

call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")
write (u, "(A)")  "* Probe library API:"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active" = ", &
lib%is_active ()
write (u, "(1x,A,I0)")  "n_processes" = ", &
lib%get_n_processes ()

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_6"

end subroutine prc_omega_6

```

Generate matrix element diagrams

The same process as before. No amplitude is computed here, instead we just generate Feynman (and color flow) diagrams, and check whether PS and PDF files have been generated. This test is only run if event analysis is possible.

```

<Omega interface: execute diags tests>≡
  call test (prc_omega_diags_1, "prc_omega_diags_1", &
    "generate Feynman diagrams", &
    u, results)

<Omega interface: test declarations>+≡
  public :: prc_omega_diags_1

<Omega interface: tests>+≡
  subroutine prc_omega_diags_1 (u)
    integer, intent(in) :: u
    type(process_library_t) :: lib
    class(prc_core_def_t), allocatable :: def
    type(process_def_entry_t), pointer :: entry
    type(os_data_t) :: os_data
    type(string_t) :: model_name
    type(string_t), dimension(:), allocatable :: prt_in, prt_out
    type(string_t) :: diags_file, pdf_file, ps_file
    logical :: exist, exist_pdf, exist_ps
    integer :: iostat, u_diags

```

```

character(128) :: buffer

write (u, "(A)")  "* Test output: prc_omega_diags_1"
write (u, "(A)")  "*   Purpose: generate Feynman diagrams"
write (u, "(A)")

write (u, "(A)")  "* Initialize a process library with one entry"
write (u, "(A)")
call lib%init (var_str ("prc_omega_diags_1_lib"))
call os_data%init ()

model_name = "SM"

allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("u"), var_str ("ubar")]
prt_out = [var_str ("d"), var_str ("dbar")]

allocate (omega_def_t :: def)
select type (def)
type is (omega_def_t)
    call def%init (model_name, prt_in, prt_out, &
        ufo = .false., ovm = .false., &
        diags = .true., diags_color = .true.)
end select
allocate (entry)
call entry%init (var_str ("prc_omega_diags_1_p"), model_name = model_name, &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call lib%append (entry)

write (u, "(A)")  "* Configure and compile process"
write (u, "(A)")  "    and generate diagrams"
write (u, "(A)")
call lib%configure (os_data)
call lib%write_makefile &
    (os_data, force = .true., verbose = .false., testflag = .true.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

write (u, "(A)")  "* Probe library API"
write (u, "(A)")

write (u, "(1x,A,L1)")  "is active = ", lib%is_active ()

write (u, "(A)")  "* Check produced diagram files"
write (u, "(A)")

diags_file = "prc_omega_diags_1_p_i1_diags.tex"
ps_file = "prc_omega_diags_1_p_i1_diags.ps"

```

```

pdf_file = "prc_omega_diags_1_p_i1_diags.pdf"
inquire (file = char (diags_file), exist = exist)
if (exist) then
  u_diags = free_unit ()
  open (u_diags, file = char (diags_file), action = "read", status = "old")
  iostat = 0
  do while (iostat == 0)
    read (u_diags, "(A)", iostat = iostat) buffer
    if (iostat == 0) write (u, "(A)") trim (buffer)
  end do
  close (u_diags)
else
  write (u, "(A)") "[Feynman diagrams LaTeX file is missing]"
end if
inquire (file = char (ps_file), exist = exist_ps)
if (exist_ps) then
  write (u, "(A)") "[Feynman diagrams Postscript file exists and is nonempty]"
else
  write (u, "(A)") "[Feynman diagrams Postscript file is missing/non-regular]"
end if
inquire (file = char (pdf_file), exist = exist_pdf)
if (exist_pdf) then
  write (u, "(A)") "[Feynman diagrams PDF file exists and is nonempty]"
else
  write (u, "(A)") "[Feynman diagrams PDF file is missing/non-regular]"
end if

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call lib%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: prc_omega_diags_1"

end subroutine prc_omega_diags_1

```

17.5 External matrix elements (squared)

This defines an abstract framework that can handle matrix elements which are computed outside of WHIZARD. Such matrix elements typically (i) require extra code or libraries to be configured linked at execution time, and (ii) provide only plain or correlated squared matrix elements instead of amplitudes.

In particular, matrix-element libraries that conform to the BLHA standard belong to this class. They have their own (also abstract) extension of the abstract `prc_external_t` type introduced here. `prc_external_t`-type.

```

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

```

```

use, intrinsic :: iso_c_binding !NODEP!

use kinds
use constants
use io_units
<Use strings>
<Use debug>
use system_defs, only: TAB
use physics_defs, only: CF
use diagnostics
use os_interface
use lorentz
use interactions
use sm_qcd
use sm_qed
use variables, only: var_list_t

use model_data
use prclib_interfaces
use prc_core_def
use prc_core
use prc_omega, only: omega_state_t

use sf_base
use sf_pdf_builtin, only: pdf_builtin_t
use sf_lhapdf, only: lhpdf_t
use pdg_arrays, only: is_gluon, is_quark

<Standard module head>

<Prc external: public>

<Prc external: parameters>

<Prc external: types>

<Prc external: interfaces>

contains

<Prc external: procedures>

end module prc_external

```

17.5.1 Handling of structure functions

External matrix elements do not have access to the structure functions stored in the evaluators. The current solution to this problem is to just apply them explicitly after the computation of the matrix element.

```

<Prc external: parameters>≡
  integer, parameter :: LEPTONS = 1
  integer, parameter :: HADRONS = 2

```

```

<Prc external: types>≡
  type :: sf_handler_t
    integer :: initial_state_type = 0
    integer :: n_sf = -1
    real(default) :: val = one
  contains
  <Prc external: sf handler: TBP>
  end type sf_handler_t

<Prc external: sf handler: TBP>≡
  procedure :: init => sf_handler_init

<Prc external: procedures>≡
  subroutine sf_handler_init (sf_handler, sf_chain)
    class(sf_handler_t), intent(out) :: sf_handler
    type(sf_chain_instance_t), intent(in) :: sf_chain
    integer :: i
    sf_handler%n_sf = size (sf_chain%sf)
    if (sf_handler%n_sf == 0) then
      sf_handler%initial_state_type = LEPTONS
    else
      do i = 1, sf_handler%n_sf
        select type (int => sf_chain%sf(i)%int)
          type is (pdf_builtin_t)
            sf_handler%initial_state_type = HADRONS
          type is (lhpdf_t)
            sf_handler%initial_state_type = HADRONS
          class default
            sf_handler%initial_state_type = LEPTONS
        end select
      end do
    end if
  end subroutine sf_handler_init

<Prc external: sf handler: TBP>+≡
  procedure :: init_dummy => sf_handler_init_dummy

<Prc external: procedures>+≡
  subroutine sf_handler_init_dummy (sf_handler)
    class(sf_handler_t), intent(out) :: sf_handler
    sf_handler%n_sf = 0
    sf_handler%initial_state_type = LEPTONS
  end subroutine sf_handler_init_dummy

<Prc external: sf handler: TBP>+≡
  procedure :: apply_structure_functions => sf_handler_apply_structure_functions

<Prc external: procedures>+≡
  subroutine sf_handler_apply_structure_functions (sf_handler, sf_chain, flavors)
    class(sf_handler_t), intent(inout) :: sf_handler
    type(sf_chain_instance_t), intent(in) :: sf_chain
    integer, intent(in), dimension(2) :: flavors
    integer :: i
    real(default), dimension(:), allocatable :: f

```

```

if (sf_handler%n_sf < 0) call msg_fatal ("sf_handler not initialized")
sf_handler%val = one
do i = 1, sf_handler%n_sf
  select case (sf_handler%initial_state_type)
  case (HADRONS)
    sf_handler%val = sf_handler%val * sf_handler%get_pdf (sf_chain, i, flavors(i))
  case (LEPTONS)
    call sf_chain%get_matrix_elements (i, f)
    sf_handler%val = sf_handler%val * f(1)
  case default
    call msg_fatal ("sf_handler not initialized")
  end select
end do
end subroutine sf_handler_apply_structure_functions

```

```

<Prc external: sf handler: TBP>+≡
  procedure :: get_pdf => sf_handler_get_pdf

<Prc external: procedures>+≡
  function sf_handler_get_pdf (sf_handler, sf_chain, i, flavor) result (f)
    real(default) :: f
    class(sf_handler_t), intent(in) :: sf_handler
    type(sf_chain_instance_t), intent(in) :: sf_chain
    integer, intent(in) :: i, flavor
    integer :: k
    real(default), dimension(:), allocatable :: ff
    integer, parameter :: n_flv_light = 6

    call sf_chain%get_matrix_elements (i, ff)

    if (is_gluon (flavor)) then
      k = n_flv_light + 1
    else if (is_quark (abs(flavor))) then
      k = n_flv_light + 1 + flavor
    else
      call msg_fatal ("Not a colored particle")
    end if

    f = ff(k)
  end function sf_handler_get_pdf

```

17.5.2 Abstract interface to external matrix elements

This process class allows us to factor out common necessities of processes that involve external code or libraries.

Workspace

This is the workspace that is available for external matrix elements.

```

<Prc external: public>≡
  public :: prc_external_state_t

```



```

<Prc external: types>+≡
  type, abstract, extends (prc_core_state_t) :: prc_external_state_t
    logical :: new_kinematics = .true.
    real(default) :: alpha_qcd = -1
  contains
    <Prc external: external state: TBP>
  end type prc_external_state_t

<Prc external: external state: TBP>≡
  procedure :: reset_new_kinematics => prc_external_state_reset_new_kinematics

<Prc external: procedures>+≡
  subroutine prc_external_state_reset_new_kinematics (object)
    class(prc_external_state_t), intent(inout) :: object
    object%new_kinematics = .true.
  end subroutine prc_external_state_reset_new_kinematics

<Prc external: external state: TBP>+≡
  procedure :: get_alpha_qcd => prc_external_state_get_alpha_qcd

<Prc external: procedures>+≡
  function prc_external_state_get_alpha_qcd (object) result (alpha_qcd)
    real(default) :: alpha_qcd
    class(prc_external_state_t), intent(in) :: object
    alpha_qcd = object%alpha_qcd
  end function prc_external_state_get_alpha_qcd

```

Driver

We have to add two O'Mega-routines to the external matrix-element driver to ensure proper process setup. The problem is that during the setup of the real component, the particle and flavor data are taken from the Born component to set up the subtraction terms. However, the Born component expects this data to be obtained from the Omega code, accessed by the driver.

```

<Prc external: public>+≡
  public :: prc_external_driver_t

<Prc external: types>+≡
  type, abstract, extends (prc_core_driver_t) :: prc_external_driver_t
    procedure(omega_update_alpha_s), nopass, pointer :: &
      update_alpha_s => null ()
    procedure(omega_is_allowed), nopass, pointer :: &
      is_allowed => null ()
  end type prc_external_driver_t

```

Core

```

<Prc external: public>+≡
  public :: prc_external_t

```

```

<Prc external: types>+≡
  type, abstract, extends (prc_core_t) :: prc_external_t
  type(qcd_t) :: qcd
  type(qed_t) :: qed
  integer :: n_flv = 1
  real(default), dimension(:), allocatable :: par
  integer :: scheme = 0
  type(sf_handler_t) :: sf_handler
  real(default) :: maximum_accuracy = 10000.0
contains
  <Prc external: prc external: TBP>
end type prc_external_t

```

By definition, this class of process-core types require extra code.

```

<Prc external: prc external: TBP>≡
  procedure, nopass :: needs_external_code => &
    prc_external_needs_external_code

<Prc external: procedures>+≡
  function prc_external_needs_external_code () result (flag)
    logical :: flag
    flag = .true.
  end function prc_external_needs_external_code

<Prc external: prc external: TBP>+≡
  procedure :: get_n_flvs => prc_external_get_n_flvs

<Prc external: procedures>+≡
  pure function prc_external_get_n_flvs (object, i_flv) result (n)
    integer :: n
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv
    n = size (object%data%flv_state (:,i_flv))
  end function prc_external_get_n_flvs

<Prc external: prc external: TBP>+≡
  procedure :: get_flv_state => prc_external_get_flv_state

<Prc external: procedures>+≡
  function prc_external_get_flv_state (object, i_flv) result (flv)
    integer, dimension(:), allocatable :: flv
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv
    allocate (flv (size (object%data%flv_state (:,i_flv))))
    flv = object%data%flv_state (:,i_flv)
  end function prc_external_get_flv_state

```

Return one single squared test matrix element. It is fixed to 1, therefore the integration output will be the phase space volume.

```

<Prc external: prc external: TBP>+≡
  procedure :: compute_sqme => prc_external_compute_sqme

```

```

<Prc external: procedures>+≡
  subroutine prc_external_compute_sqme (object, i_flv, i_hel, p, &
    ren_scale, sqme, bad_point)
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(out) :: sqme
    logical, intent(out) :: bad_point
    sqme = one
    bad_point = .false.
  end subroutine prc_external_compute_sqme

```

Return an array of 4 numbers corresponding to the BLHA output convention.
Used for testing.

```

<Prc external: prc external: TBP>+≡
  procedure :: compute_sqme_virt => prc_external_compute_sqme_virt

<Prc external: procedures>+≡
  subroutine prc_external_compute_sqme_virt (object, i_flv, i_hel, &
    p, ren_scale, es_scale, loop_method, sqme, bad_point)
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: ren_scale, es_scale
    integer, intent(in) :: loop_method
    logical, intent(out) :: bad_point
    real(default), dimension(4), intent(out) :: sqme
    if (debug_on) call msg_debug2 (D_ME_METHODS, "prc_external_compute_sqme_virt")
    sqme(1) = 0.001_default
    sqme(2) = 0.001_default
    sqme(3) = 0.001_default
    sqme(4) = 0.0015_default
    bad_point = .false.
  end subroutine prc_external_compute_sqme_virt

```

Also return test output for color-correlated matrix elements. We only give a sensible result for the processes used in the functional tests, which have 2 -> 2 topology. All other processes will obtain a vanishing dummy color-correlation. This effectively switches off the subtraction contributions, reproducing the real phase-space volume.

```

<Prc external: prc external: TBP>+≡
  procedure :: compute_sqme_color_c => prc_external_compute_sqme_color_c

<Prc external: procedures>+≡
  subroutine prc_external_compute_sqme_color_c (object, i_flv, i_hel, p, &
    ren_scale, born_color_c, bad_point, born_out)
    class(prc_external_t), intent(inout) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(inout), dimension(:,:) :: born_color_c
    logical, intent(out) :: bad_point

```

```

real(default), intent(out), optional :: born_out
if (debug_on) call msg_debug2 (D_ME_METHODS, "prc_external_compute_sqme_color_c")
if (size (p) == 4) then
  if (present (born_out)) then
    born_out = 0.0015_default
    born_color_c = zero
    born_color_c(3,3) = - CF * born_out
    born_color_c(4,4) = - CF * born_out
    born_color_c(3,4) = CF * born_out
    born_color_c(4,3) = born_color_c(3,4)
    bad_point = .false.
  end if
else
  if (present (born_out)) born_out = zero
  born_color_c = zero
end if
end subroutine prc_external_compute_sqme_color_c

```

```

<Prc external: prc external: TBP>+≡
  procedure :: compute_alpha_s => prc_external_compute_alpha_s

```

```

<Prc external: procedures>+≡
  subroutine prc_external_compute_alpha_s &
    (object, core_state, ren_scale)
    class(prc_external_t), intent(in) :: object
    class(prc_external_state_t), intent(inout) :: core_state
    real(default), intent(in) :: ren_scale
    core_state%alpha_qcd = object%qcd%alpha%get (ren_scale)
  end subroutine prc_external_compute_alpha_s

```

```

<Prc external: prc external: TBP>+≡
  procedure :: get_alpha_s => prc_external_get_alpha_s

```

```

<Prc external: procedures>+≡
  function prc_external_get_alpha_s (object, core_state) result (alpha_qcd)
    class(prc_external_t), intent(in) :: object
    class(prc_core_state_t), intent(in), allocatable :: core_state
    real(default) :: alpha_qcd
    if (allocated (core_state)) then
      select type (core_state)
      class is (prc_external_state_t)
        alpha_qcd = core_state%alpha_qcd
      type is (omega_state_t)
        alpha_qcd = core_state%alpha_qcd
      class default
        alpha_qcd = zero
      end select
    else
      alpha_qcd = zero
    end if
  end function prc_external_get_alpha_s

```

Getter for alpha_qed

<Prc external: prc external: TBP>+≡

```
procedure :: get_alpha_qed => prc_external_get_alpha_qed
```

<Prc external: procedures>+≡

```
function prc_external_get_alpha_qed (object) result (alpha_qed)
  class(prc_external_t), intent(in) :: object
  real(default) :: alpha_qed
  alpha_qed = object%qed%get_alpha_qed ()
end function prc_external_get_alpha_qed
```

<Prc external: prc external: TBP>+≡

```
procedure :: is_allowed => prc_external_is_allowed
```

<Prc external: procedures>+≡

```
function prc_external_is_allowed (object, i_term, f, h, c) result (flag)
  class(prc_external_t), intent(in) :: object
  integer, intent(in) :: i_term, f, h, c
  logical :: flag
  logical(c_bool) :: cflag
  select type (driver => object%driver)
  class is (prc_external_driver_t)
    call driver%is_allowed (f, h, c, cflag)
    flag = cflag
  class default
    call msg_fatal &
      ("Driver does not fit to prc_external_t")
  end select
end function prc_external_is_allowed
```

<Prc external: prc external: TBP>+≡

```
procedure :: get_nflv => prc_external_get_nflv
```

<Prc external: procedures>+≡

```
function prc_external_get_nflv (object) result (n_flv)
  class(prc_external_t), intent(in) :: object
  integer :: n_flv
  n_flv = object%n_flv
end function prc_external_get_nflv
```

<Prc external: prc external: TBP>+≡

```
procedure :: compute_hard_kinematics => prc_external_compute_hard_kinematics
```

<Prc external: procedures>+≡

```
subroutine prc_external_compute_hard_kinematics &
  (object, p_seed, i_term, int_hard, core_state)
  class(prc_external_t), intent(in) :: object
  type(vector4_t), dimension(:), intent(in) :: p_seed
  integer, intent(in) :: i_term
  type(interaction_t), intent(inout) :: int_hard
  class(prc_core_state_t), intent(inout), allocatable :: core_state
  call int_hard%set_momenta (p_seed)
  if (allocated (core_state)) then
    select type (core_state)
```

```

        class is (prc_external_state_t); core_state%new_kinematics = .true.
    end select
end if
end subroutine prc_external_compute_hard_kinematics

<Prc external: prc external: TBP>+≡
    procedure :: compute_eff_kinematics => prc_external_compute_eff_kinematics

<Prc external: procedures>+≡
    subroutine prc_external_compute_eff_kinematics &
        (object, i_term, int_hard, int_eff, core_state)
    class(prc_external_t), intent(in) :: object
    integer, intent(in) :: i_term
    type(interaction_t), intent(in) :: int_hard
    type(interaction_t), intent(inout) :: int_eff
    class(prc_core_state_t), intent(inout), allocatable :: core_state
end subroutine prc_external_compute_eff_kinematics

<Prc external: prc external: TBP>+≡
    procedure :: set_parameters => prc_external_set_parameters

<Prc external: procedures>+≡
    subroutine prc_external_set_parameters (object, qcd, model)
    class(prc_external_t), intent(inout) :: object
    type(qcd_t), intent(in) :: qcd
    type(qed_t) :: qed
    class(model_data_t), intent(in), target, optional :: model
    object%qcd = qcd
    if (present (model)) then
        if (.not. allocated (object%par)) &
            allocate (object%par (model%get_n_real ()))
        call model%real_parameters_to_array (object%par)
        object%scheme = model%get_scheme_num ()
        if (associated (model%get_par_data_ptr (var_str ('alpha_em_i')))) then
            call qed%set_alpha_qed (one / model%get_real (var_str ('alpha_em_i')))
        end if
        object%qed = qed
    end if
end subroutine prc_external_set_parameters

<Prc external: prc external: TBP>+≡
    procedure :: update_alpha_s => prc_external_update_alpha_s

<Prc external: procedures>+≡
    subroutine prc_external_update_alpha_s (object, core_state, fac_scale)
    class(prc_external_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    real(default), intent(in) :: fac_scale
    real(default) :: alpha_qcd
    if (allocated (object%qcd%alpha)) then
        alpha_qcd = object%qcd%alpha%get (fac_scale)
        select type (driver => object%driver)
        class is (prc_external_driver_t)
            call driver%update_alpha_s (alpha_qcd)

```

```

        end select
        select type (core_state)
        class is (prc_external_state_t)
            core_state%alpha_qcd = alpha_qcd
        type is (omega_state_t)
            core_state%alpha_qcd = alpha_qcd
        end select
    end if
end subroutine prc_external_update_alpha_s

<Prc external: prc external: TBP>+≡
    procedure :: init_sf_handler => prc_external_init_sf_handler

<Prc external: procedures>+≡
    subroutine prc_external_init_sf_handler (core, sf_chain)
        class(prc_external_t), intent(inout) :: core
        type(sf_chain_instance_t), intent(in) :: sf_chain
        if (allocated (sf_chain%sf)) then
            call core%sf_handler%init (sf_chain)
        else
            call core%sf_handler%init_dummy ()
        end if
    end subroutine prc_external_init_sf_handler

<Prc external: prc external: TBP>+≡
    procedure :: init_sf_handler_dummy => prc_external_init_sf_handler_dummy

<Prc external: procedures>+≡
    subroutine prc_external_init_sf_handler_dummy (core)
        class(prc_external_t), intent(inout) :: core
        call core%sf_handler%init_dummy ()
    end subroutine prc_external_init_sf_handler_dummy

<Prc external: prc external: TBP>+≡
    procedure :: apply_structure_functions => prc_external_apply_structure_functions

<Prc external: procedures>+≡
    subroutine prc_external_apply_structure_functions (core, sf_chain, flavors)
        class(prc_external_t), intent(inout) :: core
        type(sf_chain_instance_t), intent(in) :: sf_chain
        integer, dimension(2), intent(in) :: flavors
        call core%sf_handler%apply_structure_functions (sf_chain, flavors)
    end subroutine prc_external_apply_structure_functions

<Prc external: prc external: TBP>+≡
    procedure :: get_sf_value => prc_external_get_sf_value

<Prc external: procedures>+≡
    function prc_external_get_sf_value (core) result (val)
        real(default) :: val
        class(prc_external_t), intent(in) :: core
        val = core%sf_handler%val
    end function prc_external_get_sf_value

```

```

<Prc external: prc external: TBP>+≡
  procedure(prc_external_includes_polarization), deferred :: &
    includes_polarization
<Prc external: interfaces>≡
  abstract interface
    function prc_external_includes_polarization (object) result (polarized)
      import
      logical :: polarized
      class(prc_external_t), intent(in) :: object
    end function prc_external_includes_polarization
  end interface

```

Configuration

This is the abstract external matrix-element interface.

```

<Prc external: public>+≡
  public :: prc_external_def_t
<Prc external: types>+≡
  type, abstract, extends (prc_core_def_t) :: prc_external_def_t
    type(string_t) :: basename
  contains
    <Prc external: external def: TBP>
  end type prc_external_def_t

<Prc external: external def: TBP>≡
  procedure :: set_active_writer => prc_external_def_set_active_writer
<Prc external: procedures>+≡
  subroutine prc_external_def_set_active_writer (def, active)
    class(prc_external_def_t), intent(inout) :: def
    logical, intent(in) :: active
    select type (writer => def%writer)
      class is (prc_external_writer_t)
        writer%active = active
      end select
  end subroutine prc_external_def_set_active_writer

<Prc external: external def: TBP>+≡
  procedure, nopass :: get_features => prc_external_def_get_features
<Prc external: procedures>+≡
  subroutine prc_external_def_get_features (features)
    type(string_t), dimension(:), allocatable, intent(out) :: features
    allocate (features (6))
    features = [ &
      var_str ("init"), &
      var_str ("update_alpha_s"), &
      var_str ("reset_helicity_selection"), &
      var_str ("is_allowed"), &
      var_str ("new_event"), &
      var_str ("get_amplitude")]
  end subroutine prc_external_def_get_features

```



```

<Prc external: external def: TBP>+≡
  procedure :: connect => prc_external_def_connect
  procedure :: omega_connect => prc_external_def_connect

<Prc external: procedures>+≡
  subroutine prc_external_def_connect (def, lib_driver, i, proc_driver)
    class(prc_external_def_t), intent(in) :: def
    class(prclib_driver_t), intent(in) :: lib_driver
    integer, intent(in) :: i
    class(prc_core_driver_t), intent(inout) :: proc_driver
    integer :: pid, fid
    type(c_funptr) :: fptr
    select type (proc_driver)
    class is (prc_external_driver_t)
      pid = i
      fid = 2
      call lib_driver%get_fptr (pid, fid, fptr)
      call c_f_procpointer (fptr, proc_driver%update_alpha_s)
      fid = 4
      call lib_driver%get_fptr (pid, fid, fptr)
      call c_f_procpointer (fptr, proc_driver%is_allowed)
    end select
  end subroutine prc_external_def_connect

<Prc external: external def: TBP>+≡
  procedure, nopass :: needs_code => prc_external_def_needs_code

<Prc external: procedures>+≡
  function prc_external_def_needs_code () result (flag)
    logical :: flag
    flag = .true.
  end function prc_external_def_needs_code

<Prc external: interfaces>+≡
  abstract interface
    subroutine omega_update_alpha_s (alpha_s) bind(C)
      import
      real(c_default_float), intent(in) :: alpha_s
    end subroutine omega_update_alpha_s
  end interface

  abstract interface
    subroutine omega_is_allowed (flv, hel, col, flag) bind(C)
      import
      integer(c_int), intent(in) :: flv, hel, col
      logical(c_bool), intent(out) :: flag
    end subroutine omega_is_allowed
  end interface

```

Writer

```

<Prc external: public>+≡
  public :: prc_external_writer_t

```

```

<Prc external: types>+≡
  type, abstract, extends (prc_writer_f_module_t) :: prc_external_writer_t
    type(string_t) :: model_name
    type(string_t) :: process_mode
    type(string_t) :: process_string
    type(string_t) :: restrictions
    integer :: n_in = 0
    integer :: n_out = 0
    logical :: active = .true.
    logical :: amp_triv = .true.
  contains
    <Prc external: external writer: TBP>
  end type prc_external_writer_t

```

```

<Prc external: external writer: TBP>≡
  procedure :: init => prc_external_writer_init
  procedure :: base_init => prc_external_writer_init

```

```

<Prc external: procedures>+≡
  pure subroutine prc_external_writer_init &
    (writer, model_name, prt_in, prt_out, restrictions)
    class(prc_external_writer_t), intent(inout) :: writer
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    type(string_t), intent(in), optional :: restrictions
    integer :: i
    writer%model_name = model_name
    if (present (restrictions)) then
      writer%restrictions = restrictions
    else
      writer%restrictions = ""
    end if
    writer%n_in = size (prt_in)
    writer%n_out = size (prt_out)
    select case (size (prt_in))
      case(1); writer%process_mode = " -decay"
      case(2); writer%process_mode = " -scatter"
    end select
    associate (s => writer%process_string)
      s = " '"
      do i = 1, size (prt_in)
        if (i > 1) s = s // " "
        s = s // prt_in(i)
      end do
      s = s // " ->"
      do i = 1, size (prt_out)
        s = s // " " // prt_out(i)
      end do
      s = s // "' "
    end associate
  end subroutine prc_external_writer_init

```

```

<Prc external: external writer: TBP>+≡
  procedure, nopass :: get_module_name => prc_external_writer_get_module_name

```

```

<Prc external: procedures>+≡
function prc_external_writer_get_module_name (id) result (name)
    type(string_t) :: name
    type(string_t), intent(in) :: id
    name = "opr_" // id
end function prc_external_writer_get_module_name

<Prc external: external writer: TBP>+≡
procedure :: write_wrapper => prc_external_writer_write_wrapper

<Prc external: procedures>+≡
subroutine prc_external_writer_write_wrapper (writer, unit, id, feature)
    class(prc_external_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id, feature
    type(string_t) :: name
    name = writer%get_c_procname (id, feature)
    write (unit, *)
    select case (char (feature))
    case ("init")
        write (unit, "(9A)") "subroutine ", char (name), &
            " (par, scheme) bind(C)"
        write (unit, "(2x,9A)") "use iso_c_binding"
        write (unit, "(2x,9A)") "use kinds"
        write (unit, "(2x,9A)") "use opr_", char (id)
        write (unit, "(2x,9A)") "real(c_default_float), dimension(*), &
            &intent(in) :: par"
        write (unit, "(2x,9A)") "integer(c_int), intent(in) :: scheme"
        if (c_default_float == default .and. c_int == kind (1)) then
            write (unit, "(2x,9A)") "call ", char (feature), " (par, scheme)"
        end if
        write (unit, "(9A)") "end subroutine ", char (name)
    case ("update_alpha_s")
        write (unit, "(9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
        write (unit, "(2x,9A)") "use iso_c_binding"
        write (unit, "(2x,9A)") "use kinds"
        write (unit, "(2x,9A)") "use opr_", char (id)
        if (c_default_float == default) then
            write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
                &:: alpha_s"
            write (unit, "(2x,9A)") "call ", char (feature), " (alpha_s)"
        end if
        write (unit, "(9A)") "end subroutine ", char (name)
    case ("reset_helicity_selection")
        write (unit, "(9A)") "subroutine ", char (name), &
            " (threshold, cutoff) bind(C)"
        write (unit, "(2x,9A)") "use iso_c_binding"
        write (unit, "(2x,9A)") "use kinds"
        write (unit, "(2x,9A)") "use opr_", char (id)
        if (c_default_float == default) then
            write (unit, "(2x,9A)") "real(c_default_float), intent(in) &
                &:: threshold"
            write (unit, "(2x,9A)") "integer(c_int), intent(in) :: cutoff"
            write (unit, "(2x,9A)") "call ", char (feature), &

```

```

        " (threshold, int (cutoff))"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
case ("is_allowed")
    write (unit, "(9A)") "subroutine ", char (name), &
        " (flv, hel, col, flag) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
    write (unit, "(2x,9A)") "logical(c_bool), intent(out) :: flag"
    write (unit, "(2x,9A)") "flag = ", char (feature), &
        " (int (flv), int (hel), int (col))"
    write (unit, "(9A)") "end subroutine ", char (name)
case ("new_event")
    write (unit, "(9A)") "subroutine ", char (name), " (p) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    if (c_default_float == default) then
        write (unit, "(2x,9A)") "real(c_default_float), dimension(0:3,*), &
            &intent(in) :: p"
        write (unit, "(2x,9A)") "call ", char (feature), " (p)"
    end if
    write (unit, "(9A)") "end subroutine ", char (name)
case ("get_amplitude")
    write (unit, "(9A)") "subroutine ", char (name), &
        " (flv, hel, col, amp) bind(C)"
    write (unit, "(2x,9A)") "use iso_c_binding"
    write (unit, "(2x,9A)") "use kinds"
    write (unit, "(2x,9A)") "use opr_", char (id)
    write (unit, "(2x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
    write (unit, "(2x,9A)") "complex(c_default_complex), intent(out) &
        &:: amp"
    write (unit, "(2x,9A)") "amp = ", char (feature), &
        " (int (flv), int (hel), int (col))"
    write (unit, "(9A)") "end subroutine ", char (name)
end select

```

```

end subroutine prc_external_writer_write_wrapper

```

<Prc external: external writer: TBP>+≡

```

procedure :: write_interface => prc_external_writer_write_interface

```

<Prc external: procedures>+≡

```

subroutine prc_external_writer_write_interface (writer, unit, id, feature)
    class(prc_external_writer_t), intent(in) :: writer
    integer, intent(in) :: unit
    type(string_t), intent(in) :: id
    type(string_t), intent(in) :: feature
    type(string_t) :: name
    name = writer%get_c_procname (id, feature)
    write (unit, "(2x,9A)") "interface"
    select case (char (feature))

```

```

case ("init")
  write (unit, "(5x,9A)") "subroutine ", char (name), &
    " (par, scheme) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "real(c_default_float), dimension(*), &
    &intent(in) :: par"
  write (unit, "(7x,9A)") "integer(c_int), intent(in) :: scheme"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("update_alpha_s")
  write (unit, "(5x,9A)") "subroutine ", char (name), " (alpha_s) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: alpha_s"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("reset_helicity_selection")
  write (unit, "(5x,9A)") "subroutine ", char (name), " &
    &(threshold, cutoff) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "real(c_default_float), intent(in) :: threshold"
  write (unit, "(7x,9A)") "integer(c_int), intent(in) :: cutoff"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("is_allowed")
  write (unit, "(5x,9A)") "subroutine ", char (name), " &
    &(flv, hel, col, flag) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
  write (unit, "(7x,9A)") "logical(c_bool), intent(out) :: flag"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("new_event")
  write (unit, "(5x,9A)") "subroutine ", char (name), " (p) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "real(c_default_float), dimension(0:3,*), &
    &intent(in) :: p"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
case ("get_amplitude")
  write (unit, "(5x,9A)") "subroutine ", char (name), " &
    &(flv, hel, col, amp) bind(C)"
  write (unit, "(7x,9A)") "import"
  write (unit, "(7x,9A)") "integer(c_int), intent(in) :: flv, hel, col"
  write (unit, "(7x,9A)") "complex(c_default_complex), intent(out) &
    &:: amp"
  write (unit, "(5x,9A)") "end subroutine ", char (name)
end select
write (unit, "(2x,9A)") "end interface"
end subroutine prc_external_writer_write_interface

```

Empty, but can be overridden.

<Prc external: external writer: TBP>+≡

```

  procedure :: write_source_code => prc_external_writer_write_source_code

```

<Prc external: procedures>+≡

```

  subroutine prc_external_writer_write_source_code (writer, id)
    class(prc_external_writer_t), intent(in) :: writer
    type(string_t), intent(in) :: id
    if (debug_on) call msg_debug (D_ME_METHODS, &

```

```

        "prc_external_writer_write_source_code (no-op)")
    !!! This is a dummy
end subroutine prc_external_writer_write_source_code

```

Empty, but can be overridden.

```

<Prc external: external writer: TBP>+≡
    procedure :: before_compile => prc_external_writer_before_compile
    procedure :: after_compile => prc_external_writer_after_compile

<Prc external: procedures>+≡
    subroutine prc_external_writer_before_compile (writer, id)
        class(prc_external_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
        if (debug_on) call msg_debug (D_ME_METHODS, &
            "prc_external_writer_before_compile (no-op)")
        !!! This is a dummy
    end subroutine prc_external_writer_before_compile

    subroutine prc_external_writer_after_compile (writer, id)
        class(prc_external_writer_t), intent(in) :: writer
        type(string_t), intent(in) :: id
        if (debug_on) call msg_debug (D_ME_METHODS, &
            "prc_external_writer_after_compile (no-op)")
        !!! This is a dummy
    end subroutine prc_external_writer_after_compile

```

Standard Makefile, set up to call O'MEGA. Additionally, the O'MEGA output can be exploited for its data-management parts.

```

<Prc external: external writer: TBP>+≡
    procedure :: write_makefile_code => prc_external_writer_write_makefile_code
    procedure :: base_write_makefile_code => prc_external_writer_write_makefile_code

<Prc external: procedures>+≡
    subroutine prc_external_writer_write_makefile_code &
        (writer, unit, id, os_data, verbose, testflag)
        class(prc_external_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        type(string_t), intent(in) :: id
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: testflag
        type(string_t) :: omega_binary, omega_path
        type(string_t) :: restrictions_string, amp_triv_string
        omega_binary = "omega_" // writer%model_name // ".opt"
        omega_path = os_data%whizard_omega_binpath // "/" // omega_binary
        if (.not. verbose) omega_path = "@" // omega_path
        if (writer%restrictions /= "") then
            restrictions_string = " -cascade '" // writer%restrictions // "'"
        else
            restrictions_string = ""
        end if
        amp_triv_string = ""
        if (writer%amp_triv) amp_triv_string = " -target:amp_triv"
        write (unit, "(5A)") "OBJECTS += ", char (id), ".lo"
    end subroutine

```

```

write (unit, "(5A)") char (id), ".f90:"
if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " OMEGA ', trim (char (id)), '.f90"'
end if
write (unit, "(99A)") TAB, char (omega_path), &
    " -o ", char (id), ".f90", &
    " -target:whizard", char (amp_triv_string), &
    " -target:parameter_module parameters_", char (writer%model_name), &
    " -target:module opr_", char (id), &
    " -target:md5sum '", writer%md5sum, "'", &
    char (writer%process_mode), char (writer%process_string), &
    char (restrictions_string)
write (unit, "(5A)") "clean-", char (id), ":"
write (unit, "(5A)") TAB, "rm -f ", char (id), ".f90"
write (unit, "(5A)") TAB, "rm -f opr_", char (id), ".mod"
write (unit, "(5A)") TAB, "rm -f ", char (id), ".lo"
write (unit, "(5A)") "CLEAN_SOURCES += ", char (id), ".f90"
write (unit, "(5A)") "CLEAN_OBJECTS += opr_", char (id), ".mod"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), ".lo"
write (unit, "(5A)") char (id), ".lo: ", char (id), ".f90"
if (.not. verbose) then
    write (unit, "(5A)") TAB // '@echo " FC " $@"
end if
write (unit, "(5A)") TAB, "$ (LTF_COMPILE) $<"

end subroutine prc_external_writer_write_makefile_code

```

```

<Prc external: external writer: TBP>+≡
    procedure, nopass:: get_procname => prc_external_writer_writer_get_procname

<Prc external: procedures>+≡
    function prc_external_writer_writer_get_procname (feature) result (name)
        type(string_t) :: name
        type(string_t), intent(in) :: feature
        select case (char (feature))
            case ("n_in"); name = "number_particles_in"
            case ("n_out"); name = "number_particles_out"
            case ("n_flv"); name = "number_flavor_states"
            case ("n_hel"); name = "number_spin_states"
            case ("n_col"); name = "number_color_flows"
            case ("n_cin"); name = "number_color_indices"
            case ("n_cf"); name = "number_color_factors"
            case ("flv_state"); name = "flavor_states"
            case ("hel_state"); name = "spin_states"
            case ("col_state"); name = "color_flows"
            case default
                name = feature
            end select
        end function prc_external_writer_writer_get_procname

```

17.5.3 external test

Writer

```
<Prc external: public>+≡
  public :: prc_external_test_writer_t
<Prc external: types>+≡
  type, extends (prc_external_writer_t) :: prc_external_test_writer_t
  contains
  <Prc external: external test writer: TBP>
  end type prc_external_test_writer_t

<Prc external: external test writer: TBP>≡
  procedure, nopass :: type_name => prc_external_test_writer_type_name
<Prc external: procedures>+≡
  function prc_external_test_writer_type_name () result (string)
    type(string_t) :: string
    string = "External matrix element dummy"
  end function prc_external_test_writer_type_name
```

Workspace

This looks pretty useless. Why don't we make `prc_external_state_t` nonabstract and remove this?

```
<Prc external: public>+≡
  public :: prc_external_test_state_t
<Prc external: types>+≡
  type, extends (prc_external_state_t) :: prc_external_test_state_t
  contains
  <Prc external: external test state: TBP>
  end type prc_external_test_state_t

<Prc external: external test state: TBP>≡
  procedure :: write => prc_external_test_state_write
<Prc external: procedures>+≡
  subroutine prc_external_test_state_write (object, unit)
    class(prc_external_test_state_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine prc_external_test_state_write
```

Driver

```
<Prc external: public>+≡
  public :: prc_external_test_driver_t
<Prc external: types>+≡
  type, extends (prc_external_driver_t) :: prc_external_test_driver_t
  contains
  <Prc external: external test driver: TBP>
  end type prc_external_test_driver_t
```



```

<Prc external: external test driver: TBP>≡
    procedure, nopass :: type_name => prc_external_test_driver_type_name

<Prc external: procedures>+≡
    function prc_external_test_driver_type_name () result (type)
        type(string_t) :: type
        type = "External matrix element dummy"
    end function prc_external_test_driver_type_name

```

Configuration

A external test definition.

```

<Prc external: public>+≡
    public :: prc_external_test_def_t

<Prc external: types>+≡
    type, extends (prc_external_def_t) :: prc_external_test_def_t
    contains
    <Prc external: external test def: TBP>
    end type prc_external_test_def_t

<Prc external: external test def: TBP>≡
    procedure :: init => prc_external_test_def_init

<Prc external: procedures>+≡
    subroutine prc_external_test_def_init (object, basename, model_name, &
        prt_in, prt_out)
        class(prc_external_test_def_t), intent(inout) :: object
        type(string_t), intent(in) :: basename, model_name
        type(string_t), dimension(:), intent(in) :: prt_in, prt_out
        object%basename = basename
        allocate (prc_external_test_writer_t :: object%writer)
        select type (writer => object%writer)
            type is (prc_external_test_writer_t)
                call writer%init (model_name, prt_in, prt_out)
            end select
    end subroutine prc_external_test_def_init

<Prc external: external test def: TBP>+≡
    procedure, nopass :: type_string => prc_external_test_def_type_string

<Prc external: procedures>+≡
    function prc_external_test_def_type_string () result (string)
        type(string_t) :: string
        string = "external test dummy"
    end function prc_external_test_def_type_string

<Prc external: external test def: TBP>+≡
    procedure :: write => prc_external_test_def_write

```

```

<Prc external: procedures>+≡
  subroutine prc_external_test_def_write (object, unit)
    class(prc_external_test_def_t), intent(in) :: object
    integer, intent(in) :: unit
  end subroutine prc_external_test_def_write

<Prc external: external test def: TBP>+≡
  procedure :: read => prc_external_test_def_read

<Prc external: procedures>+≡
  subroutine prc_external_test_def_read (object, unit)
    class(prc_external_test_def_t), intent(out) :: object
    integer, intent(in) :: unit
  end subroutine prc_external_test_def_read

<Prc external: external test def: TBP>+≡
  procedure :: allocate_driver => prc_external_test_def_allocate_driver

<Prc external: procedures>+≡
  subroutine prc_external_test_def_allocate_driver (object, driver, basename)
    class(prc_external_test_def_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    if (.not. allocated (driver)) allocate (prc_external_test_driver_t :: driver)
  end subroutine prc_external_test_def_allocate_driver

```

Core

This external test just returns $|\mathcal{M}|^2 = 1$ and thus the result of the integration is the n-particle-phase-space volume.

```

<Prc external: public>+≡
  public :: prc_external_test_t

<Prc external: types>+≡
  type, extends (prc_external_t) :: prc_external_test_t
  contains
  <Prc external: prc test: TBP>
  end type prc_external_test_t

<Prc external: prc test: TBP>≡
  procedure :: write => prc_external_test_write

<Prc external: procedures>+≡
  subroutine prc_external_test_write (object, unit)
    class(prc_external_test_t), intent(in) :: object
    integer, intent(in), optional :: unit
    call msg_message ("Test external matrix elements")
  end subroutine prc_external_test_write

<Prc external: prc test: TBP>+≡
  procedure :: write_name => prc_external_test_write_name

```

```

<Prc external: procedures>+≡
  subroutine prc_external_test_write_name (object, unit)
    class(prc_external_test_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u,"(1x,A)") "Core: external test"
  end subroutine prc_external_test_write_name

<Prc external: prc test: TBP>+≡
  procedure :: compute_amplitude => prc_external_test_compute_amplitude

<Prc external: procedures>+≡
  function prc_external_test_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
     core_state) result (amp)
    class(prc_external_test_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale
    real(default), intent(in), allocatable :: alpha_qcd_forced
    class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
    complex(default) :: amp
    select type (core_state)
    class is (prc_external_test_state_t)
      core_state%alpha_qcd = object%qcd%alpha%get (fac_scale)
    end select
    amp = 0.0
  end function prc_external_test_compute_amplitude

<Prc external: prc test: TBP>+≡
  procedure :: allocate_workspace => prc_external_test_allocate_workspace

<Prc external: procedures>+≡
  subroutine prc_external_test_allocate_workspace (object, core_state)
    class(prc_external_test_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    allocate (prc_external_test_state_t :: core_state)
  end subroutine prc_external_test_allocate_workspace

<Prc external: prc test: TBP>+≡
  procedure :: includes_polarization => prc_external_test_includes_polarization

<Prc external: procedures>+≡
  function prc_external_test_includes_polarization (object) result (polarized)
    logical :: polarized
    class(prc_external_test_t), intent(in) :: object
    polarized = .false.
  end function prc_external_test_includes_polarization

<Prc external: prc test: TBP>+≡
  procedure :: prepare_external_code => &
    prc_external_test_prepare_external_code

```

```

<Prc external: procedures>+≡
  subroutine prc_external_test_prepare_external_code &
    (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
    class(prc_external_test_t), intent(inout) :: core
    integer, intent(in), dimension(:,:), allocatable :: flv_states
    type(var_list_t), intent(in) :: var_list
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: libname
    type(model_data_t), intent(in), target :: model
    integer, intent(in) :: i_core
    logical, intent(in) :: is_nlo
  end subroutine prc_external_test_prepare_external_code

```

17.5.4 Threshold

```

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

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    use constants
    use numeric_utils
    use string_utils, only: lower_case
    use io_units
  <Use strings>
  <Use debug>
    use physics_defs
    use system_defs, only: TAB
    use diagnostics
    use os_interface
    use lorentz
    use interactions
    use sm_qcd
    use model_data
    use variables, only: var_list_t

    use prclib_interfaces
    use process_libraries
    use prc_core_def
    use prc_core
    use prc_external

  <Standard module head>

  <Prc Threshold: public>

  <Prc Threshold: interfaces>

  <Prc Threshold: types>

  contains

```

```
<Prc Threshold: procedures>
```

```
end module prc_threshold
```

Writer

```
<Prc Threshold: public>≡
```

```
public :: threshold_writer_t
```

```
<Prc Threshold: types>≡
```

```
type, extends (prc_external_writer_t) :: threshold_writer_t
```

```
integer :: nlo_type
```

```
contains
```

```
<Prc Threshold: threshold writer: TBP>
```

```
end type threshold_writer_t
```

```
<Prc Threshold: threshold writer: TBP>≡
```

```
procedure :: init => threshold_writer_init
```

```
<Prc Threshold: procedures>≡
```

```
pure subroutine threshold_writer_init &
```

```
(writer, model_name, prt_in, prt_out, restrictions)
```

```
class(threshold_writer_t), intent(inout) :: writer
```

```
type(string_t), intent(in) :: model_name
```

```
type(string_t), dimension(:), intent(in) :: prt_in, prt_out
```

```
type(string_t), intent(in), optional :: restrictions
```

```
call writer%base_init (model_name, prt_in, prt_out, restrictions)
```

```
writer%amp_triv = .false.
```

```
end subroutine threshold_writer_init
```

```
<Prc Threshold: threshold writer: TBP>+≡
```

```
procedure :: write_makefile_extra => threshold_writer_write_makefile_extra
```

```
<Prc Threshold: procedures>+≡
```

```
subroutine threshold_writer_write_makefile_extra &
```

```
(writer, unit, id, os_data, verbose, nlo_type)
```

```
class(threshold_writer_t), intent(in) :: writer
```

```
integer, intent(in) :: unit
```

```
type(string_t), intent(in) :: id
```

```
type(os_data_t), intent(in) :: os_data
```

```
logical, intent(in) :: verbose
```

```
integer, intent(in) :: nlo_type
```

```
type(string_t) :: f90in, f90, lo, extra
```

```
if (debug_on) call msg_debug (D_ME_METHODS, "threshold_writer_write_makefile_extra")
```

```
if (nlo_type /= BORN) then
```

```
extra = "_" // component_status (nlo_type)
```

```
else
```

```
extra = var_str ("")
```

```
end if
```

```
f90 = id // "_threshold" // extra // ".f90"
```

```
f90in = f90 // ".in"
```

```
lo = id // "_threshold" // extra // ".lo"
```

```
write (unit, "(A)") "OBJECTS += " // char (lo)
```

```

write (unit, "(A)") char (f90in) // ":"
write (unit, "(A)") char (TAB // "if ! test -f " // f90in // &
"; then cp " // os_data%whizard_sharepath // &
"/SM_tt_threshold_data/threshold" // extra // ".f90 " // &
f90in // "; fi")
write (unit, "(A)") char(f90) // ": " // char (f90in)
write (unit, "(A)") TAB // "sed 's/@ID@/" // char (id) // "/" " // &
char (f90in) // " > " // char (f90)
write (unit, "(5A)") "CLEAN_SOURCES += ", char (f90)
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (f90in)
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (id), "_threshold.mod"
write (unit, "(5A)") "CLEAN_OBJECTS += ", char (lo)
write (unit, "(A)") char(lo) // ": " // char (f90) // " " // &
char(id) // ".f90"
write (unit, "(5A)") TAB, "$ (LTF_COMPILE) $<"
if (.not. verbose) then
write (unit, "(5A)") TAB // '@echo " FC " $@"
end if
end subroutine threshold_writer_write_makefile_extra

```

<Prc Threshold: threshold writer: TBP>+≡

```

procedure :: write_makefile_code => threshold_writer_write_makefile_code

```

<Prc Threshold: procedures>+≡

```

subroutine threshold_writer_write_makefile_code &
(writer, unit, id, os_data, verbose, testflag)
class(threshold_writer_t), intent(in) :: writer
integer, intent(in) :: unit
type(string_t), intent(in) :: id
type(os_data_t), intent(in) :: os_data
logical, intent(in) :: verbose
logical, intent(in), optional :: testflag
if (debug_on) &
call msg_debug (D_ME_METHODS, "threshold_writer_write_makefile_code")
call writer%base_write_makefile_code &
(unit, id, os_data, verbose, testflag = testflag)
call writer%write_makefile_extra (unit, id, os_data, verbose, BORN)
if (writer%nlo_type == NLO_VIRTUAL .and. writer%active) &
call writer%write_makefile_extra (unit, id, os_data, verbose, writer%nlo_type)
end subroutine threshold_writer_write_makefile_code

```

<Prc Threshold: threshold writer: TBP>+≡

```

procedure, nopass :: type_name => threshold_writer_type_name

```

<Prc Threshold: procedures>+≡

```

function threshold_writer_type_name () result (string)
type(string_t) :: string
string = "Threshold"
end function threshold_writer_type_name

```

Driver

<Prc Threshold: public>+≡

```

    public :: threshold_set_process_mode
<Prc Threshold: interfaces>≡
    interface
        subroutine threshold_set_process_mode (mode) bind(C)
            import
            integer(kind = c_int), intent(in) :: mode
        end subroutine threshold_set_process_mode
    end interface

<Prc Threshold: public>+≡
    public :: threshold_get_amp_squared

<Prc Threshold: interfaces>+≡
    interface
        subroutine threshold_get_amp_squared (amp2, p_ofs, p_ons, leg, n_tot, sel_hel_beam) bind(C)
            import
            real(c_default_float), intent(out) :: amp2
            real(c_default_float), dimension(0:3,*), intent(in) :: p_ofs
            real(c_default_float), dimension(0:3,*), intent(in) :: p_ons
            integer(kind = c_int) :: n_tot, leg, sel_hel_beam
        end subroutine threshold_get_amp_squared
    end interface

<Prc Threshold: public>+≡
    public :: threshold_olp_eval2

<Prc Threshold: interfaces>+≡
    interface
        subroutine threshold_olp_eval2 (i_flg, alpha_s_c, parray, mu_c, &
            sel_hel_beam, sqme_c, acc_c) bind(C)
            import
            integer(c_int), intent(in) :: i_flg
            real(c_default_float), intent(in) :: alpha_s_c
            real(c_default_float), dimension(0:3,*), intent(in) :: parray
            real(c_default_float), intent(in) :: mu_c
            integer, intent(in) :: sel_hel_beam
            real(c_default_float), dimension(4), intent(out) :: sqme_c
            real(c_default_float), intent(out) :: acc_c
        end subroutine threshold_olp_eval2
    end interface

<Prc Threshold: public>+≡
    public :: threshold_init

<Prc Threshold: interfaces>+≡
    interface
        subroutine threshold_init (par, scheme) bind(C)
            import
            real(c_default_float), dimension(*), intent(in) :: par
            integer(c_int), intent(in) :: scheme
        end subroutine threshold_init
    end interface

```

```

<Prc Threshold: public>+≡
    public :: threshold_start_openloops

<Prc Threshold: interfaces>+≡
    interface
        subroutine threshold_start_openloops () bind(C)
            import
        end subroutine threshold_start_openloops
    end interface

<Prc Threshold: public>+≡
    public :: threshold_driver_t

<Prc Threshold: types>+≡
    type, extends (prc_external_driver_t) :: threshold_driver_t
        procedure(threshold_olp_eval2), nopass, pointer :: &
            olp_eval2 => null ()
        procedure(threshold_set_process_mode), nopass, pointer :: &
            set_process_mode => null ()
        procedure(threshold_get_amp_squared), nopass, pointer :: &
            get_amp_squared => null ()
        procedure(threshold_start_openloops), nopass, pointer :: &
            start_openloops => null ()
        procedure(threshold_init), nopass, pointer :: &
            init => null ()
        type(string_t) :: id
        integer :: nlo_type = BORN
    contains
        <Prc Threshold: threshold driver: TBP>
    end type threshold_driver_t

<Prc Threshold: threshold driver: TBP>≡
    procedure, nopass :: type_name => threshold_driver_type_name

<Prc Threshold: procedures>+≡
    function threshold_driver_type_name () result (type)
        type(string_t) :: type
        type = "Threshold"
    end function threshold_driver_type_name

<Prc Threshold: threshold driver: TBP>+≡
    procedure :: load => threshold_driver_load

<Prc Threshold: procedures>+≡
    subroutine threshold_driver_load (threshold_driver, dlaccess)
        class(threshold_driver_t), intent(inout) :: threshold_driver
        type(dlaccess_t), intent(inout) :: dlaccess
        type(c_funptr) :: c_fptr
        type(string_t) :: lower_case_id
        if (debug_on) call msg_debug (D_ME_METHODS, "threshold_driver_load")
        lower_case_id = lower_case (threshold_driver%id)
        c_fptr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_set_process_mode")
        call c_f_procpointer (c_fptr, threshold_driver%set_process_mode)
        call check_for_error (lower_case_id // "_set_process_mode")

```



```

c_fpnr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_get_amp_squared")
call c_f_procpnter (c_fpnr, threshold_driver%get_amp_squared)
call check_for_error (lower_case_id // "_get_amp_squared")
c_fpnr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_threshold_init")
call c_f_procpnter (c_fpnr, threshold_driver%init)
call check_for_error (lower_case_id // "_threshold_init")
select type (threshold_driver)
type is (threshold_driver_t)
  if (threshold_driver%nlo_type == NLO_VIRTUAL) then
    c_fpnr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_start_openloops")
    call c_f_procpnter (c_fpnr, threshold_driver%start_openloops)
    call check_for_error (lower_case_id // "_start_openloops")
    c_fpnr = dlaccess_get_c_funptr (dlaccess, lower_case_id // "_olp_eval2")
    call c_f_procpnter (c_fpnr, threshold_driver%olp_eval2)
    call check_for_error (lower_case_id // "_olp_eval2")
  end if
end select
call msg_message ("Loaded extra threshold functions")
contains
  subroutine check_for_error (function_name)
    type(string_t), intent(in) :: function_name
    if (dlaccess_has_error (dlaccess)) &
      call msg_fatal (char ("Loading of " // function_name // " failed!"))
  end subroutine check_for_error
end subroutine threshold_driver_load

```

Configuration

```

<Prc Threshold: public>+≡
  public :: threshold_def_t

<Prc Threshold: types>+≡
  type, extends (prc_external_def_t) :: threshold_def_t
    integer :: nlo_type
  contains
  <Prc Threshold: threshold def: TBP>
  end type threshold_def_t

<Prc Threshold: threshold def: TBP>≡
  procedure :: init => threshold_def_init

<Prc Threshold: procedures>+≡
  subroutine threshold_def_init (object, basename, model_name, &
    prt_in, prt_out, nlo_type, restrictions)
    class(threshold_def_t), intent(inout) :: object
    type(string_t), intent(in) :: basename, model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    integer, intent(in) :: nlo_type
    type(string_t), intent(in), optional :: restrictions
    if (debug_on) call msg_debug (D_ME_METHODS, "threshold_def_init")
    object%basename = basename
    object%nlo_type = nlo_type
    allocate (threshold_writer_t :: object%writer)

```

```

        select type (writer => object%writer)
        type is (threshold_writer_t)
            call writer%init (model_name, prt_in, prt_out, restrictions)
            writer%nlo_type = nlo_type
        end select
    end subroutine threshold_def_init

<Prc Threshold: threshold def: TBP>+≡
    procedure, nopass :: type_string => threshold_def_type_string

<Prc Threshold: procedures>+≡
    function threshold_def_type_string () result (string)
        type(string_t) :: string
        string = "threshold computation"
    end function threshold_def_type_string

write and read could be put in the abstract version

<Prc Threshold: threshold def: TBP>+≡
    procedure :: write => threshold_def_write

<Prc Threshold: procedures>+≡
    subroutine threshold_def_write (object, unit)
        class(threshold_def_t), intent(in) :: object
        integer, intent(in) :: unit
    end subroutine threshold_def_write

<Prc Threshold: threshold def: TBP>+≡
    procedure :: read => threshold_def_read

<Prc Threshold: procedures>+≡
    subroutine threshold_def_read (object, unit)
        class(threshold_def_t), intent(out) :: object
        integer, intent(in) :: unit
    end subroutine threshold_def_read

<Prc Threshold: threshold def: TBP>+≡
    procedure :: allocate_driver => threshold_def_allocate_driver

<Prc Threshold: procedures>+≡
    subroutine threshold_def_allocate_driver (object, driver, basename)
        class(threshold_def_t), intent(in) :: object
        class(prc_core_driver_t), intent(out), allocatable :: driver
        type(string_t), intent(in) :: basename
        if (debug_on) call msg_debug (D_ME_METHODS, "threshold_def_allocate_driver")
        if (.not. allocated (driver)) allocate (threshold_driver_t :: driver)
        select type (driver)
        type is (threshold_driver_t)
            driver%id = basename
            driver%nlo_type = object%nlo_type
        end select
    end subroutine threshold_def_allocate_driver

<Prc Threshold: threshold def: TBP>+≡
    procedure :: connect => threshold_def_connect

```

```

<Prc Threshold: procedures>+≡
subroutine threshold_def_connect (def, lib_driver, i, proc_driver)
  class(threshold_def_t), intent(in) :: def
  class(prclib_driver_t), intent(in) :: lib_driver
  integer, intent(in) :: i
  class(prc_core_driver_t), intent(inout) :: proc_driver
  type(dlaccess_t) :: dlaccess
  logical :: skip
  if (debug_on) call msg_debug (D_ME_METHODS, "threshold_def_connect")
  call def%omega_connect (lib_driver, i, proc_driver)
  select type (lib_driver)
  class is (prclib_driver_dynamic_t)
    dlaccess = lib_driver%dlaccess
  end select
  select type (proc_driver)
  class is (threshold_driver_t)
    select type (writer => def%writer)
    type is (threshold_writer_t)
      skip = writer%nlo_type == NLO_VIRTUAL .and. .not. writer%active
      if (.not. skip) call proc_driver%load (dlaccess)
    end select
  end select
end subroutine threshold_def_connect

```

Core state

```

<Prc Threshold: public>+≡
public :: threshold_state_t

<Prc Threshold: types>+≡
type, extends (prc_external_state_t) :: threshold_state_t
contains
  <Prc Threshold: threshold state: TBP>
end type threshold_state_t

```

```

<Prc Threshold: threshold state: TBP>≡
procedure :: write => threshold_state_write

```

```

<Prc Threshold: procedures>+≡
subroutine threshold_state_write (object, unit)
  class(threshold_state_t), intent(in) :: object
  integer, intent(in), optional :: unit
end subroutine threshold_state_write

```

Core

```

<Prc Threshold: public>+≡
public :: prc_threshold_t

<Prc Threshold: types>+≡
type, extends (prc_external_t) :: prc_threshold_t
  real(default), dimension(:, :), allocatable :: parray_ofs

```

```

        real(default), dimension(:,:), allocatable :: parray_ons
        integer :: leg
        logical :: has_beam_pol = .false.
contains
<Prc Threshold: prc threshold: TBP>
end type prc_threshold_t

<Prc Threshold: prc threshold: TBP>≡
procedure :: write => prc_threshold_write

<Prc Threshold: procedures>+≡
subroutine prc_threshold_write (object, unit)
    class(prc_threshold_t), intent(in) :: object
    integer, intent(in), optional :: unit
    call msg_message ("Supply amplitudes squared for threshold computation")
end subroutine prc_threshold_write

<Prc Threshold: prc threshold: TBP>+≡
procedure :: write_name => prc_threshold_write_name

<Prc Threshold: procedures>+≡
subroutine prc_threshold_write_name (object, unit)
    class(prc_threshold_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u,"(1x,A)") "Core: Threshold"
end subroutine prc_threshold_write_name

This core type has the beam polarization as an extra parameter.

<Prc Threshold: prc threshold: TBP>+≡
procedure :: set_beam_pol => prc_threshold_set_beam_pol

<Prc Threshold: procedures>+≡
subroutine prc_threshold_set_beam_pol (object, has_beam_pol)
    class(prc_threshold_t), intent(inout) :: object
    logical, intent(in), optional :: has_beam_pol
    if (present (has_beam_pol)) then
        object%has_beam_pol = has_beam_pol
    end if
end subroutine prc_threshold_set_beam_pol

<Prc Threshold: prc threshold: TBP>+≡
procedure :: compute_amplitude => prc_threshold_compute_amplitude

<Prc Threshold: procedures>+≡
function prc_threshold_compute_amplitude &
    (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
    core_state) result (amp)
    class(prc_threshold_t), intent(in) :: object
    integer, intent(in) :: j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in) :: fac_scale, ren_scale

```

```

real(default), intent(in), allocatable :: alpha_qcd_forced
class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
complex(default) :: amp
select type (core_state)
class is (prc_external_test_state_t)
    core_state%alpha_qcd = object%qcd%alpha%get (fac_scale)
end select
amp = 0
end function prc_threshold_compute_amplitude

```

<Prc Threshold: prc threshold: TBP>+≡

```

procedure :: allocate_workspace => prc_threshold_allocate_workspace

```

<Prc Threshold: procedures>+≡

```

subroutine prc_threshold_allocate_workspace (object, core_state)
class(prc_threshold_t), intent(in) :: object
class(prc_core_state_t), intent(inout), allocatable :: core_state
allocate (threshold_state_t :: core_state)
end subroutine prc_threshold_allocate_workspace

```

<Prc Threshold: prc threshold: TBP>+≡

```

procedure :: set_offshell_momenta => prc_threshold_set_offshell_momenta

```

<Prc Threshold: procedures>+≡

```

subroutine prc_threshold_set_offshell_momenta (object, p)
class(prc_threshold_t), intent(inout) :: object
type(vector4_t), intent(in), dimension(:) :: p
integer :: i
do i = 1, size(p)
    object%parray_ofs(:,i) = p(i)%p
end do
end subroutine prc_threshold_set_offshell_momenta

```

<Prc Threshold: prc threshold: TBP>+≡

```

procedure :: set_onshell_momenta => prc_threshold_set_onshell_momenta

```

<Prc Threshold: procedures>+≡

```

subroutine prc_threshold_set_onshell_momenta (object, p)
class(prc_threshold_t), intent(inout) :: object
type(vector4_t), intent(in), dimension(:) :: p
integer :: i
do i = 1, size(p)
    object%parray_ons(:,i) = p(i)%p
end do
end subroutine prc_threshold_set_onshell_momenta

```

<Prc Threshold: prc threshold: TBP>+≡

```

procedure :: set_leg => prc_threshold_set_leg

```

<Prc Threshold: procedures>+≡

```

subroutine prc_threshold_set_leg (object, leg)
class(prc_threshold_t), intent(inout) :: object
integer, intent(in) :: leg
object%leg = leg

```

```

end subroutine prc_threshold_set_leg

<Prc Threshold: prc threshold: TBP>+≡
  procedure :: set_process_mode => prc_threshold_set_process_mode

<Prc Threshold: procedures>+≡
  subroutine prc_threshold_set_process_mode (object, mode)
    class(prc_threshold_t), intent(in) :: object
    integer(kind = c_int), intent(in) :: mode
    select type (driver => object%driver)
    class is (threshold_driver_t)
      if (associated (driver%set_process_mode)) &
        call driver%set_process_mode (mode)
    end select
  end subroutine prc_threshold_set_process_mode

<Prc Threshold: prc threshold: TBP>+≡
  procedure :: compute_sqme => prc_threshold_compute_sqme

<Prc Threshold: procedures>+≡
  subroutine prc_threshold_compute_sqme (object, i_flv, i_hel, p, &
    ren_scale, sqme, bad_point)
    class(prc_threshold_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(out) :: sqme
    logical, intent(out) :: bad_point
    integer :: n_tot
    if (debug_on) call msg_debug2 (D_ME_METHODS, "prc_threshold_compute_sqme")
    n_tot = size (p)
    select type (driver => object%driver)
    class is (threshold_driver_t)
      if (object%has_beam_pol) then
        call driver%get_amp_squared (sqme, object%pararray_ofs, &
          object%pararray_ons, object%leg, n_tot, i_flv - 1)
      else
        call driver%get_amp_squared (sqme, object%pararray_ofs, &
          object%pararray_ons, object%leg, n_tot, -1)
      end if
    end select
    bad_point = .false.
  end subroutine prc_threshold_compute_sqme

<Prc Threshold: prc threshold: TBP>+≡
  procedure :: compute_sqme_virt => prc_threshold_compute_sqme_virt

<Prc Threshold: procedures>+≡
  subroutine prc_threshold_compute_sqme_virt (object, i_flv, i_hel, &
    p, ren_scale, es_scale, loop_method, sqme, bad_point)
    class(prc_threshold_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: ren_scale, es_scale

```

```

integer, intent(in) :: loop_method
real(default), dimension(4), intent(out) :: sqme
real(c_default_float), dimension(:, :), allocatable, save :: parray
logical, intent(out) :: bad_point
integer :: n_tot, i
real(default) :: mu
real(c_default_float), dimension(4) :: sqme_c
real(c_default_float) :: mu_c, acc_c, alpha_s_c
integer(c_int) :: i_flv_c
if (debug_on) call msg_debug2 (D_ME_METHODS, "prc_threshold_compute_sqme_virt")
n_tot = size (p)
if (allocated (parray)) then
    if (size(parray) /= n_tot) deallocate (parray)
end if
if (.not. allocated (parray)) allocate (parray (0:3, n_tot))
forall (i = 1:n_tot) parray(:, i) = p(i)%p

if (vanishes (ren_scale)) then
    mu = sqrt (2* (p(1)*p(2)))
else
    mu = ren_scale
end if
mu_c = mu
alpha_s_c = object%qcd%alpha%get (mu)
i_flv_c = i_flv
select type (driver => object%driver)
class is (threshold_driver_t)
    if (associated (driver%olp_eval2)) then
        if (object%has_beam_pol) then
            call driver%olp_eval2 (1, alpha_s_c, &
                parray, mu_c, i_flv_c - 1, sqme_c, acc_c)
        else
            call driver%olp_eval2 (i_flv_c, alpha_s_c, &
                parray, mu_c, -1, sqme_c, acc_c)
        end if
        bad_point = real(acc_c, kind=default) > object%maximum_accuracy
        sqme = sqme_c
    else
        sqme = 0._default
        bad_point = .true.
    end if
end select
end subroutine prc_threshold_compute_sqme_virt

```

<Prc Threshold: prc threshold: TBP>+≡
 procedure :: init => prc_threshold_init

<Prc Threshold: procedures>+≡
 subroutine prc_threshold_init (object, def, lib, id, i_component)
 class(prc_threshold_t), intent(inout) :: object
 class(prc_core_def_t), intent(in), target :: def
 type(process_library_t), intent(in), target :: lib
 type(string_t), intent(in) :: id
 integer, intent(in) :: i_component

```

integer :: n_tot
call object%base_init (def, lib, id, i_component)
n_tot = object%data%n_in + object%data%n_out
allocate (object%pararray_ofs (0:3,n_tot), object%pararray_ons (0:3,n_tot))
if (n_tot == 4) then
    call object%set_process_mode (PROC_MODE_TT)
else
    call object%set_process_mode (PROC_MODE_WBWB)
end if
call object%activate_parameters ()
end subroutine prc_threshold_init

```

Activate the stored parameters by transferring them to the external matrix element.

```

<Prc Threshold: prc threshold: TBP>+≡
    procedure :: activate_parameters => prc_threshold_activate_parameters

<Prc Threshold: procedures>+≡
    subroutine prc_threshold_activate_parameters (object)
        class (prc_threshold_t), intent(inout) :: object
        if (debug_on) call msg_debug (D_ME_METHODS, "prc_threshold_activate_parameters")
        if (allocated (object%driver)) then
            if (allocated (object%par)) then
                select type (driver => object%driver)
                type is (threshold_driver_t)
                    if (associated (driver%init)) then
                        call driver%init (object%par, object%scheme)
                    end if
                end select
            else
                call msg_bug ("prc_threshold_activate: parameter set is not allocated")
            end if
        else
            call msg_bug ("prc_threshold_activate: driver is not allocated")
        end if
    end subroutine prc_threshold_activate_parameters

<Prc Threshold: prc threshold: TBP>+≡
    procedure :: prepare_external_code => &
        prc_threshold_prepare_external_code

<Prc Threshold: procedures>+≡
    subroutine prc_threshold_prepare_external_code &
        (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
        class(prc_threshold_t), intent(inout) :: core
        integer, intent(in), dimension(:,:), allocatable :: flv_states
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: libname
        type(model_data_t), intent(in), target :: model
        integer, intent(in) :: i_core
        logical, intent(in) :: is_nlo
        if (debug_on) call msg_debug (D_ME_METHODS, &
            "prc_threshold_prepare_external_code")

```



```

if (allocated (core%driver)) then
  select type (driver => core%driver)
  type is (threshold_driver_t)
    if (driver%nlo_type == NLO_VIRTUAL) call driver%start_openloops ()
  end select
else
  call msg_bug ("prc_threshold_prepare_external_code: " &
    // "driver is not allocated")
end if
end subroutine prc_threshold_prepare_external_code

```

```

<Prc Threshold: prc threshold: TBP>+≡
  procedure :: includes_polarization => prc_threshold_includes_polarization

<Prc Threshold: procedures>+≡
  function prc_threshold_includes_polarization (object) result (polarized)
    logical :: polarized
    class(prc_threshold_t), intent(in) :: object
    polarized = object%has_beam_pol
  end function prc_threshold_includes_polarization

```

Chapter 18

Generic Event Handling

Event records allow the MC to communicate with the outside world. The event record should exhibit the observable contents of a physical event. We should be able to read and write events. The actual implementation of the event need not be defined yet, for that purpose.

We have the following basic modules:

event_base Abstract base type for event records. The base type contains a reference to a **particle_set.t** object as the event core, and it holds some data that we should always expect, such as the squared matrix element and event weight.

eio_data Transparent container for the metadata of an event sample.

eio_base Abstract base type for event-record input and output. The implementations of this base type represent specific event I/O formats.

These are the implementation modules:

eio_checkpoints Auxiliary output format. The only purpose is to provide screen diagnostics during event output.

eio_callback Auxiliary output format. The only purpose is to execute a callback procedure, so we have a hook for external access during event output.

eio_weights Print some event summary data, no details. The main use is for testing purposes.

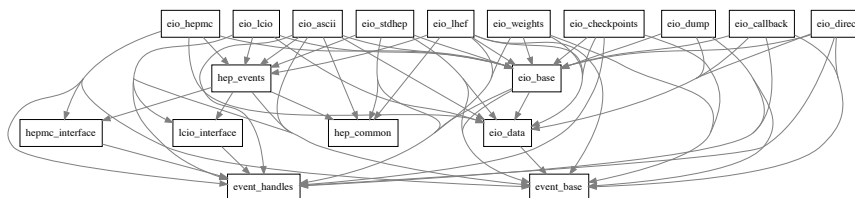


Figure 18.1: Module dependencies in `src/events`.

eio_dump Dump the contents of WHIZARD's `particle_set` internal record, using the `write` method of that record as-is. The main use is for testing purposes.

hep_common Implements traditional HEP common blocks that are (still) used by some of the event I/O formats below.

hepmc_interface Access particle objects of the HepMC package. Functional only if this package is linked. The interface is working both for HepMC2 and HepMC3.

lcio_interface Access objects of the LCIO package. Functional only if this package is linked.

hep_events Interface between the event record and the common blocks.

eio_ascii Collection of event output formats that write ASCII files.

eio_lhef LHEF for input and output.

eio_stdhep Support for the StdHEP format (binary, machine-independent).

eio_hepmc Support for the HepMC format (C++).

eio_lcio Support for the LCIO format (C++).

18.1 Generic Event Handling

We introduce events first in form of an abstract type, together with some utilities. Abstract events can be used by other modules, in particular event I/O, without introducing an explicit dependency on the event implementation.

```

<event_base.f90>≡
  <File header>

  module event_base

    <Use kinds>
    use kinds, only: i64
    <Use strings>
    use io_units
    use string_utils, only: lower_case
    use diagnostics
    use model_data
    use particles

    <Standard module head>

    <Event base: public>

    <Event base: parameters>

    <Event base: types>

    <Event base: interfaces>

```

```

contains

  <Event base: procedures>

end module event_base

```

18.1.1 generic event type

```

<Event base: public>≡
  public :: generic_event_t

<Event base: types>≡
  type, abstract :: generic_event_t
    !private
    logical :: particle_set_is_valid = .false.
    type(particle_set_t), pointer :: particle_set => null ()
    logical :: sqme_ref_known = .false.
    real(default) :: sqme_ref = 0
    logical :: sqme_prc_known = .false.
    real(default) :: sqme_prc = 0
    logical :: weight_ref_known = .false.
    real(default) :: weight_ref = 0
    logical :: weight_prc_known = .false.
    real(default) :: weight_prc = 0
    logical :: excess_prc_known = .false.
    real(default) :: excess_prc = 0
    logical :: n_dropped_known = .false.
    integer :: n_dropped = 0
    integer :: n_alt = 0
    logical :: sqme_alt_known = .false.
    real(default), dimension(:), allocatable :: sqme_alt
    logical :: weight_alt_known = .false.
    real(default), dimension(:), allocatable :: weight_alt
  contains
    <Event base: generic event: TBP>
  end type generic_event_t

```

18.1.2 Initialization

This determines the number of alternate weights and sqme values.

```

<Event base: generic event: TBP>≡
  procedure :: base_init => generic_event_init

<Event base: procedures>≡
  subroutine generic_event_init (event, n_alt)
    class(generic_event_t), intent(out) :: event
    integer, intent(in) :: n_alt
    event%n_alt = n_alt
    allocate (event%sqme_alt (n_alt))
    allocate (event%weight_alt (n_alt))
  end subroutine generic_event_init

```

18.1.3 Access particle set

The particle set is the core of the event. We allow access to it via a pointer, and we maintain the information whether the particle set is valid, i.e., has been filled with meaningful data.

```
<Event base: generic event: TBP>+≡
  procedure :: has_valid_particle_set => generic_event_has_valid_particle_set
  procedure :: accept_particle_set => generic_event_accept_particle_set
  procedure :: discard_particle_set => generic_event_discard_particle_set

<Event base: procedures>+≡
  function generic_event_has_valid_particle_set (event) result (flag)
    class(generic_event_t), intent(in) :: event
    logical :: flag
    flag = event%particle_set_is_valid
  end function generic_event_has_valid_particle_set

  subroutine generic_event_accept_particle_set (event)
    class(generic_event_t), intent(inout) :: event
    event%particle_set_is_valid = .true.
  end subroutine generic_event_accept_particle_set

  subroutine generic_event_discard_particle_set (event)
    class(generic_event_t), intent(inout) :: event
    event%particle_set_is_valid = .false.
  end subroutine generic_event_discard_particle_set
```

These procedures deal with the particle set directly. Return the pointer:

```
<Event base: generic event: TBP>+≡
  procedure :: get_particle_set_ptr => generic_event_get_particle_set_ptr

<Event base: procedures>+≡
  function generic_event_get_particle_set_ptr (event) result (ptr)
    class(generic_event_t), intent(in) :: event
    type(particle_set_t), pointer :: ptr
    ptr => event%particle_set
  end function generic_event_get_particle_set_ptr
```

Let it point to some existing particle set:

```
<Event base: generic event: TBP>+≡
  procedure :: link_particle_set => generic_event_link_particle_set

<Event base: procedures>+≡
  subroutine generic_event_link_particle_set (event, particle_set)
    class(generic_event_t), intent(inout) :: event
    type(particle_set_t), intent(in), target :: particle_set
    event%particle_set => particle_set
    call event%accept_particle_set ()
  end subroutine generic_event_link_particle_set
```

18.1.4 Access sqme and weight

There are several incarnations: the current value, a reference value, alternate values.

(Event base: generic event: TBP)+≡

```
procedure :: sqme_prc_is_known => generic_event_sqme_prc_is_known
procedure :: sqme_ref_is_known => generic_event_sqme_ref_is_known
procedure :: sqme_alt_is_known => generic_event_sqme_alt_is_known
procedure :: weight_prc_is_known => generic_event_weight_prc_is_known
procedure :: weight_ref_is_known => generic_event_weight_ref_is_known
procedure :: weight_alt_is_known => generic_event_weight_alt_is_known
procedure :: excess_prc_is_known => generic_event_excess_prc_is_known
```

(Event base: procedures)+≡

```
function generic_event_sqme_prc_is_known (event) result (flag)
  class(generic_event_t), intent(in) :: event
  logical :: flag
  flag = event%sqme_prc_known
end function generic_event_sqme_prc_is_known

function generic_event_sqme_ref_is_known (event) result (flag)
  class(generic_event_t), intent(in) :: event
  logical :: flag
  flag = event%sqme_ref_known
end function generic_event_sqme_ref_is_known

function generic_event_sqme_alt_is_known (event) result (flag)
  class(generic_event_t), intent(in) :: event
  logical :: flag
  flag = event%sqme_alt_known
end function generic_event_sqme_alt_is_known

function generic_event_weight_prc_is_known (event) result (flag)
  class(generic_event_t), intent(in) :: event
  logical :: flag
  flag = event%weight_prc_known
end function generic_event_weight_prc_is_known

function generic_event_weight_ref_is_known (event) result (flag)
  class(generic_event_t), intent(in) :: event
  logical :: flag
  flag = event%weight_ref_known
end function generic_event_weight_ref_is_known

function generic_event_weight_alt_is_known (event) result (flag)
  class(generic_event_t), intent(in) :: event
  logical :: flag
  flag = event%weight_alt_known
end function generic_event_weight_alt_is_known

function generic_event_excess_prc_is_known (event) result (flag)
  class(generic_event_t), intent(in) :: event
  logical :: flag
  flag = event%excess_prc_known
end function generic_event_excess_prc_is_known
```

```

(Event base: generic event: TBP)+≡
    procedure :: get_n_alt => generic_event_get_n_alt

(Event base: procedures)+≡
    function generic_event_get_n_alt (event) result (n)
        class(generic_event_t), intent(in) :: event
        integer :: n
        n = event%n_alt
    end function generic_event_get_n_alt

(Event base: generic event: TBP)+≡
    procedure :: get_sqme_prc => generic_event_get_sqme_prc
    procedure :: get_sqme_ref => generic_event_get_sqme_ref
    generic :: get_sqme_alt => &
        generic_event_get_sqme_alt_0, generic_event_get_sqme_alt_1
    procedure :: generic_event_get_sqme_alt_0
    procedure :: generic_event_get_sqme_alt_1
    procedure :: get_weight_prc => generic_event_get_weight_prc
    procedure :: get_weight_ref => generic_event_get_weight_ref
    generic :: get_weight_alt => &
        generic_event_get_weight_alt_0, generic_event_get_weight_alt_1
    procedure :: generic_event_get_weight_alt_0
    procedure :: generic_event_get_weight_alt_1
    procedure :: get_n_dropped => generic_event_get_n_dropped
    procedure :: get_excess_prc => generic_event_get_excess_prc

(Event base: procedures)+≡
    function generic_event_get_sqme_prc (event) result (sqme)
        class(generic_event_t), intent(in) :: event
        real(default) :: sqme
        if (event%sqme_prc_known) then
            sqme = event%sqme_prc
        else
            sqme = 0
        end if
    end function generic_event_get_sqme_prc

    function generic_event_get_sqme_ref (event) result (sqme)
        class(generic_event_t), intent(in) :: event
        real(default) :: sqme
        if (event%sqme_ref_known) then
            sqme = event%sqme_ref
        else
            sqme = 0
        end if
    end function generic_event_get_sqme_ref

    function generic_event_get_sqme_alt_0 (event, i) result (sqme)
        class(generic_event_t), intent(in) :: event
        integer, intent(in) :: i
        real(default) :: sqme
        if (event%sqme_alt_known) then
            sqme = event%sqme_alt(i)
        end if
    end function generic_event_get_sqme_alt_0

```

```

else
    sqme = 0
end if
end function generic_event_get_sqme_alt_0

function generic_event_get_sqme_alt_1 (event) result (sqme)
    class(generic_event_t), intent(in) :: event
    real(default), dimension(event%n_alt) :: sqme
    sqme = event%sqme_alt
end function generic_event_get_sqme_alt_1

function generic_event_get_weight_prc (event) result (weight)
    class(generic_event_t), intent(in) :: event
    real(default) :: weight
    if (event%weight_prc_known) then
        weight = event%weight_prc
    else
        weight = 0
    end if
end function generic_event_get_weight_prc

function generic_event_get_weight_ref (event) result (weight)
    class(generic_event_t), intent(in) :: event
    real(default) :: weight
    if (event%weight_ref_known) then
        weight = event%weight_ref
    else
        weight = 0
    end if
end function generic_event_get_weight_ref

function generic_event_get_weight_alt_0 (event, i) result (weight)
    class(generic_event_t), intent(in) :: event
    integer, intent(in) :: i
    real(default) :: weight
    if (event%weight_alt_known) then
        weight = event%weight_alt(i)
    else
        weight = 0
    end if
end function generic_event_get_weight_alt_0

function generic_event_get_weight_alt_1 (event) result (weight)
    class(generic_event_t), intent(in) :: event
    real(default), dimension(event%n_alt) :: weight
    weight = event%weight_alt
end function generic_event_get_weight_alt_1

function generic_event_get_excess_prc (event) result (excess)
    class(generic_event_t), intent(in) :: event
    real(default) :: excess
    if (event%excess_prc_known) then
        excess = event%excess_prc
    else

```



```

        excess = 0
    end if
end function generic_event_get_excess_prc

function generic_event_get_n_dropped (event) result (n_dropped)
    class(generic_event_t), intent(in) :: event
    integer :: n_dropped
    if (event%n_dropped_known) then
        n_dropped = event%n_dropped
    else
        n_dropped = 0
    end if
end function generic_event_get_n_dropped

```

(Event base: generic event: TBP)+≡

```

procedure :: set_sqme_prc => generic_event_set_sqme_prc
procedure :: set_sqme_ref => generic_event_set_sqme_ref
procedure :: set_sqme_alt => generic_event_set_sqme_alt
procedure :: set_weight_prc => generic_event_set_weight_prc
procedure :: set_weight_ref => generic_event_set_weight_ref
procedure :: set_weight_alt => generic_event_set_weight_alt
procedure :: set_excess_prc => generic_event_set_excess_prc
procedure :: set_n_dropped => generic_event_set_n_dropped

```

(Event base: procedures)+≡

```

subroutine generic_event_set_sqme_prc (event, sqme)
    class(generic_event_t), intent(inout) :: event
    real(default), intent(in) :: sqme
    event%sqme_prc = sqme
    event%sqme_prc_known = .true.
end subroutine generic_event_set_sqme_prc

subroutine generic_event_set_sqme_ref (event, sqme)
    class(generic_event_t), intent(inout) :: event
    real(default), intent(in) :: sqme
    event%sqme_ref = sqme
    event%sqme_ref_known = .true.
end subroutine generic_event_set_sqme_ref

subroutine generic_event_set_sqme_alt (event, sqme)
    class(generic_event_t), intent(inout) :: event
    real(default), dimension(:), intent(in) :: sqme
    event%sqme_alt = sqme
    event%sqme_alt_known = .true.
end subroutine generic_event_set_sqme_alt

subroutine generic_event_set_weight_prc (event, weight)
    class(generic_event_t), intent(inout) :: event
    real(default), intent(in) :: weight
    event%weight_prc = weight
    event%weight_prc_known = .true.
end subroutine generic_event_set_weight_prc

subroutine generic_event_set_weight_ref (event, weight)

```

```

class(generic_event_t), intent(inout) :: event
real(default), intent(in) :: weight
event%weight_ref = weight
event%weight_ref_known = .true.
end subroutine generic_event_set_weight_ref

subroutine generic_event_set_weight_alt (event, weight)
class(generic_event_t), intent(inout) :: event
real(default), dimension(:), intent(in) :: weight
event%weight_alt = weight
event%weight_alt_known = .true.
end subroutine generic_event_set_weight_alt

subroutine generic_event_set_excess_prc (event, excess)
class(generic_event_t), intent(inout) :: event
real(default), intent(in) :: excess
event%excess_prc = excess
event%excess_prc_known = .true.
end subroutine generic_event_set_excess_prc

subroutine generic_event_set_n_dropped (event, n_dropped)
class(generic_event_t), intent(inout) :: event
integer, intent(in) :: n_dropped
event%n_dropped = n_dropped
event%n_dropped_known = .true.
end subroutine generic_event_set_n_dropped

```

Set the appropriate entry directly.

(Event base: generic event: TBP)+≡

```

procedure :: set => generic_event_set

```

(Event base: procedures)+≡

```

subroutine generic_event_set (event, &
    weight_ref, weight_prc, weight_alt, &
    excess_prc, n_dropped, &
    sqme_ref, sqme_prc, sqme_alt)
class(generic_event_t), intent(inout) :: event
real(default), intent(in), optional :: weight_ref, weight_prc
real(default), intent(in), optional :: sqme_ref, sqme_prc
real(default), dimension(:), intent(in), optional :: sqme_alt, weight_alt
real(default), intent(in), optional :: excess_prc
integer, intent(in), optional :: n_dropped
if (present (sqme_prc)) then
    call event%set_sqme_prc (sqme_prc)
end if
if (present (sqme_ref)) then
    call event%set_sqme_ref (sqme_ref)
end if
if (present (sqme_alt)) then
    call event%set_sqme_alt (sqme_alt)
end if
if (present (weight_prc)) then
    call event%set_weight_prc (weight_prc)
end if

```

```

    if (present (weight_ref)) then
        call event%set_weight_ref (weight_ref)
    end if
    if (present (weight_alt)) then
        call event%set_weight_alt (weight_alt)
    end if
    if (present (excess_prc)) then
        call event%set_excess_prc (excess_prc)
    end if
    if (present (n_dropped)) then
        call event%set_n_dropped (n_dropped)
    end if
end subroutine generic_event_set

```

18.1.5 Pure Virtual Methods

These procedures can only be implemented in the concrete implementation.

Output (verbose, depending on parameters).

```

(Event base: generic event: TBP)+≡
    procedure (generic_event_write), deferred :: write

```

```

(Event base: interfaces)≡
    abstract interface
        subroutine generic_event_write (object, unit, &
            show_process, show_transforms, &
            show_decay, verbose, testflag)
        import
        class(generic_event_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_process
        logical, intent(in), optional :: show_transforms
        logical, intent(in), optional :: show_decay
        logical, intent(in), optional :: verbose
        logical, intent(in), optional :: testflag
    end subroutine generic_event_write
end interface

```

Generate an event, based on a selector index `i_mci`, and optionally on an extra set of random numbers `r`. For the main bunch of random numbers that the generator needs, the event object should contain its own generator.

```

(Event base: generic event: TBP)+≡
    procedure (generic_event_generate), deferred :: generate

(Event base: interfaces)+≡
    abstract interface
        subroutine generic_event_generate (event, i_mci, r, i_nlo)
        import
        class(generic_event_t), intent(inout) :: event
        integer, intent(in) :: i_mci
        real(default), dimension(:), intent(in), optional :: r
        integer, intent(in), optional :: i_nlo
    end subroutine generic_event_generate

```

```
end interface
```

Alternative : inject a particle set that is supposed to represent the hard process.
How this determines the event, is dependent on the event structure, therefore
this is a deferred method.

```
<Event base: generic event: TBP>+≡
  procedure (generic_event_set_hard_particle_set), deferred :: &
    set_hard_particle_set

<Event base: interfaces>+≡
  abstract interface
    subroutine generic_event_set_hard_particle_set (event, particle_set)
      import
      class(generic_event_t), intent(inout) :: event
      type(particle_set_t), intent(in) :: particle_set
    end subroutine generic_event_set_hard_particle_set
  end interface
```

Event index handlers.

```
<Event base: generic event: TBP>+≡
  procedure (generic_event_set_index), deferred :: set_index
  procedure (generic_event_handler), deferred :: reset_index
  procedure (generic_event_increment_index), deferred :: increment_index

<Event base: interfaces>+≡
  abstract interface
    subroutine generic_event_set_index (event, index)
      import
      class(generic_event_t), intent(inout) :: event
      integer, intent(in) :: index
    end subroutine generic_event_set_index
  end interface

  abstract interface
    subroutine generic_event_handler (event)
      import
      class(generic_event_t), intent(inout) :: event
    end subroutine generic_event_handler
  end interface

  abstract interface
    subroutine generic_event_increment_index (event, offset)
      import
      class(generic_event_t), intent(inout) :: event
      integer, intent(in), optional :: offset
    end subroutine generic_event_increment_index
  end interface
```

Evaluate any expressions associated with the event. No argument needed.

```
<Event base: generic event: TBP>+≡
  procedure (generic_event_handler), deferred :: evaluate_expressions
```

Select internal parameters

```
<Event base: generic event: TBP>+≡
  procedure (generic_event_select), deferred :: select

<Event base: interfaces>+≡
  abstract interface
    subroutine generic_event_select (event, i_mci, i_term, channel)
      import
      class(generic_event_t), intent(inout) :: event
      integer, intent(in) :: i_mci, i_term, channel
    end subroutine generic_event_select
  end interface
```

Return a pointer to the model for the currently active process.

```
<Event base: generic event: TBP>+≡
  procedure (generic_event_get_model_ptr), deferred :: get_model_ptr

<Event base: interfaces>+≡
  abstract interface
    function generic_event_get_model_ptr (event) result (model)
      import
      class(generic_event_t), intent(in) :: event
      class(model_data_t), pointer :: model
    end function generic_event_get_model_ptr
  end interface
```

Return data used by external event formats.

```
<Event base: generic event: TBP>+≡
  procedure (generic_event_has_index), deferred :: has_index
  procedure (generic_event_get_index), deferred :: get_index
  procedure (generic_event_get_fac_scale), deferred :: get_fac_scale
  procedure (generic_event_get_alpha_s), deferred :: get_alpha_s
  procedure (generic_event_get_sqrts), deferred :: get_sqrts
  procedure (generic_event_get_polarization), deferred :: get_polarization
  procedure (generic_event_get_beam_file), deferred :: get_beam_file
  procedure (generic_event_get_process_name), deferred :: &
    get_process_name

<Event base: interfaces>+≡
  abstract interface
    function generic_event_has_index (event) result (flag)
      import
      class(generic_event_t), intent(in) :: event
      logical :: flag
    end function generic_event_has_index
  end interface

  abstract interface
    function generic_event_get_index (event) result (index)
      import
      class(generic_event_t), intent(in) :: event
      integer :: index
    end function generic_event_get_index
  end interface
```

```

abstract interface
  function generic_event_get_fac_scale (event) result (fac_scale)
    import
    class(generic_event_t), intent(in) :: event
    real(default) :: fac_scale
  end function generic_event_get_fac_scale
end interface

abstract interface
  function generic_event_get_alpha_s (event) result (alpha_s)
    import
    class(generic_event_t), intent(in) :: event
    real(default) :: alpha_s
  end function generic_event_get_alpha_s
end interface

abstract interface
  function generic_event_get_sqrts (event) result (sqrts)
    import
    class(generic_event_t), intent(in) :: event
    real(default) :: sqrts
  end function generic_event_get_sqrts
end interface

abstract interface
  function generic_event_get_polarization (event) result (pol)
    import
    class(generic_event_t), intent(in) :: event
    real(default), dimension(2) :: pol
  end function generic_event_get_polarization
end interface

abstract interface
  function generic_event_get_beam_file (event) result (file)
    import
    class(generic_event_t), intent(in) :: event
    type(string_t) :: file
  end function generic_event_get_beam_file
end interface

abstract interface
  function generic_event_get_process_name (event) result (name)
    import
    class(generic_event_t), intent(in) :: event
    type(string_t) :: name
  end function generic_event_get_process_name
end interface

```

Set data used by external event formats.

(Event base: generic event: TBP)+≡

```

  procedure (generic_event_set_alpha_qcd_forced), deferred :: &
    set_alpha_qcd_forced

```

```

    procedure (generic_event_set_scale_forced), deferred :: &
        set_scale_forced
<Event base: interfaces>+≡
    abstract interface
        subroutine generic_event_set_alpha_qcd_forced (event, alpha_qcd)
            import
            class(generic_event_t), intent(inout) :: event
            real(default), intent(in) :: alpha_qcd
        end subroutine generic_event_set_alpha_qcd_forced
    end interface

    abstract interface
        subroutine generic_event_set_scale_forced (event, scale)
            import
            class(generic_event_t), intent(inout) :: event
            real(default), intent(in) :: scale
        end subroutine generic_event_set_scale_forced
    end interface

```

18.1.6 Utilities

Applying this, current event contents are marked as incomplete but are not deleted. In particular, the initialization is kept.

```

<Event base: generic event: TBP>+≡
    procedure :: reset_contents => generic_event_reset_contents
    procedure :: base_reset_contents => generic_event_reset_contents

<Event base: procedures>+≡
    subroutine generic_event_reset_contents (event)
        class(generic_event_t), intent(inout) :: event
        call event%discard_particle_set ()
        event%sqme_ref_known = .false.
        event%sqme_prc_known = .false.
        event%sqme_alt_known = .false.
        event%weight_ref_known = .false.
        event%weight_prc_known = .false.
        event%weight_alt_known = .false.
        event%excess_prc_known = .false.
    end subroutine generic_event_reset_contents

```

Pacify particle set.

```

<Event base: generic event: TBP>+≡
    procedure :: pacify_particle_set => generic_event_pacify_particle_set

<Event base: procedures>+≡
    subroutine generic_event_pacify_particle_set (event)
        class(generic_event_t), intent(inout) :: event
        if (event%has_valid_particle_set ()) call pacify (event%particle_set)
    end subroutine generic_event_pacify_particle_set

```

18.1.7 Event normalization

The parameters for event normalization. For unweighted events, `NORM_UNIT` is intended as default, while for weighted events, it is `NORM_SIGMA`.

Note: the unit test for this is in `eio_data_2` below.

```
<Event base: parameters>≡
  integer, parameter, public :: NORM_UNDEFINED = 0
  integer, parameter, public :: NORM_UNIT = 1
  integer, parameter, public :: NORM_N_EVT = 2
  integer, parameter, public :: NORM_SIGMA = 3
  integer, parameter, public :: NORM_S_N = 4
```

These functions translate between the user representation and the internal one.

```
<Event base: public>+≡
  public :: event_normalization_mode
  public :: event_normalization_string

<Event base: procedures>+≡
  function event_normalization_mode (string, unweighted) result (mode)
    integer :: mode
    type(string_t), intent(in) :: string
    logical, intent(in) :: unweighted
    select case (lower_case (char (string)))
    case ("auto")
      if (unweighted) then
        mode = NORM_UNIT
      else
        mode = NORM_SIGMA
      end if
    case ("1")
      mode = NORM_UNIT
    case ("1/n")
      mode = NORM_N_EVT
    case ("sigma")
      mode = NORM_SIGMA
    case ("sigma/n")
      mode = NORM_S_N
    case default
      call msg_fatal ("Event normalization: unknown value '" &
        // char (string) // "'")
    end select
  end function event_normalization_mode

  function event_normalization_string (norm_mode) result (string)
    integer, intent(in) :: norm_mode
    type(string_t) :: string
    select case (norm_mode)
    case (NORM_UNDEFINED); string = "[undefined]"
    case (NORM_UNIT);      string = "'1'"
    case (NORM_N_EVT);     string = "'1/n'"
    case (NORM_SIGMA);     string = "'sigma'"
    case (NORM_S_N);       string = "'sigma/n'"
    case default;          string = "???"
    end select
```



```
end function event_normalization_string
```

We place this here as a generic helper, so we can update event weights whenever we need, not just in connection with an event sample data object.

```
<Event base: public>+≡
  public :: event_normalization_update

<Event base: procedures>+≡
  subroutine event_normalization_update (weight, sigma, n, mode_new, mode_old)
    real(default), intent(inout) :: weight
    real(default), intent(in) :: sigma
    integer, intent(in) :: n
    integer, intent(in) :: mode_new, mode_old
    if (mode_new /= mode_old) then
      if (sigma > 0 .and. n > 0) then
        weight = weight / factor (mode_old) * factor (mode_new)
      else
        call msg_fatal ("Event normalization update: null sample")
      end if
    end if
  contains
    function factor (mode)
      real(default) :: factor
      integer, intent(in) :: mode
      select case (mode)
        case (NORM_UNIT);   factor = 1._default
        case (NORM_N_EVT);   factor = 1._default / n
        case (NORM_SIGMA);   factor = sigma
        case (NORM_S_N);     factor = sigma / n
        case default
          call msg_fatal ("Event normalization update: undefined mode")
        end select
      end function factor
    end subroutine event_normalization_update
```

18.1.8 Callback container

This derived type contains a callback procedure that can be executed during event I/O. The callback procedure is given the event object (with class `generic_event`) and an event index.

This is a simple wrapper. The object is abstract, so the the actual procedure is introduced by overriding the deferred one. We use the PASS attribute, so we may supplement runtime data in the callback object if desired.

```
<Event base: public>+≡
  public :: event_callback_t

<Event base: types>+≡
  type, abstract :: event_callback_t
    private
  contains
    procedure(event_callback_write), deferred :: write
    procedure(event_callback_proc), deferred :: proc
```

```
end type event_callback_t
```

Identify the callback procedure in output

<Event base: interfaces>+≡

```
abstract interface
  subroutine event_callback_write (event_callback, unit)
    import
    class(event_callback_t), intent(in) :: event_callback
    integer, intent(in), optional :: unit
  end subroutine event_callback_write
end interface
```

This is the procedure interface.

<Event base: interfaces>+≡

```
abstract interface
  subroutine event_callback_proc (event_callback, i, event)
    import
    class(event_callback_t), intent(in) :: event_callback
    integer(i64), intent(in) :: i
    class(generic_event_t), intent(in) :: event
  end subroutine event_callback_proc
end interface
```

A dummy implementation for testing and fallback.

<Event base: public>+≡

```
public :: event_callback_nop_t
```

<Event base: types>+≡

```
type, extends (event_callback_t) :: event_callback_nop_t
private
contains
  procedure :: write => event_callback_nop_write
  procedure :: proc => event_callback_nop
end type event_callback_nop_t
```

<Event base: procedures>+≡

```
subroutine event_callback_nop_write (event_callback, unit)
  class(event_callback_nop_t), intent(in) :: event_callback
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "NOP"
end subroutine event_callback_nop_write

subroutine event_callback_nop (event_callback, i, event)
  class(event_callback_nop_t), intent(in) :: event_callback
  integer(i64), intent(in) :: i
  class(generic_event_t), intent(in) :: event
end subroutine event_callback_nop
```

18.2 Event Handle

This module defines an abstract base type that allows us to communicate any type of event record within the program. The concrete extensions are expected to consist of pointers, such as the C pointers for HepMC or LCIO events, so the communication object is a very light-weight one.

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

```
  module event_handles
```

```
    <Standard module head>
```

```
    <Event handle: public>
```

```
    <Event handle: types>
```

```
  end module event_handles
```

There is only one abstract type.

```
<Event handle: public>≡
```

```
  public :: event_handle_t
```

```
<Event handle: types>≡
```

```
  type, abstract :: event_handle_t
```

```
  end type event_handle_t
```

18.3 Event Sample Data

We define a simple and transparent container for (meta)data that are associated with an event sample.

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

```
  module eio_data
```

```
    <Use kinds>
```

```
    <Use strings>
```

```
      use io_units
```

```
      use numeric_utils
```

```
      use diagnostics
```

```
      use event_base
```

```
    <Standard module head>
```

```
    <EIO data: public>
```

```
    <EIO data: types>
```

```
  contains
```

```

    <EIO data: procedures>

```

```

end module eio_data

```

18.3.1 Event Sample Data

These are data that apply to an event sample as a whole. They are given in an easily portable form (no fancy structure) and are used for initializing event formats.

There are two MD5 sums here. `md5sum_proc` depends only on the definition of the contributing processes. A sample with matching checksum can be rescanned with modified model parameters, beam structure etc, to recalculate observables. `md5sum_config` includes all relevant data. Rescanning a sample with matching checksum will produce identical observables. (A third checksum might be added which depends on the event sample itself. This is not needed, so far.)

If alternate weights are part of the event sample (`n_alt` nonzero), there is a configuration MD5 sum for each of them.

```

<EIO data: public>≡

```

```

    public :: event_sample_data_t

```

```

<EIO data: types>≡

```

```

    type :: event_sample_data_t
        character(32) :: md5sum_prc = ""
        character(32) :: md5sum_cfg = ""
        logical :: unweighted = .true.
        logical :: negative_weights = .false.
        integer :: norm_mode = NORM_UNDEFINED
        integer :: n_beam = 0
        integer, dimension(2) :: pdg_beam = 0
        real(default), dimension(2) :: energy_beam = 0
        integer :: n_proc = 0
        integer :: n_evt = 0
        integer :: nlo_multiplier = 1
        integer :: split_n_evt = 0
        integer :: split_n_kbytes = 0
        integer :: split_index = 0
        real(default) :: total_cross_section = 0
        integer, dimension(:), allocatable :: proc_num_id
        integer :: n_alt = 0
        character(32), dimension(:), allocatable :: md5sum_alt
        real(default), dimension(:), allocatable :: cross_section
        real(default), dimension(:), allocatable :: error
    contains
        <EIO data: event sample data: TBP>
    end type event_sample_data_t

```

Initialize: allocate for the number of processes

```

<EIO data: event sample data: TBP>≡

```

```

    procedure :: init => event_sample_data_init

```

```

<EIO data: procedures>≡
subroutine event_sample_data_init (data, n_proc, n_alt)
  class(event_sample_data_t), intent(out) :: data
  integer, intent(in) :: n_proc
  integer, intent(in), optional :: n_alt
  data%n_proc = n_proc
  allocate (data%proc_num_id (n_proc), source = 0)
  allocate (data%cross_section (n_proc), source = 0._default)
  allocate (data%error (n_proc), source = 0._default)
  if (present (n_alt)) then
    data%n_alt = n_alt
    allocate (data%md5sum_alt (n_alt))
    data%md5sum_alt = ""
  end if
end subroutine event_sample_data_init

```

Output.

```

<EIO data: event sample data: TBP>+≡
  procedure :: write => event_sample_data_write

<EIO data: procedures>+≡
subroutine event_sample_data_write (data, unit)
  class(event_sample_data_t), intent(in) :: data
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Event sample properties:"
  write (u, "(3x,A,A,A)") "MD5 sum (proc) = ", data%md5sum_prc, ""
  write (u, "(3x,A,A,A)") "MD5 sum (config) = ", data%md5sum_cfg, ""
  write (u, "(3x,A,L1)") "unweighted = ", data%unweighted
  write (u, "(3x,A,L1)") "negative weights = ", data%negative_weights
  write (u, "(3x,A,A)") "normalization = ", &
    char (event_normalization_string (data%norm_mode))
  write (u, "(3x,A,I0)") "number of beams = ", data%n_beam
  write (u, "(5x,A,2(1x,I19))") "PDG = ", &
    data%pdg_beam(:data%n_beam)
  write (u, "(5x,A,2(1x,ES19.12))") "Energy = ", &
    data%energy_beam(:data%n_beam)
  if (data%n_evt > 0) then
    write (u, "(3x,A,I0)") "number of events = ", data%n_evt
  end if
  if (.not. vanishes (data%total_cross_section)) then
    write (u, "(3x,A,ES19.12)") "total cross sec. = ", &
      data%total_cross_section
  end if
  write (u, "(3x,A,I0)") "num of processes = ", data%n_proc
  do i = 1, data%n_proc
    write (u, "(3x,A,I0)") "Process #", data%proc_num_id (i)
    select case (data%n_beam)
    case (1)
      write (u, "(5x,A,ES19.12)") "Width = ", data%cross_section(i)
    case (2)
      write (u, "(5x,A,ES19.12)") "CSec = ", data%cross_section(i)
    end select
  end do
end subroutine event_sample_data_write

```

```

        write (u, "(5x,A,ES19.12)") "Error = ", data%error(i)
    end do
    if (data%n_alt > 0) then
        write (u, "(3x,A,I0)") "num of alt wgt  = ", data%n_alt
        do i = 1, data%n_alt
            write (u, "(5x,A,A,A,1x,I0)") "MD5 sum (cfg) = ', &
                data%md5sum_alt(i), "'", i
        end do
    end if
end subroutine event_sample_data_write

```

18.3.2 Unit tests

Test module, followed by the corresponding implementation module.

<eio_data.ut.f90>≡

<File header>

```

module eio_data_ut
    use unit_tests
    use eio_data_util

```

<Standard module head>

<EIO data: public test>

contains

<EIO data: test driver>

```

end module eio_data_ut

```

<eio_data_util.f90>≡

<File header>

```

module eio_data_util

```

<Use kinds>

<Use strings>

```

    use event_base

```

```

    use eio_data

```

<Standard module head>

<EIO data: test declarations>

contains

<EIO data: tests>

```

end module eio_data_util

```

```

⟨EIO data: public test⟩≡
    public :: eio_data_test

⟨EIO data: test driver⟩≡
    subroutine eio_data_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    ⟨EIO data: execute tests⟩
    end subroutine eio_data_test

```

Print the contents of a sample data block.

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```

call data%init (2)
data%n_beam = 2
data%pdg_beam = [2212, -2212]
data%energy_beam = [8._default, 10._default]

data%norm_mode = NORM_SIGMA

data%proc_num_id = [12, 34]
data%cross_section = [100._default, 88._default]
data%error = [1._default, 0.1_default]

call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_data_1"

end subroutine eio_data_1

```

Event Normalization

Check the functions for translating modes and updating weights.

```

<EIO data: execute tests>+≡
call test (eio_data_2, "eio_data_2", &
  "event normalization", &
  u, results)

<EIO data: test declarations>+≡
public :: eio_data_2

<EIO data: tests>+≡
subroutine eio_data_2 (u)
  integer, intent(in) :: u
  type(string_t) :: s
  logical :: unweighted
  real(default) :: w, w0, sigma
  integer :: n

  write (u, "(A)")  "* Test output: eio_data_2"
  write (u, "(A)")  "* Purpose: handle event normalization"
  write (u, "(A)")

  write (u, "(A)")  "* Normalization strings"
  write (u, "(A)")

  s = "auto"
  unweighted = .true.
  write (u, "(1x,A,1x,L1,1x,A)") char (s), unweighted, &
    char (event_normalization_string &
      (event_normalization_mode (s, unweighted)))
  s = "AUTO"
  unweighted = .false.
  write (u, "(1x,A,1x,L1,1x,A)") char (s), unweighted, &
    char (event_normalization_string &

```



```

(event_normalization_mode (s, unweighted)))

unweighted = .true.

s = "1"
write (u, "(2(1x,A))") char (s), char (event_normalization_string &
(event_normalization_mode (s, unweighted)))
s = "1/n"
write (u, "(2(1x,A))") char (s), char (event_normalization_string &
(event_normalization_mode (s, unweighted)))
s = "Sigma"
write (u, "(2(1x,A))") char (s), char (event_normalization_string &
(event_normalization_mode (s, unweighted)))
s = "sigma/N"
write (u, "(2(1x,A))") char (s), char (event_normalization_string &
(event_normalization_mode (s, unweighted)))

write (u, "(A)")
write (u, "(A)")  "* Normalization update"
write (u, "(A)")

sigma = 5
n = 2

w0 = 1

w = w0
call event_normalization_update (w, sigma, n, NORM_UNIT, NORM_UNIT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_N_EVT, NORM_UNIT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_SIGMA, NORM_UNIT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_S_N, NORM_UNIT)
write (u, "(2(F6.3))") w0, w

write (u, *)

w0 = 0.5

w = w0
call event_normalization_update (w, sigma, n, NORM_UNIT, NORM_N_EVT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_N_EVT, NORM_N_EVT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_SIGMA, NORM_N_EVT)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_S_N, NORM_N_EVT)

```

```

write (u, "(2(F6.3))") w0, w

write (u, *)

w0 = 5.0

w = w0
call event_normalization_update (w, sigma, n, NORM_UNIT, NORM_SIGMA)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_N_EVT, NORM_SIGMA)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_SIGMA, NORM_SIGMA)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_S_N, NORM_SIGMA)
write (u, "(2(F6.3))") w0, w

write (u, *)

w0 = 2.5

w = w0
call event_normalization_update (w, sigma, n, NORM_UNIT, NORM_S_N)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_N_EVT, NORM_S_N)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_SIGMA, NORM_S_N)
write (u, "(2(F6.3))") w0, w
w = w0
call event_normalization_update (w, sigma, n, NORM_S_N, NORM_S_N)
write (u, "(2(F6.3))") w0, w

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_data_2"

end subroutine eio_data_2

```

18.4 Abstract I/O Handler

This module defines an abstract object for event I/O and the associated methods.

There are **output** and **input** methods which write or read a single event from/to the I/O stream, respectively. The I/O stream itself may be a file, a common block, or an externally linked structure, depending on the concrete implementation.

A **write** method prints the current content of the implementation-dependent event record in human-readable form.

The `init_in/init_out` and `final` prepare and finalize the I/O stream, respectively. There is also a `switch_inout` method which turns an input stream into an output stream where events can be appended.

Optionally, output files can be split in chunks of well-defined size. The `split_out` method takes care of this.

```

⟨eio_base.f90⟩≡
  ⟨File header⟩

  module eio_base

    use kinds, only: i64
  ⟨Use strings⟩
    use io_units
    use diagnostics
    use model_data
    use event_base
    use event_handles, only: event_handle_t
    use eio_data

  ⟨Standard module head⟩

  ⟨EIO base: public⟩

  ⟨EIO base: types⟩

  ⟨EIO base: interfaces⟩

  contains

  ⟨EIO base: procedures⟩

  end module eio_base

```

18.4.1 Type

We can assume that most implementations will need the file extension as a fixed string and, if they support file splitting, the current file index.

The fallback model is useful for implementations that are able to read unknown files which may contain hadrons etc., not in the current hard-interaction model.

```

⟨EIO base: public⟩≡
  public :: eio_t

⟨EIO base: types⟩≡
  type, abstract :: eio_t
    type(string_t) :: sample
    type(string_t) :: extension
    type(string_t) :: filename
    logical :: has_file = .false.
    logical :: split = .false.
    integer :: split_n_evt = 0
    integer :: split_n_kbytes = 0
    integer :: split_index = 0

```

```

integer :: split_count = 0
class(model_data_t), pointer :: fallback_model => null ()
contains
  <EIO base: eio: TBP>≡
end type eio_t

```

Write to screen. If possible, this should display the contents of the current event, i.e., the last one that was written or read.

```

<EIO base: eio: TBP>≡
  procedure (eio_write), deferred :: write
<EIO base: interfaces>≡
  abstract interface
    subroutine eio_write (object, unit)
      import
      class(eio_t), intent(in) :: object
      integer, intent(in), optional :: unit
    end subroutine eio_write
  end interface

```

Finalize. This should write/read footer data and close input/output channels.

```

<EIO base: eio: TBP>+≡
  procedure (eio_final), deferred :: final
<EIO base: interfaces>+≡
  abstract interface
    subroutine eio_final (object)
      import
      class(eio_t), intent(inout) :: object
    end subroutine eio_final
  end interface

```

Determine splitting parameters from the event sample data.

```

<EIO base: eio: TBP>+≡
  procedure :: set_splitting => eio_set_splitting
<EIO base: procedures>≡
  subroutine eio_set_splitting (eio, data)
    class(eio_t), intent(inout) :: eio
    type(event_sample_data_t), intent(in) :: data
    eio%split = data%split_n_evt > 0 .or. data%split_n_kbytes > 0
    if (eio%split) then
      eio%split_n_evt = data%split_n_evt
      eio%split_n_kbytes = data%split_n_kbytes
      eio%split_index = data%split_index
      eio%split_count = 0
    end if
  end subroutine eio_set_splitting

```

Update the byte count and check if it has increased. We use integer division to determine the number of `n_kbytes` blocks that are in the event file.

```

<EIO base: eio: TBP>+≡
  procedure :: update_split_count => eio_update_split_count

```

```

<EIO base: procedures>+=
subroutine eio_update_split_count (eio, increased)
  class(eio_t), intent(inout) :: eio
  logical, intent(out) :: increased
  integer :: split_count_old
  if (eio%split_n_kbytes > 0) then
    split_count_old = eio%split_count
    eio%split_count = eio%file_size_kbytes () / eio%split_n_kbytes
    increased = eio%split_count > split_count_old
  end if
end subroutine eio_update_split_count

```

Generate a filename, taking a possible split index into account.

```

<EIO base: eio: TBP>+=
procedure :: set_filename => eio_set_filename

<EIO base: procedures>+=
subroutine eio_set_filename (eio)
  class(eio_t), intent(inout) :: eio
  character(32) :: buffer
  if (eio%split) then
    write (buffer, "(I0,'.')") eio%split_index
    eio%filename = eio%sample // "." // trim (buffer) // eio%extension
    eio%has_file = .true.
  else
    eio%filename = eio%sample // "." // eio%extension
    eio%has_file = .true.
  end if
end subroutine eio_set_filename

```

Set the fallback model.

```

<EIO base: eio: TBP>+=
procedure :: set_fallback_model => eio_set_fallback_model

<EIO base: procedures>+=
subroutine eio_set_fallback_model (eio, model)
  class(eio_t), intent(inout) :: eio
  class(model_data_t), intent(in), target :: model
  eio%fallback_model => model
end subroutine eio_set_fallback_model

```

Initialize for output. We provide process names. This should open an event file if appropriate and write header data. Some methods may require event sample data.

```

<EIO base: eio: TBP>+=
procedure (eio_init_out), deferred :: init_out

<EIO base: interfaces>+=
abstract interface
  subroutine eio_init_out (eio, sample, data, success, extension)
    import
    class(eio_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample

```

```

        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        type(string_t), intent(in), optional :: extension
    end subroutine eio_init_out
end interface

```

Initialize for input. We provide process names. This should open an event file if appropriate and read header data. The `md5sum` can be used to check the integrity of the configuration, it provides a checksum to compare with. In case the extension has changed the extension is also given as an argument.

The `data` argument is `intent(inout)`: we may read part of it and keep other parts and/or check them against the data in the file.

```

<EIO base: eio: TBP>+≡
    procedure (eio_init_in), deferred :: init_in

<EIO base: interfaces>+≡
    abstract interface
        subroutine eio_init_in (eio, sample, data, success, extension)
            import
            class(eio_t), intent(inout) :: eio
            type(string_t), intent(in) :: sample
            type(event_sample_data_t), intent(inout), optional :: data
            logical, intent(out), optional :: success
            type(string_t), intent(in), optional :: extension
        end subroutine eio_init_in
    end interface

```

Re-initialize for output. This should change the status of any event file from input to output and position it for appending new events.

```

<EIO base: eio: TBP>+≡
    procedure (eio_switch_inout), deferred :: switch_inout

<EIO base: interfaces>+≡
    abstract interface
        subroutine eio_switch_inout (eio, success)
            import
            class(eio_t), intent(inout) :: eio
            logical, intent(out), optional :: success
        end subroutine eio_switch_inout
    end interface

```

This is similar: split the output, i.e., close the current file and open a new one. The default implementation does nothing. For the feature to work, an implementation must override this.

```

<EIO base: eio: TBP>+≡
    procedure :: split_out => eio_split_out

<EIO base: procedures>+≡
    subroutine eio_split_out (eio)
        class(eio_t), intent(inout) :: eio
    end subroutine eio_split_out

```

Determine the file size in kilobytes. More exactly, determine the size in units of 1024 storage units, as returned by the INQUIRE statement.

The implementation returns zero if there is no file. The `has_file` flag is set by the `set_filename` method, so we can be confident that the `inquire` call is meaningful. If this algorithm doesn't apply for a particular format, we still can override the procedure.

```

(EIO base: eio: TBP)+≡
  procedure :: file_size_kbytes => eio_file_size_kbytes

(EIO base: procedures)+≡
  function eio_file_size_kbytes (eio) result (kbytes)
    class(eio_t), intent(in) :: eio
    integer :: kbytes
    integer(i64) :: bytes
    if (eio%has_file) then
      inquire (file = char (eio%filename), size = bytes)
      if (bytes > 0) then
        kbytes = bytes / 1024
      else
        kbytes = 0
      end if
    else
      kbytes = 0
    end if
  end function eio_file_size_kbytes

```

Output an event. All data can be taken from the `event` record. The index `i_prc` identifies the process among the processes that are contained in the current sample. The `reading` flag, if present, indicates that the event was read from file, not generated.

The `passed` flag tells us that this event has passed the selection criteria. Depending on the event format, we may choose to skip events that have not passed.

```

(EIO base: eio: TBP)+≡
  procedure (eio_output), deferred :: output

(EIO base: interfaces)+≡
  abstract interface
    subroutine eio_output &
      (eio, event, i_prc, reading, passed, pacify, event_handle)
    import
    class(eio_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    integer, intent(in) :: i_prc
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
  end subroutine eio_output
  end interface

```

Input an event. This should fill all event data that cannot be inferred from the associated process.

The input is broken down into two parts. First we read the `i_prc` index. So we know which process to expect in the subsequent event. If we have reached end of file, we also will know. Then, we read the event itself.

The parameter `iostat` is supposed to be set as the Fortran standard requires, negative for EOF and positive for error.

```

<EIO base: eio: TBP>+≡
  procedure (eio_input_i_prc), deferred :: input_i_prc
  procedure (eio_input_event), deferred :: input_event

<EIO base: interfaces>+≡
  abstract interface
    subroutine eio_input_i_prc (eio, i_prc, iostat)
      import
      class(eio_t), intent(inout) :: eio
      integer, intent(out) :: i_prc
      integer, intent(out) :: iostat
    end subroutine eio_input_i_prc
  end interface

  abstract interface
    subroutine eio_input_event (eio, event, iostat, event_handle)
      import
      class(eio_t), intent(inout) :: eio
      class(generic_event_t), intent(inout), target :: event
      integer, intent(out) :: iostat
      class(event_handle_t), intent(inout), optional :: event_handle
    end subroutine eio_input_event
  end interface

<EIO base: eio: TBP>+≡
  procedure (eio_skip), deferred :: skip

<EIO base: interfaces>+≡
  abstract interface
    subroutine eio_skip (eio, iostat)
      import
      class(eio_t), intent(inout) :: eio
      integer, intent(out) :: iostat
    end subroutine eio_skip
  end interface

```

18.4.2 Unit tests

Test module, followed by the corresponding implementation module.

```

<eio_base.ut.f90>≡
  <File header>

  module eio_base_ut
    use unit_tests
    use eio_base_ut_i

    <Standard module head>

```



```

    <EIO base: public test>

    <EIO base: public test auxiliary>

    contains

    <EIO base: test driver>

    end module eio_base_ut

    <eio_base.uti.f90>≡
    <File header>

    module eio_base_uti

    <Use kinds>
    <Use strings>
        use io_units
        use lorentz
        use model_data
        use particles
        use event_base
        use event_handles, only: event_handle_t
        use eio_data

        use eio_base

    <Standard module head>

    <EIO base: public test auxiliary>

    <EIO base: test declarations>

    <EIO base: test types>

    <EIO base: test variables>

    contains

    <EIO base: tests>

    <EIO base: test auxiliary>

    end module eio_base_uti
API: driver for the unit tests below.
    <EIO base: public test>≡
        public :: eio_base_test
    <EIO base: test driver>≡
        subroutine eio_base_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <EIO base: execute tests>
        end subroutine eio_base_test

```

The caller has to provide procedures that prepare and cleanup the test environment. They depend on modules that are not available here.

```

<EIO base: test types>≡
  abstract interface
    subroutine eio_prepare_event (event, unweighted, n_alt, sample_norm)
      import
      class(generic_event_t), intent(inout), pointer :: event
      logical, intent(in), optional :: unweighted
      integer, intent(in), optional :: n_alt
      type(string_t), intent(in), optional :: sample_norm
    end subroutine eio_prepare_event
  end interface

  abstract interface
    subroutine eio_cleanup_event (event)
      import
      class(generic_event_t), intent(inout), pointer :: event
    end subroutine eio_cleanup_event
  end interface

```

We store pointers to the test-environment handlers as module variables. This allows us to call them from the test routines themselves, which don't allow for extra arguments.

```

<EIO base: public test auxiliary>≡
  public :: eio_prepare_test, eio_cleanup_test

<EIO base: test types>+≡
  procedure(eio_prepare_event), pointer :: eio_prepare_test => null ()
  procedure(eio_cleanup_event), pointer :: eio_cleanup_test => null ()

```

Similarly, for the fallback (hadron) model that some eio tests require:

```

<EIO base: test types>+≡
  abstract interface
    subroutine eio_prepare_model (model)
      import
      class(model_data_t), intent(inout), pointer :: model
    end subroutine eio_prepare_model
  end interface

  abstract interface
    subroutine eio_cleanup_model (model)
      import
      class(model_data_t), intent(inout), target :: model
    end subroutine eio_cleanup_model
  end interface

<EIO base: public test auxiliary>+≡
  public :: eio_prepare_fallback_model, eio_cleanup_fallback_model

<EIO base: test variables>≡
  procedure(eio_prepare_model), pointer :: eio_prepare_fallback_model => null ()

```

```
procedure(eio_cleanup_model), pointer :: eio_cleanup_fallback_model => null ()
```

Test type for event I/O

The contents simulate the contents of an external file. We have the `sample` string as the file name and the array of momenta `event_p` as the list of events. The second index is the event index. The `event_i` component is the pointer to the current event, `event_n` is the total number of stored events.

```
<EIO base: test types>+≡
type, extends (eio_t) :: eio_test_t
  integer :: event_n = 0
  integer :: event_i = 0
  integer :: i_prc = 0
  type(vector4_t), dimension(:,,:), allocatable :: event_p
contains
  <EIO base: eio test: TBP>
end type eio_test_t
```

Write to screen. Pretend that this is an actual event format.

```
<EIO base: eio test: TBP>≡
  procedure :: write => eio_test_write

<EIO base: test auxiliary>≡
  subroutine eio_test_write (object, unit)
    class(eio_test_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Test event stream"
    if (object%event_i /= 0) then
      write (u, "(1x,A,I0,A)") "Event #", object%event_i, ":"
      do i = 1, size (object%event_p, 1)
        call vector4_write (object%event_p(i, object%event_i), u)
      end do
    end if
  end subroutine eio_test_write
```

Finalizer. For the test case, we just reset the event count, but keep the stored “events”. For the real implementations, the events would be stored on an external medium, so we would delete the object contents.

```
<EIO base: eio test: TBP>+≡
  procedure :: final => eio_test_final

<EIO base: test auxiliary>+≡
  subroutine eio_test_final (object)
    class(eio_test_t), intent(inout) :: object
    object%event_i = 0
  end subroutine eio_test_final
```

Initialization: We store the process IDs and the energy from the beam-data object. We also allocate the momenta (i.e., the simulated event record) for a fixed maximum size of 10 events, 2 momenta each. There is only a single process.

```

(EIO base: eio test: TBP)+≡
  procedure :: init_out => eio_test_init_out

(EIO base: test auxiliary)+≡
  subroutine eio_test_init_out (eio, sample, data, success, extension)
    class(eio_test_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(event_sample_data_t), intent(in), optional :: data
    logical, intent(out), optional :: success
    type(string_t), intent(in), optional :: extension
    eio%sample = sample
    eio%event_n = 0
    eio%event_i = 0
    allocate (eio%event_p (2, 10))
    if (present (success)) success = .true.
  end subroutine eio_test_init_out

```

Initialization for input. Nothing to do for the test type.

```

(EIO base: eio test: TBP)+≡
  procedure :: init_in => eio_test_init_in

(EIO base: test auxiliary)+≡
  subroutine eio_test_init_in (eio, sample, data, success, extension)
    class(eio_test_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(event_sample_data_t), intent(inout), optional :: data
    logical, intent(out), optional :: success
    type(string_t), intent(in), optional :: extension
    if (present (success)) success = .true.
  end subroutine eio_test_init_in

```

Switch from output to input. Again, nothing to do for the test type.

```

(EIO base: eio test: TBP)+≡
  procedure :: switch_inout => eio_test_switch_inout

(EIO base: test auxiliary)+≡
  subroutine eio_test_switch_inout (eio, success)
    class(eio_test_t), intent(inout) :: eio
    logical, intent(out), optional :: success
    if (present (success)) success = .true.
  end subroutine eio_test_switch_inout

```

Output. Increment the event counter and store the momenta of the current event.

```

(EIO base: eio test: TBP)+≡
  procedure :: output => eio_test_output

```

```

(EIO base: test auxiliary)+≡
subroutine eio_test_output &
  (eio, event, i_prc, reading, passed, pacify, event_handle)
  class(eio_test_t), intent(inout) :: eio
  class(generic_event_t), intent(in), target :: event
  logical, intent(in), optional :: reading, passed, pacify
  class(event_handle_t), intent(inout), optional :: event_handle
  integer, intent(in) :: i_prc
  type(particle_set_t), pointer :: pset
  type(particle_t) :: prt
  eio%event_n = eio%event_n + 1
  eio%event_i = eio%event_n
  eio%i_prc = i_prc
  pset => event%get_particle_set_ptr ()
  prt = pset%get_particle (3)
  eio%event_p(1, eio%event_i) = prt%get_momentum ()
  prt = pset%get_particle (4)
  eio%event_p(2, eio%event_i) = prt%get_momentum ()
end subroutine eio_test_output

```

Input. Increment the event counter and retrieve the momenta of the current event. For the test case, we do not actually modify the current event.

```

(EIO base: eio test: TBP)+≡
procedure :: input_i_prc => eio_test_input_i_prc
procedure :: input_event => eio_test_input_event

(EIO base: test auxiliary)+≡
subroutine eio_test_input_i_prc (eio, i_prc, iostat)
  class(eio_test_t), intent(inout) :: eio
  integer, intent(out) :: i_prc
  integer, intent(out) :: iostat
  i_prc = eio%i_prc
  iostat = 0
end subroutine eio_test_input_i_prc

subroutine eio_test_input_event (eio, event, iostat, event_handle)
  class(eio_test_t), intent(inout) :: eio
  class(generic_event_t), intent(inout), target :: event
  integer, intent(out) :: iostat
  class(event_handle_t), intent(inout), optional :: event_handle
  eio%event_i = eio%event_i + 1
  iostat = 0
end subroutine eio_test_input_event

(EIO base: eio test: TBP)+≡
procedure :: skip => eio_test_skip

(EIO base: test auxiliary)+≡
subroutine eio_test_skip (eio, iostat)
  class(eio_test_t), intent(inout) :: eio
  integer, intent(out) :: iostat
  iostat = 0
end subroutine eio_test_skip

```

Test I/O methods

<EIO base: execute tests>≡

```
call test (eio_base_1, "eio_base_1", &
          "read and write event contents", &
          u, results)
```

<EIO base: test declarations>≡

```
public :: eio_base_1
```

<EIO base: tests>≡

```
subroutine eio_base_1 (u)
  integer, intent(in) :: u
  class(generic_event_t), pointer :: event
  class(eio_t), allocatable :: eio
  integer :: i_prc, iostat
  type(string_t) :: sample

  write (u, "(A)")  "* Test output: eio_base_1"
  write (u, "(A)")  "* Purpose: generate and read/write an event"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize test process"

  call eio_prepare_test (event, unweighted = .false.)

  write (u, "(A)")
  write (u, "(A)")  "* Generate and write an event"
  write (u, "(A)")

  sample = "eio_test1"

  allocate (eio_test_t :: eio)

  call eio%init_out (sample)
  call event%generate (1, [0._default, 0._default])
  call eio%output (event, 42)
  call eio%write (u)
  call eio%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Re-read the event"
  write (u, "(A)")

  call eio%init_in (sample)
  call eio%input_i_prc (i_prc, iostat)
  call eio%input_event (event, iostat)
  call eio%write (u)
  write (u, "(A)")
  write (u, "(1x,A,I0)")  "i = ", i_prc

  write (u, "(A)")
  write (u, "(A)")  "* Generate and append another event"
  write (u, "(A)")

  call eio%switch_inout ()
```

```

call event%generate (1, [0._default, 0._default])
call eio%output (event, 5)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* Re-read both events"
write (u, "(A)")

call eio%init_in (sample)
call eio%input_i_prc (i_prc, iostat)
call eio%input_event (event, iostat)
call eio%input_i_prc (i_prc, iostat)
call eio%input_event (event, iostat)
call eio%write (u)
write (u, "(A)")
write (u, "(1x,A,I0)")  "i = ", i_prc

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
deallocate (eio)

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_base_1"

end subroutine eio_base_1

```

18.5 Direct Event Access

As a convenient application of the base type, we construct an event handler that allows us of setting and retrieving events just in the same way as an file I/O format, but directly dealing with particle data and momenta. This is an input and output format, but we do not care about counting events.

`<eio_direct.f90>`≡
<File header>

```

module eio_direct

<Use kinds>
<Use strings>
  use io_units
  use diagnostics
  use cputime
  use lorentz, only: vector4_t
  use particles, only: particle_set_t
  use model_data, only: model_data_t
  use event_base

```

```

    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

```

<Standard module head>

<EIO direct: public>

<EIO direct: types>

contains

<EIO direct: procedures>

end module eio_direct

18.5.1 Type

<EIO direct: public>≡

```

    public :: eio_direct_t

```

<EIO direct: types>≡

```

    type, extends (eio_t) :: eio_direct_t

```

```

        private

```

```

            logical :: i_evt_set = .false.

```

```

            integer :: i_evt = 0

```

```

            integer :: i_prc = 0

```

```

            integer :: i_mci = 0

```

```

            integer :: i_term = 0

```

```

            integer :: channel = 0

```

```

            logical :: passed_set = .false.

```

```

            logical :: passed = .true.

```

```

            type(particle_set_t) :: pset

```

```

        contains

```

```

            <EIO direct: eio direct: TBP>

```

```

        end type eio_direct_t

```

18.5.2 Common Methods

Output.

<EIO direct: eio direct: TBP>≡

```

    procedure :: write => eio_direct_write

```

<EIO direct: procedures>≡

```

    subroutine eio_direct_write (object, unit)

```

```

        class(eio_direct_t), intent(in) :: object

```

```

        integer, intent(in), optional :: unit

```

```

        integer :: u

```

```

        u = given_output_unit (unit)

```

```

        write (u, "(1x,A)") "Event direct access:"

```

```

        if (object%i_evt_set) then

```

```

            write (u, "(3x,A,1x,I0)") "i_evt =", object%i_evt

```

```

        else

```



```

        write (u, "(3x,A)") "i_evt = [undefined]"
    end if
    write (u, "(3x,A,1x,I0)") "i_prc =", object%i_prc
    write (u, "(3x,A,1x,I0)") "i_mci =", object%i_prc
    write (u, "(3x,A,1x,I0)") "i_term =", object%i_prc
    write (u, "(3x,A,1x,I0)") "channel =", object%i_prc
    if (object%passed_set) then
        write (u, "(3x,A,1x,L1)") "passed =", object%passed
    else
        write (u, "(3x,A)") "passed = [N/A]"
    end if
    call object%pset%write (u)
end subroutine eio_direct_write

```

Finalizer: trivial.

```

(EIO direct: eio direct: TBP)+≡
    procedure :: final => eio_direct_final
(EIO direct: procedures)+≡
    subroutine eio_direct_final (object)
        class(eio_direct_t), intent(inout) :: object
        call object%pset%final ()
    end subroutine eio_direct_final

```

Initialize for input and/or output, both are identical

```

(EIO direct: eio direct: TBP)+≡
    procedure :: init_out => eio_direct_init_out
(EIO direct: procedures)+≡
    subroutine eio_direct_init_out (eio, sample, data, success, extension)
        class(eio_direct_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        if (present (success)) success = .true.
    end subroutine eio_direct_init_out

```

```

(EIO direct: eio direct: TBP)+≡
    procedure :: init_in => eio_direct_init_in
(EIO direct: procedures)+≡
    subroutine eio_direct_init_in (eio, sample, data, success, extension)
        class(eio_direct_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        if (present (success)) success = .true.
    end subroutine eio_direct_init_in

```

Switch from input to output: no-op

```

(EIO direct: eio direct: TBP)+≡
    procedure :: switch_inout => eio_direct_switch_inout

```

```

<EIO direct: procedures>+≡
  subroutine eio_direct_switch_inout (eio, success)
    class(eio_direct_t), intent(inout) :: eio
    logical, intent(out), optional :: success
    if (present (success)) success = .true.
  end subroutine eio_direct_switch_inout

```

Output: transfer event contents from the `event` object to the `eio` object. Note that finalization of the particle set is not (yet) automatic.

```

<EIO direct: eio direct: TBP>+≡
  procedure :: output => eio_direct_output

<EIO direct: procedures>+≡
  subroutine eio_direct_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_direct_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    integer, intent(in) :: i_prc
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    type(particle_set_t), pointer :: pset_ptr
    call eio%pset%final ()
    if (event%has_index ()) then
      call eio%set_event_index (event%get_index ())
    else
      call eio%reset_event_index ()
    end if
    if (present (passed)) then
      eio%passed = passed
      eio%passed_set = .true.
    else
      eio%passed_set = .false.
    end if
    pset_ptr => event%get_particle_set_ptr ()
    if (associated (pset_ptr)) then
      eio%i_prc = i_prc
      eio%pset = pset_ptr
    end if
  end subroutine eio_direct_output

```

Input: transfer event contents from the `eio` object to the `event` object. The `i_prc` parameter has been stored inside the `eio` record before.

```

<EIO direct: eio direct: TBP>+≡
  procedure :: input_i_prc => eio_direct_input_i_prc
  procedure :: input_event => eio_direct_input_event

<EIO direct: procedures>+≡
  subroutine eio_direct_input_i_prc (eio, i_prc, iostat)
    class(eio_direct_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
    i_prc = eio%i_prc
    iostat = 0
  end subroutine eio_direct_input_i_prc

```

```

subroutine eio_direct_input_event (eio, event, iostat, event_handle)
  class(eio_direct_t), intent(inout) :: eio
  class(generic_event_t), intent(inout), target :: event
  integer, intent(out) :: iostat
  class(event_handle_t), intent(inout), optional :: event_handle
  call event%select (eio%i_mci, eio%i_term, eio%channel)
  if (eio%has_event_index ()) then
    call event%set_index (eio%get_event_index ())
  else
    call event%reset_index ()
  end if
  call event%set_hard_particle_set (eio%pset)
end subroutine eio_direct_input_event

```

No-op.

```

<EIO direct: eio direct: TBP>+≡
  procedure :: skip => eio_direct_skip

<EIO direct: procedures>+≡
  subroutine eio_direct_skip (eio, iostat)
    class(eio_direct_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    iostat = 0
  end subroutine eio_direct_skip

```

18.5.3 Retrieve individual contents

```

<EIO direct: eio direct: TBP>+≡
  procedure :: has_event_index => eio_direct_has_event_index
  procedure :: get_event_index => eio_direct_get_event_index
  procedure :: passed_known => eio_direct_passed_known
  procedure :: has_passed => eio_direct_has_passed
  procedure :: get_n_in => eio_direct_get_n_in
  procedure :: get_n_out => eio_direct_get_n_out
  procedure :: get_n_tot => eio_direct_get_n_tot

<EIO direct: procedures>+≡
  function eio_direct_has_event_index (eio) result (flag)
    class(eio_direct_t), intent(in) :: eio
    logical :: flag
    flag = eio%i_evt_set
  end function eio_direct_has_event_index

  function eio_direct_get_event_index (eio) result (index)
    class(eio_direct_t), intent(in) :: eio
    integer :: index
    if (eio%has_event_index ()) then
      index = eio%i_evt
    else
      index = 0
    end if
  end function eio_direct_get_event_index

```

```

function eio_direct_passed_known (eio) result (flag)
  class(eio_direct_t), intent(in) :: eio
  logical :: flag
  flag = eio%pset%passed_set
end function eio_direct_passed_known

function eio_direct_has_passed (eio) result (flag)
  class(eio_direct_t), intent(in) :: eio
  logical :: flag
  if (eio%pset%passed_known ()) then
    flag = eio%pset%passed
  else
    flag = .true.
  end if
end function eio_direct_has_passed

function eio_direct_get_n_in (eio) result (n_in)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_in
  n_in = eio%pset%get_n_in ()
end function eio_direct_get_n_in

function eio_direct_get_n_out (eio) result (n_out)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_out
  n_out = eio%pset%get_n_out ()
end function eio_direct_get_n_out

function eio_direct_get_n_tot (eio) result (n_tot)
  class(eio_direct_t), intent(in) :: eio
  integer :: n_tot
  n_tot = eio%pset%get_n_tot ()
end function eio_direct_get_n_tot

```

All momenta as a single allocatable array.

```

<EIO direct: eio direct: TBP>+≡
  procedure :: get_momentum_array => eio_direct_get_momentum_array

<EIO direct: procedures>+≡
  subroutine eio_direct_get_momentum_array (eio, p)
    class(eio_direct_t), intent(in) :: eio
    type(vector4_t), dimension(:), allocatable, intent(out) :: p
    integer :: n
    n = eio%get_n_tot ()
    allocate (p (n))
    p(:) = eio%pset%get_momenta ()
  end subroutine eio_direct_get_momentum_array

```

18.5.4 Manual access

Build the contained particle set from scratch.

```

<EIO direct: eio direct: TBP>+≡

```

```

    procedure :: init_direct => eio_direct_init_direct
  <EIO direct: procedures>+≡
    subroutine eio_direct_init_direct &
      (eio, n_beam, n_in, n_rem, n_vir, n_out, pdg, model)
      class(eio_direct_t), intent(out) :: eio
      integer, intent(in) :: n_beam
      integer, intent(in) :: n_in
      integer, intent(in) :: n_rem
      integer, intent(in) :: n_vir
      integer, intent(in) :: n_out
      integer, dimension(:), intent(in) :: pdg
      class(model_data_t), intent(in), target :: model
      call eio%pset%init_direct (n_beam, n_in, n_rem, n_vir, n_out, pdg, model)
    end subroutine eio_direct_init_direct

```

Set/reset the event index, which is optional.

```

  <EIO direct: eio direct: TBP>+≡
    procedure :: set_event_index => eio_direct_set_event_index
    procedure :: reset_event_index => eio_direct_reset_event_index

  <EIO direct: procedures>+≡
    subroutine eio_direct_set_event_index (eio, index)
      class(eio_direct_t), intent(inout) :: eio
      integer, intent(in) :: index
      eio%i_evt = index
      eio%i_evt_set = .true.
    end subroutine eio_direct_set_event_index

    subroutine eio_direct_reset_event_index (eio)
      class(eio_direct_t), intent(inout) :: eio
      eio%i_evt_set = .false.
    end subroutine eio_direct_reset_event_index

```

Set the selection indices. This is supposed to select the `i_prc`, `i_mci`, `i_term`, and `channel` entries of the event where the momentum set has to be stored, respectively. The selection indices determine the process, MCI set, calculation term, and phase-space channel is to be used for recalculation. The index values must not be zero, even if they do not apply.

```

  <EIO direct: eio direct: TBP>+≡
    procedure :: set_selection_indices => eio_direct_set_selection_indices

  <EIO direct: procedures>+≡
    subroutine eio_direct_set_selection_indices &
      (eio, i_prc, i_mci, i_term, channel)
      class(eio_direct_t), intent(inout) :: eio
      integer, intent(in) :: i_prc
      integer, intent(in) :: i_mci
      integer, intent(in) :: i_term
      integer, intent(in) :: channel
      eio%i_prc = i_prc
      eio%i_mci = i_mci
      eio%i_term = i_term
      eio%channel = channel

```

```
end subroutine eio_direct_set_selection_indices
```

Set momentum (or momenta – elemental).

<EIO direct: eio direct: TBP>+≡

```
generic :: set_momentum => set_momentum_single
generic :: set_momentum => set_momentum_all
procedure :: set_momentum_single => eio_direct_set_momentum_single
procedure :: set_momentum_all => eio_direct_set_momentum_all
```

<EIO direct: procedures>+≡

```
subroutine eio_direct_set_momentum_single (eio, i, p, p2, on_shell)
  class(eio_direct_t), intent(inout) :: eio
  integer, intent(in) :: i
  type(vector4_t), intent(in) :: p
  real(default), intent(in), optional :: p2
  logical, intent(in), optional :: on_shell
  call eio%pset%set_momentum (i, p, p2, on_shell)
end subroutine eio_direct_set_momentum_single

subroutine eio_direct_set_momentum_all (eio, p, p2, on_shell)
  class(eio_direct_t), intent(inout) :: eio
  type(vector4_t), dimension(:), intent(in) :: p
  real(default), dimension(:), intent(in), optional :: p2
  logical, intent(in), optional :: on_shell
  call eio%pset%set_momentum (p, p2, on_shell)
end subroutine eio_direct_set_momentum_all
```

18.5.5 Unit tests

Test module, followed by the corresponding implementation module.

<eio_direct_ut.f90>≡

<File header>

```
module eio_direct_ut
  use unit_tests
  use eio_direct_util
```

<Standard module head>

<EIO direct: public test>

contains

<EIO direct: test driver>

```
end module eio_direct_ut
```

<eio_direct_util.f90>≡

<File header>

```
module eio_direct_util
```

<Use kinds>

```

    <Use strings>
    use lorentz, only: vector4_t
    use model_data, only: model_data_t
    use event_base
    use eio_data
    use eio_base

    use eio_direct

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO direct: test declarations>

contains

    <EIO direct: tests>

end module eio_direct_util

API: driver for the unit tests below.
<EIO direct: public test>≡
    public :: eio_direct_test
<EIO direct: test driver>≡
    subroutine eio_direct_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <EIO direct: execute tests>
    end subroutine eio_direct_test

```

Test I/O methods

We test the implementation of all I/O methods.

```

<EIO direct: execute tests>≡
    call test (eio_direct_1, "eio_direct_1", &
        "read and write event contents", &
        u, results)

<EIO direct: test declarations>≡
    public :: eio_direct_1

<EIO direct: tests>≡
    subroutine eio_direct_1 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        class(eio_t), allocatable :: eio
        type(event_sample_data_t) :: data
        type(string_t) :: sample
        type(vector4_t), dimension(:), allocatable :: p
        class(model_data_t), pointer :: model
        integer :: i, n_events, iostat, i_prc

        write (u, "(A)")  "* Test output: eio_direct_1"
    end subroutine eio_direct_1

```

```

write (u, "(A)")  "*" Purpose: generate and read/write an event"
write (u, "(A)")

write (u, "(A)")  "*" Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

write (u, "(A)")
write (u, "(A)")  "*" Initial state"
write (u, "(A)")

allocate (eio_direct_t :: eio)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "*" Extract an empty event"
write (u, "(A)")

call eio%output (event, 1)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "*" Retrieve contents"
write (u, "(A)")

select type (eio)
class is (eio_direct_t)
  if (eio%has_event_index ()) write (u, "(A,1x,I0)") "index =", eio%get_event_index ()
  if (eio%passed_known ()) write (u, "(A,1x,L1)") "passed =", eio%has_passed ()
  write (u, "(A,1x,I0)") "n_in =", eio%get_n_in ()
  write (u, "(A,1x,I0)") "n_out =", eio%get_n_out ()
end select

write (u, "(A)")
write (u, "(A)")  "*" Generate and extract an event"
write (u, "(A)")

call event%generate (1, [0._default, 0._default])
call event%set_index (42)
model => event%get_model_ptr ()

sample = ""
call eio%init_out (sample)
call eio%output (event, 1, passed = .true.)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "*" Retrieve contents"
write (u, "(A)")

select type (eio)
class is (eio_direct_t)
  if (eio%has_event_index ()) write (u, "(A,1x,I0)") "index =", eio%get_event_index ()
  if (eio%passed_known ()) write (u, "(A,1x,L1)") "passed =", eio%has_passed ()

```



```

        write (u, "(A,1x,I0)") "n_in =", eio%get_n_in ()
        write (u, "(A,1x,I0)") "n_out =", eio%get_n_out ()
    end select

    select type (eio)
    class is (eio_direct_t)
        call eio%get_momentum_array (p)
        if (allocated (p)) then
            write (u, "(A)") "p[3] ="
            call p(3)%write (u)
        end if
    end select

    write (u, "(A)")
    write (u, "(A)")  "* Re-create an eio event record: initialization"
    write (u, "(A)")

    call eio%final ()

    select type (eio)
    class is (eio_direct_t)
        call eio%init_direct ( &
            n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 2, &
            pdg = [25, 25, 25, 25], model = model)
        call eio%set_event_index (42)
        call eio%set_selection_indices (1, 1, 1, 1)
        call eio%write (u)
    end select

    write (u, "(A)")
    write (u, "(A)")  "* Re-create an eio event record: &
        &set momenta, interchanged"
    write (u, "(A)")

    select type (eio)
    class is (eio_direct_t)
        call eio%set_momentum (p([1,2,4,3]), on_shell=.true.)
        call eio%write (u)
    end select

    write (u, "(A)")
    write (u, "(A)")  "* 'read' i_prc"
    write (u, "(A)")

    call eio%input_i_prc (i_prc, iostat)
    write (u, "(1x,A,1x,I0)") "i_prc =", i_prc
    write (u, "(1x,A,1x,I0)") "iostat =", iostat

    write (u, "(A)")
    write (u, "(A)")  "* 'read' (fill) event"
    write (u, "(A)")

    call eio%input_event (event, iostat)
    write (u, "(1x,A,1x,I0)") "iostat =", iostat

```

```

write (u, "(A)")

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
deallocate (eio)

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_direct_1"

end subroutine eio_direct_1

```

18.6 Event Generation Checkpoints

This is an output-only format. Its only use is to write screen messages every n events, to inform the user about progress.

```

(eio_checkpoints.f90)≡
  <File header>

  module eio_checkpoints

    <Use strings>
    use io_units
    use diagnostics
    use cputime
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

    <Standard module head>

    <EIO checkpoints: public>

    <EIO checkpoints: parameters>

    <EIO checkpoints: types>

    contains

    <EIO checkpoints: procedures>

  end module eio_checkpoints

```

18.6.1 Type

```
<EIO checkpoints: public>≡
  public :: eio_checkpoints_t
<EIO checkpoints: types>≡
  type, extends (eio_t) :: eio_checkpoints_t
    logical :: active = .false.
    logical :: running = .false.
    integer :: val = 0
    integer :: n_events = 0
    integer :: n_read = 0
    integer :: i_evt = 0
    logical :: blank = .false.
    type(timer_t) :: timer
  contains
    <EIO checkpoints: eio checkpoints: TBP>
  end type eio_checkpoints_t
```

18.6.2 Specific Methods

Set parameters that are specifically used for checkpointing.

```
<EIO checkpoints: eio checkpoints: TBP>≡
  procedure :: set_parameters => eio_checkpoints_set_parameters
<EIO checkpoints: procedures>≡
  subroutine eio_checkpoints_set_parameters (eio, checkpoint, blank)
    class(eio_checkpoints_t), intent(inout) :: eio
    integer, intent(in) :: checkpoint
    logical, intent(in), optional :: blank
    eio%val = checkpoint
    if (present (blank)) eio%blank = blank
  end subroutine eio_checkpoints_set_parameters
```

18.6.3 Common Methods

Output. This is not the actual event format, but a readable account of the current status.

```
<EIO checkpoints: eio checkpoints: TBP>+≡
  procedure :: write => eio_checkpoints_write
<EIO checkpoints: procedures>+≡
  subroutine eio_checkpoints_write (object, unit)
    class(eio_checkpoints_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    if (object%active) then
      write (u, "(1x,A)") "Event-sample checkpoints: active"
      write (u, "(3x,A,I0)") "interval = ", object%val
      write (u, "(3x,A,I0)") "n_events = ", object%n_events
      write (u, "(3x,A,I0)") "n_read = ", object%n_read
```

```

        write (u, "(3x,A,I0)") "n_current = ", object%i_evt
        write (u, "(3x,A,L1)") "blanking = ", object%blank
        call object%timer%write (u)
    else
        write (u, "(1x,A)") "Event-sample checkpoints: off"
    end if
end subroutine eio_checkpoints_write

```

Finalizer: trivial.

```

<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: final => eio_checkpoints_final
<EIO checkpoints: procedures>+≡
    subroutine eio_checkpoints_final (object)
        class(eio_checkpoints_t), intent(inout) :: object
        object%active = .false.
    end subroutine eio_checkpoints_final

```

Activate checkpointing for event generation or writing.

```

<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: init_out => eio_checkpoints_init_out
<EIO checkpoints: procedures>+≡
    subroutine eio_checkpoints_init_out (eio, sample, data, success, extension)
        class(eio_checkpoints_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        if (present (data)) then
            if (eio%val > 0) then
                eio%active = .true.
                eio%i_evt = 0
                eio%n_read = 0
                eio%n_events = data%n_evt * data%nlo_multiplier
            end if
        end if
        if (present (success)) success = .true.
    end subroutine eio_checkpoints_init_out

```

No checkpointing for event reading.

```

<EIO checkpoints: eio checkpoints: TBP>+≡
    procedure :: init_in => eio_checkpoints_init_in
<EIO checkpoints: procedures>+≡
    subroutine eio_checkpoints_init_in (eio, sample, data, success, extension)
        class(eio_checkpoints_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        call msg_bug ("Event checkpoints: event input not supported")
        if (present (success)) success = .false.
    end subroutine eio_checkpoints_init_in

```

Switch from input to output: also not supported.

```
<EIO checkpoints: eio checkpoints: TBP>+≡
  procedure :: switch_inout => eio_checkpoints_switch_inout

<EIO checkpoints: procedures>+≡
  subroutine eio_checkpoints_switch_inout (eio, success)
    class(eio_checkpoints_t), intent(inout) :: eio
    logical, intent(out), optional :: success
    call msg_bug ("Event checkpoints: in-out switch not supported")
    if (present (success)) success = .false.
  end subroutine eio_checkpoints_switch_inout
```

Checkpoints: display progress for the current event, if applicable.

```
<EIO checkpoints: eio checkpoints: TBP>+≡
  procedure :: output => eio_checkpoints_output

<EIO checkpoints: procedures>+≡
  subroutine eio_checkpoints_output &
    (eio, event, i_prc, reading, passed, pacify, event_handle)
    class(eio_checkpoints_t), intent(inout) :: eio
    class(generic_event_t), intent(in), target :: event
    integer, intent(in) :: i_prc
    logical, intent(in), optional :: reading, passed, pacify
    class(event_handle_t), intent(inout), optional :: event_handle
    logical :: rd
    rd = .false.; if (present (reading)) rd = reading
    if (eio%active) then
      if (.not. eio%running) call eio%startup ()
      if (eio%running) then
        eio%i_evt = eio%i_evt + 1
        if (rd) then
          eio%n_read = eio%n_read + 1
        else if (mod (eio%i_evt, eio%val) == 0) then
          call eio%message (eio%blank)
        end if
        if (eio%i_evt == eio%n_events) call eio%shutdown ()
      end if
    end if
  end subroutine eio_checkpoints_output
```

When the first event is called, we have to initialize the screen output.

```
<EIO checkpoints: eio checkpoints: TBP>+≡
  procedure :: startup => eio_checkpoints_startup

<EIO checkpoints: procedures>+≡
  subroutine eio_checkpoints_startup (eio)
    class(eio_checkpoints_t), intent(inout) :: eio
    if (eio%active .and. eio%i_evt < eio%n_events) then
      call msg_message ("")
      call msg_message (checkpoint_bar)
      call msg_message (checkpoint_head)
      call msg_message (checkpoint_bar)
      write (msg_buffer, checkpoint_fmt) 0., 0, eio%n_events - eio%i_evt, "???"
      call msg_message ()
    end if
  end subroutine eio_checkpoints_startup
```

```

        eio%running = .true.
        call eio%timer%start ()
    end if
end subroutine eio_checkpoints_startup

```

This message is printed at every checkpoint.

```

(EIO checkpoints: eio checkpoints: TBP)+≡
    procedure :: message => eio_checkpoints_message

(EIO checkpoints: procedures)+≡
    subroutine eio_checkpoints_message (eio, testflag)
        class(eio_checkpoints_t), intent(inout) :: eio
        logical, intent(in), optional :: testflag
        real :: t
        type(time_t) :: time_remaining
        type(string_t) :: time_string
        call eio%timer%stop ()
        t = eio%timer
        call eio%timer%restart ()
        time_remaining = &
            nint (t / (eio%i_evt - eio%n_read) * (eio%n_events - eio%i_evt))
        time_string = time_remaining%to_string_ms (blank = testflag)
        write (msg_buffer, checkpoint_fmt) &
            100 * (eio%i_evt - eio%n_read) / real (eio%n_events - eio%n_read), &
            eio%i_evt - eio%n_read, &
            eio%n_events - eio%i_evt, &
            char (time_string)
        call msg_message ()
    end subroutine eio_checkpoints_message

```

When the last event is called, wrap up.

```

(EIO checkpoints: eio checkpoints: TBP)+≡
    procedure :: shutdown => eio_checkpoints_shutdown

(EIO checkpoints: procedures)+≡
    subroutine eio_checkpoints_shutdown (eio)
        class(eio_checkpoints_t), intent(inout) :: eio
        if (mod (eio%i_evt, eio%val) /= 0) then
            write (msg_buffer, checkpoint_fmt) &
                100., eio%i_evt - eio%n_read, 0, "0m:00s"
            call msg_message ()
        end if
        call msg_message (checkpoint_bar)
        call msg_message ("")
        eio%running = .false.
    end subroutine eio_checkpoints_shutdown

```

```

(EIO checkpoints: eio checkpoints: TBP)+≡
    procedure :: input_i_prc => eio_checkpoints_input_i_prc
    procedure :: input_event => eio_checkpoints_input_event

(EIO checkpoints: procedures)+≡
    subroutine eio_checkpoints_input_i_prc (eio, i_prc, iostat)
        class(eio_checkpoints_t), intent(inout) :: eio

```

```

integer, intent(out) :: i_prc
integer, intent(out) :: iostat
call msg_bug ("Event checkpoints: event input not supported")
i_prc = 0
iostat = 1
end subroutine eio_checkpoints_input_i_prc

subroutine eio_checkpoints_input_event (eio, event, iostat, event_handle)
class(eio_checkpoints_t), intent(inout) :: eio
class(generic_event_t), intent(inout), target :: event
integer, intent(out) :: iostat
class(event_handle_t), intent(inout), optional :: event_handle
call msg_bug ("Event checkpoints: event input not supported")
iostat = 1
end subroutine eio_checkpoints_input_event

<EIO checkpoints: eio checkpoints: TBP>+≡
procedure :: skip => eio_checkpoints_skip

<EIO checkpoints: procedures>+≡
subroutine eio_checkpoints_skip (eio, iostat)
class(eio_checkpoints_t), intent(inout) :: eio
integer, intent(out) :: iostat
iostat = 0
end subroutine eio_checkpoints_skip

```

18.6.4 Message header

```

<EIO checkpoints: parameters>≡
character(*), parameter :: &
checkpoint_head = "| % complete | events generated | events remaining &
&| time remaining"
character(*), parameter :: &
checkpoint_bar = "|=====
&=====|"
character(*), parameter :: &
checkpoint_fmt = "(' ',F5.1,T16,I9,T35,I9,T58,A)"

```

18.6.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<eio_checkpoints_ut.f90>≡
<File header>

module eio_checkpoints_ut
use unit_tests
use eio_checkpoints_util

<Standard module head>

<EIO checkpoints: public test>

```

```

contains

  <EIO checkpoints: test driver>

  end module eio_checkpoints_ut

  <eio_checkpoints_util.f90>≡
  <File header>

  module eio_checkpoints_util

    <Use kinds>
    <Use strings>
    use event_base
    use eio_data
    use eio_base

    use eio_checkpoints

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO checkpoints: test declarations>

contains

  <EIO checkpoints: tests>

  end module eio_checkpoints_util
API: driver for the unit tests below.
  <EIO checkpoints: public test>≡
    public :: eio_checkpoints_test
  <EIO checkpoints: test driver>≡
    subroutine eio_checkpoints_test (u, results)
      integer, intent(in) :: u
      type(test_results_t), intent(inout) :: results
    <EIO checkpoints: execute tests>
    end subroutine eio_checkpoints_test

```

Test I/O methods

We test the implementation of all I/O methods.

```

  <EIO checkpoints: execute tests>≡
    call test (eio_checkpoints_1, "eio_checkpoints_1", &
      "read and write event contents", &
      u, results)

  <EIO checkpoints: test declarations>≡
    public :: eio_checkpoints_1

```



```

(EIO checkpoints: tests)≡
subroutine eio_checkpoints_1 (u)
  integer, intent(in) :: u
  class(generic_event_t), pointer :: event
  class(eio_t), allocatable :: eio
  type(event_sample_data_t) :: data
  type(string_t) :: sample
  integer :: i, n_events

  write (u, "(A)")  "* Test output: eio_checkpoints_1"
  write (u, "(A)")  "* Purpose: generate a number of events &
    &with screen output"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize test process"

  call eio_prepare_test (event)

  write (u, "(A)")
  write (u, "(A)")  "* Generate events"
  write (u, "(A)")

  sample = "eio_checkpoints_1"

  allocate (eio_checkpoints_t :: eio)

  n_events = 10
  call data%init (1, 0)
  data%n_evt = n_events

  select type (eio)
  type is (eio_checkpoints_t)
    call eio%set_parameters (checkpoint = 4)
  end select

  call eio%init_out (sample, data)

  do i = 1, n_events
    call event%generate (1, [0._default, 0._default])
    call eio%output (event, i_prc = 0)
  end do

  write (u, "(A)")  "* Checkpointing status"
  write (u, "(A)")

  call eio%write (u)
  call eio%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

  call eio_cleanup_test (event)

  write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: eio_checkpoints_1"

    end subroutine eio_checkpoints_1

```

18.7 Event Generation Callback

This is an output-only format. Its only use is to write screen messages every n events, to inform the user about progress.

```

<eio_callback.f90>≡
  <File header>

  module eio_callback

    use kinds, only: i64
    <Use strings>
    use io_units
    use diagnostics
    use cputime
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

    <Standard module head>

    <EIO callback: public>

    <EIO callback: types>

    contains

    <EIO callback: procedures>

  end module eio_callback

```

18.7.1 Type

```

<EIO callback: public>≡
  public :: eio_callback_t

<EIO callback: types>≡
  type, extends (eio_t) :: eio_callback_t
    class(event_callback_t), allocatable :: callback
    integer(i64) :: i_evt = 0
    integer :: i_interval = 0
    integer :: n_interval = 0
  !   type(timer_t) :: timer
  contains
    <EIO callback: eio callback: TBP>
  end type eio_callback_t

```

18.7.2 Specific Methods

Set parameters that are specifically used for callback: the procedure and the number of events to wait until the procedure is called (again).

```
<EIO callback: eio callback: TBP>≡
  procedure :: set_parameters => eio_callback_set_parameters

<EIO callback: procedures>≡
  subroutine eio_callback_set_parameters (eio, callback, count_interval)
    class(eio_callback_t), intent(inout) :: eio
    class(event_callback_t), intent(in) :: callback
    integer, intent(in) :: count_interval
    allocate (eio%callback, source = callback)
    eio%n_interval = count_interval
  end subroutine eio_callback_set_parameters
```

18.7.3 Common Methods

Output. This is not the actual event format, but a readable account of the current status.

```
<EIO callback: eio callback: TBP>+≡
  procedure :: write => eio_callback_write

<EIO callback: procedures>+≡
  subroutine eio_callback_write (object, unit)
    class(eio_callback_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event-sample callback:"
    write (u, "(3x,A,I0)") "interval = ", object%n_interval
    write (u, "(3x,A,I0)") "evt count = ", object%i_evt
    !      call object%timer%write (u)
  end subroutine eio_callback_write
```

Finalizer: trivial.

```
<EIO callback: eio callback: TBP>+≡
  procedure :: final => eio_callback_final

<EIO callback: procedures>+≡
  subroutine eio_callback_final (object)
    class(eio_callback_t), intent(inout) :: object
  end subroutine eio_callback_final
```

Activate checkpointing for event generation or writing.

```
<EIO callback: eio callback: TBP>+≡
  procedure :: init_out => eio_callback_init_out

<EIO callback: procedures>+≡
  subroutine eio_callback_init_out (eio, sample, data, success, extension)
    class(eio_callback_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension
```

```

    type(event_sample_data_t), intent(in), optional :: data
    logical, intent(out), optional :: success
    eio%i_evt = 0
    ei0%i_interval = 0
    if (present (success)) success = .true.
end subroutine eio_callback_init_out

```

No callback for event reading.

```

<EIO callback: eio callback: TBP>+≡
    procedure :: init_in => eio_callback_init_in

<EIO callback: procedures>+≡
    subroutine eio_callback_init_in (eio, sample, data, success, extension)
        class(eio_callback_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        call msg_bug ("Event callback: event input not supported")
        if (present (success)) success = .false.
    end subroutine eio_callback_init_in

```

Switch from input to output: also not supported.

```

<EIO callback: eio callback: TBP>+≡
    procedure :: switch_inout => eio_callback_switch_inout

<EIO callback: procedures>+≡
    subroutine eio_callback_switch_inout (eio, success)
        class(eio_callback_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("Event callback: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_callback_switch_inout

```

The actual callback. First increment counters, then call the procedure if the counter hits the interval.

```

<EIO callback: eio callback: TBP>+≡
    procedure :: output => eio_callback_output

<EIO callback: procedures>+≡
    subroutine eio_callback_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_callback_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        eio%i_evt = eio%i_evt + 1
        if (eio%n_interval > 0) then
            eio%i_interval = eio%i_interval + 1
            if (eio%i_interval >= eio%n_interval) then
                call eio%callback%proc (eio%i_evt, event)
                eio%i_interval = 0
            end if
        end if
    end subroutine eio_callback_output

```

```

        end if
    end if
end subroutine eio_callback_output

```

No input.

```

<EIO callback: eio callback: TBP>+≡
    procedure :: input_i_prc => eio_callback_input_i_prc
    procedure :: input_event => eio_callback_input_event

<EIO callback: procedures>+≡
    subroutine eio_callback_input_i_prc (eio, i_prc, iostat)
        class(eio_callback_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        call msg_bug ("Event callback: event input not supported")
        i_prc = 0
        iostat = 1
    end subroutine eio_callback_input_i_prc

    subroutine eio_callback_input_event (eio, event, iostat, event_handle)
        class(eio_callback_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
        call msg_bug ("Event callback: event input not supported")
        iostat = 1
    end subroutine eio_callback_input_event

<EIO callback: eio callback: TBP>+≡
    procedure :: skip => eio_callback_skip

<EIO callback: procedures>+≡
    subroutine eio_callback_skip (eio, iostat)
        class(eio_callback_t), intent(inout) :: eio
        integer, intent(out) :: iostat
        iostat = 0
    end subroutine eio_callback_skip

```

18.8 Event Weight Output

This is an output-only format. For each event, we print the indices that identify process, process part (MCI group), and term. As numerical information we print the squared matrix element (trace) and the event weight.

```

<eio_weights.f90>≡
    <File header>

    module eio_weights

        <Use kinds>
        <Use strings>
        use io_units

```

```

    use diagnostics
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

    <Standard module head>

    <EIO weights: public>

    <EIO weights: types>

    contains

    <EIO weights: procedures>

    end module eio_weights

```

18.8.1 Type

```

<EIO weights: public>≡
    public :: eio_weights_t
<EIO weights: types>≡
    type, extends (eio_t) :: eio_weights_t
        logical :: writing = .false.
        integer :: unit = 0
        logical :: pacify = .false.
    contains
        <EIO weights: eio weights: TBP>
    end type eio_weights_t

```

18.8.2 Specific Methods

Set pacify flags.

```

<EIO weights: eio weights: TBP>≡
    procedure :: set_parameters => eio_weights_set_parameters
<EIO weights: procedures>≡
    subroutine eio_weights_set_parameters (eio, pacify)
        class(eio_weights_t), intent(inout) :: eio
        logical, intent(in), optional :: pacify
        if (present (pacify)) eio%pacify = pacify
        eio%extension = "weights.dat"
    end subroutine eio_weights_set_parameters

```

18.8.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO weights: eio weights: TBP>+≡
    procedure :: write => eio_weights_write

```

```

<EIO weights: procedures>+≡
subroutine eio_weights_write (object, unit)
  class(eio_weights_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Weight stream:"
  if (object%writing) then
    write (u, "(3x,A,A)") "Writing to file  = ", char (object%filename)
    write (u, "(3x,A,L1)") "Reduced I/O prec. = ", object%pacify
  else
    write (u, "(3x,A)") "[closed]"
  end if
end subroutine eio_weights_write

```

Finalizer: close any open file.

```

<EIO weights: eio weights: TBP>+≡
procedure :: final => eio_weights_final

<EIO weights: procedures>+≡
subroutine eio_weights_final (object)
  class(eio_weights_t), intent(inout) :: object
  if (object%writing) then
    write (msg_buffer, "(A,A,A)") "Events: closing weight stream file '", &
      char (object%filename), "'"
    call msg_message ()
    close (object%unit)
    object%writing = .false.
  end if
end subroutine eio_weights_final

```

Initialize event writing.

```

<EIO weights: eio weights: TBP>+≡
procedure :: init_out => eio_weights_init_out

<EIO weights: procedures>+≡
subroutine eio_weights_init_out (eio, sample, data, success, extension)
  class(eio_weights_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(in), optional :: data
  logical, intent(out), optional :: success
  if (present(extension)) then
    eio%extension = extension
  else
    eio%extension = "weights.dat"
  end if
  eio%filename = sample // "." // eio%extension
  eio%unit = free_unit ()
  write (msg_buffer, "(A,A,A)") "Events: writing to weight stream file '", &
    char (eio%filename), "'"
  call msg_message ()
  eio%writing = .true.
  open (eio%unit, file = char (eio%filename), &

```

```

        action = "write", status = "replace")
    if (present (success)) success = .true.
end subroutine eio_weights_init_out

```

Initialize event reading.

```

<EIO weights: eio weights: TBP>+≡
    procedure :: init_in => eio_weights_init_in

<EIO weights: procedures>+≡
    subroutine eio_weights_init_in (eio, sample, data, success, extension)
        class(eio_weights_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        call msg_bug ("Weight stream: event input not supported")
        if (present (success)) success = .false.
    end subroutine eio_weights_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO weights: eio weights: TBP>+≡
    procedure :: switch_inout => eio_weights_switch_inout

<EIO weights: procedures>+≡
    subroutine eio_weights_switch_inout (eio, success)
        class(eio_weights_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("Weight stream: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_weights_switch_inout

```

Output an event. Write first the event indices, then weight and two values of the squared matrix element: `sqme_ref` is the value stored in the event record, and `sqme_prc` is the one stored in the process instance. (They can differ: when recalculating, the former is read from file and the latter is the result of the new calculation.)

For the alternative entries, the `sqme` value is always obtained by a new calculation, and thus qualifies as `sqme_prc`.

Don't write the file if the `passed` flag is set and false.

```

<EIO weights: eio weights: TBP>+≡
    procedure :: output => eio_weights_output

<EIO weights: procedures>+≡
    subroutine eio_weights_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_weights_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        integer :: n_alt, i
        real(default) :: weight, sqme_ref, sqme_prc
        logical :: evt_pacify, evt_passed

```



```

    evt_pacify = eio%pacify; if (present (pacify)) evt_pacify = pacify
    evt_passed = .true.; if (present (passed)) evt_passed = passed
    if (eio%writing) then
        if (evt_passed) then
            weight = event%get_weight_prc ()
            sqme_ref = event%get_sqme_ref ()
            sqme_prc = event%get_sqme_prc ()
            n_alt = event%get_n_alt ()
1         format (I0,3(1x,ES17.10),3(1x,I0))
2         format (I0,3(1x,ES15.8),3(1x,I0))
            if (evt_pacify) then
                write (eio%unit, 2) 0, weight, sqme_prc, sqme_ref, &
                    i_prc
            else
                write (eio%unit, 1) 0, weight, sqme_prc, sqme_ref, &
                    i_prc
            end if
            do i = 1, n_alt
                weight = event%get_weight_alt(i)
                sqme_prc = event%get_sqme_alt(i)
                if (evt_pacify) then
                    write (eio%unit, 2) i, weight, sqme_prc
                else
                    write (eio%unit, 1) i, weight, sqme_prc
                end if
            end do
        end if
    else
        call eio%write ()
        call msg_fatal ("Weight stream file is not open for writing")
    end if
end subroutine eio_weights_output

```

Input an event.

(EIO weights: eio weights: TBP)+≡

```

    procedure :: input_i_prc => eio_weights_input_i_prc
    procedure :: input_event => eio_weights_input_event

```

(EIO weights: procedures)+≡

```

subroutine eio_weights_input_i_prc (eio, i_prc, iostat)
    class(eio_weights_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
    call msg_bug ("Weight stream: event input not supported")
    i_prc = 0
    iostat = 1
end subroutine eio_weights_input_i_prc

subroutine eio_weights_input_event (eio, event, iostat, event_handle)
    class(eio_weights_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    call msg_bug ("Weight stream: event input not supported")

```

```

        iostat = 1
    end subroutine eio_weights_input_event

    <EIO weights: eio weights: TBP>+≡
        procedure :: skip => eio_weights_skip

    <EIO weights: procedures>+≡
        subroutine eio_weights_skip (eio, iostat)
            class(eio_weights_t), intent(inout) :: eio
            integer, intent(out) :: iostat
            iostat = 0
        end subroutine eio_weights_skip

```

18.8.4 Unit tests

Test module, followed by the corresponding implementation module.

```

<eio_weights_ut.f90>≡
    <File header>

    module eio_weights_ut
        use unit_tests
        use eio_weights_uti

    <Standard module head>

    <EIO weights: public test>

    contains

    <EIO weights: test driver>

    end module eio_weights_ut

<eio_weights_uti.f90>≡
    <File header>

    module eio_weights_uti

    <Use kinds>
    <Use strings>
        use io_units
        use event_base
        use eio_data
        use eio_base

        use eio_weights

        use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO weights: test declarations>

```

contains

<EIO weights: tests>

end module eio_weights_util

API: driver for the unit tests below.

<EIO weights: public test>≡

public :: eio_weights_test

<EIO weights: test driver>≡

subroutine eio_weights_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<EIO weights: execute tests>

end subroutine eio_weights_test

Simple event

We test the implementation of all I/O methods.

<EIO weights: execute tests>≡

call test (eio_weights_1, "eio_weights_1", &
"read and write event contents", &
u, results)

<EIO weights: test declarations>≡

public :: eio_weights_1

<EIO weights: tests>≡

subroutine eio_weights_1 (u)

integer, intent(in) :: u

class(generic_event_t), pointer :: event

class(eio_t), allocatable :: eio

type(string_t) :: sample

integer :: u_file

character(80) :: buffer

write (u, "(A)") "* Test output: eio_weights_1"

write (u, "(A)") "* Purpose: generate an event and write weight to file"

write (u, "(A)")

write (u, "(A)") "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

write (u, "(A)")

write (u, "(A)") "* Generate and write an event"

write (u, "(A)")

sample = "eio_weights_1"

allocate (eio_weights_t :: eio)

call eio%init_out (sample)

call event%generate (1, [0._default, 0._default])

```

call eio%output (event, i_prc = 42)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents: &
    &(weight, sqme(evt), sqme(prc), i_prc)"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "eio_weights_1.weights.dat", &
    action = "read", status = "old")
read (u_file, "(A)") buffer
write (u, "(A)") trim (buffer)
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_weights_1"
end subroutine eio_weights_1

```

Multiple weights

Event with several weight entries set.

```

<EIO weights: execute tests>+≡
    call test (eio_weights_2, "eio_weights_2", &
        "multiple weights", &
        u, results)

<EIO weights: test declarations>+≡
    public :: eio_weights_2

<EIO weights: tests>+≡
    subroutine eio_weights_2 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, i
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_weights_2"
        write (u, "(A)")  "* Purpose: generate an event and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false., n_alt = 2)

```

```

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_weights_2"

allocate (eio_weights_t :: eio)

call eio%init_out (sample)
select type (eio)
type is (eio_weights_t)
    call eio%set_parameters (pacify = .true.)
end select
call event%generate (1, [0._default, 0._default])
call event%set (sqme_alt = [2._default, 3._default])
call event%set (weight_alt = &
    [2 * event%get_weight_prc (), 3 * event%get_weight_prc ()])

call eio%output (event, i_prc = 42)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents: &
    &(weight, sqme(evt), sqme(prc), i_prc)"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "eio_weights_2.weights.dat", &
    action = "read", status = "old")
do i = 1, 3
    read (u_file, "(A)") buffer
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_weights_2"

end subroutine eio_weights_2

```

Multiple events

Events with passed flag switched on/off.

(EIO weights: execute tests)+≡

```

call test (eio_weights_3, "eio_weights_3", &
    "check passed-flag", &
    u, results)

```

```

<EIO weights: test declarations>+=
    public :: eio_weights_3

<EIO weights: tests>+=
    subroutine eio_weights_3 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_weights_3"
        write (u, "(A)")  "*   Purpose: generate three events and write to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write events"
        write (u, "(A)")

        sample = "eio_weights_3"

        allocate (eio_weights_t :: eio)
        select type (eio)
        type is (eio_weights_t)
            call eio%set_parameters (pacify = .true.)
        end select

        call eio%init_out (sample)

        call event%generate (1, [0._default, 0._default])
        call eio%output (event, i_prc = 1)

        call event%generate (1, [0.1_default, 0._default])
        call eio%output (event, i_prc = 1, passed = .false.)

        call event%generate (1, [0.2_default, 0._default])
        call eio%output (event, i_prc = 1, passed = .true.)

        call eio%write (u)
        call eio%final ()

        write (u, "(A)")
        write (u, "(A)")  "* File contents: &
            &(weight, sqme(evt), sqme(prc), i_prc), should be just two entries"
        write (u, "(A)")

        u_file = free_unit ()
        open (u_file, file = "eio_weights_3.weights.dat", &
            action = "read", status = "old")
    do

```

```

        read (u_file, "(A)", iostat=iostat) buffer
        if (iostat /= 0) exit
        write (u, "(A)") trim (buffer)
    end do
    close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_weights_3"
end subroutine eio_weights_3

```

18.9 Event Dump Output

This is an output-only format. We simply dump the contents of the `particle_set`, using the `write` method of that type. The event-format options are the options of that procedure.

$\langle \text{eio_dump.f90} \rangle \equiv$
 $\langle \text{File header} \rangle$

```

module eio_dump

    use, intrinsic :: iso_fortran_env, only: output_unit

    use kinds, only: i64
 $\langle \text{Use strings} \rangle$ 
    use format_utils, only: write_separator
    use format_utils, only: pac_fmt
    use format_defs, only: FMT_16, FMT_19
    use io_units
    use diagnostics
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base

 $\langle \text{Standard module head} \rangle$ 

 $\langle \text{EIO dump: public} \rangle$ 

 $\langle \text{EIO dump: types} \rangle$ 

contains

 $\langle \text{EIO dump: procedures} \rangle$ 

end module eio_dump

```

18.9.1 Type

```
<EIO dump: public>≡
    public :: eio_dump_t

<EIO dump: types>≡
    type, extends (eio_t) :: eio_dump_t
        integer(i64) :: count = 0
        integer :: unit = 0
        logical :: writing = .false.
        logical :: screen = .false.
        logical :: pacify = .false.
        logical :: weights = .false.
        logical :: compressed = .false.
        logical :: summary = .false.
    contains
        <EIO dump: eio dump: TBP>
    end type eio_dump_t
```

18.9.2 Specific Methods

Set control parameters. We may provide a `unit` for input or output; this will be taken if the sample file name is empty. In that case, the unit is assumed to be open and will be kept open; no messages will be issued.

```
<EIO dump: eio dump: TBP>≡
    procedure :: set_parameters => eio_dump_set_parameters

<EIO dump: procedures>≡
    subroutine eio_dump_set_parameters (eio, extension, &
        pacify, weights, compressed, summary, screen, unit)
        class(eio_dump_t), intent(inout) :: eio
        type(string_t), intent(in), optional :: extension
        logical, intent(in), optional :: pacify
        logical, intent(in), optional :: weights
        logical, intent(in), optional :: compressed
        logical, intent(in), optional :: summary
        logical, intent(in), optional :: screen
        integer, intent(in), optional :: unit
        if (present (pacify)) eio%pacify = pacify
        if (present (weights)) eio%weights = weights
        if (present (compressed)) eio%compressed = compressed
        if (present (summary)) eio%summary = summary
        if (present (screen)) eio%screen = screen
        if (present (unit)) eio%unit = unit
        eio%extension = "pset.dat"
        if (present (extension)) eio%extension = extension
    end subroutine eio_dump_set_parameters
```

18.9.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.


```

<EIO dump: eio dump: TBP>+≡
  procedure :: write => eio_dump_write

<EIO dump: procedures>+≡
  subroutine eio_dump_write (object, unit)
    class(eio_dump_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Dump event stream:"
    if (object%writing) then
      write (u, "(3x,A,L1)") "Screen output      = ", object%screen
      write (u, "(3x,A,A,A)") "Writing to file   = '", char (object%filename), "'"
      write (u, "(3x,A,L1)") "Reduced I/O prec. = ", object%pacify
      write (u, "(3x,A,L1)") "Show weights/sqme = ", object%weights
      write (u, "(3x,A,L1)") "Compressed       = ", object%compressed
      write (u, "(3x,A,L1)") "Summary          = ", object%summary
    else
      write (u, "(3x,A)") "[closed]"
    end if
  end if
end subroutine eio_dump_write

```

Finalizer: close any open file.

```

<EIO dump: eio dump: TBP>+≡
  procedure :: final => eio_dump_final

<EIO dump: procedures>+≡
  subroutine eio_dump_final (object)
    class(eio_dump_t), intent(inout) :: object
    if (object%screen) then
      write (msg_buffer, "(A,A,A)") "Events: display complete"
      call msg_message ()
      object%screen = .false.
    end if
    if (object%writing) then
      if (object%filename /= "") then
        write (msg_buffer, "(A,A,A)") "Events: closing event dump file '", &
          char (object%filename), "'"
        call msg_message ()
        close (object%unit)
      end if
      object%writing = .false.
    end if
  end subroutine eio_dump_final

```

Initialize event writing.

```

<EIO dump: eio dump: TBP>+≡
  procedure :: init_out => eio_dump_init_out

<EIO dump: procedures>+≡
  subroutine eio_dump_init_out (eio, sample, data, success, extension)
    class(eio_dump_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(string_t), intent(in), optional :: extension

```

```

type(event_sample_data_t), intent(in), optional :: data
logical, intent(out), optional :: success
if (present(extension)) then
    eio%extension = extension
else
    eio%extension = "pset.dat"
end if
if (sample == "" .and. eio%unit /= 0) then
    eio%filename = ""
    eio%writing = .true.
else if (sample /= "") then
    eio%filename = sample // "." // eio%extension
    eio%unit = free_unit ()
    write (msg_buffer, "(A,A,A)") "Events: writing to event dump file '", &
        char (eio%filename), "'"
    call msg_message ()
    eio%writing = .true.
    open (eio%unit, file = char (eio%filename), &
        action = "write", status = "replace")
end if
if (eio%screen) then
    write (msg_buffer, "(A,A,A)") "Events: display on standard output"
    call msg_message ()
end if
eio%count = 0
if (present (success)) success = .true.
end subroutine eio_dump_init_out

```

Initialize event reading.

```

<EIO dump: eio dump: TBP>+≡
    procedure :: init_in => eio_dump_init_in

<EIO dump: procedures>+≡
    subroutine eio_dump_init_in (eio, sample, data, success, extension)
        class(eio_dump_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        call msg_bug ("Event dump: event input not supported")
        if (present (success)) success = .false.
    end subroutine eio_dump_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO dump: eio dump: TBP>+≡
    procedure :: switch_inout => eio_dump_switch_inout

<EIO dump: procedures>+≡
    subroutine eio_dump_switch_inout (eio, success)
        class(eio_dump_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("Event dump: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_dump_switch_inout

```

Output an event. Delegate the output call to the `write` method of the current particle set, if valid. Output both to file (if defined) and to screen (if requested).

(EIO dump: eio dump: TBP)+≡

```
procedure :: output => eio_dump_output
```

(EIO dump: procedures)+≡

```
subroutine eio_dump_output &
  (eio, event, i_prc, reading, passed, pacify, event_handle)
  class(eio_dump_t), intent(inout) :: eio
  class(generic_event_t), intent(in), target :: event
  integer, intent(in) :: i_prc
  logical, intent(in), optional :: reading, passed, pacify
  class(event_handle_t), intent(inout), optional :: event_handle
  character(len=7) :: fmt
  eio%count = eio%count + 1
  if (present (pacify)) then
    call pac_fmt (fmt, FMT_19, FMT_16, pacify)
  else
    call pac_fmt (fmt, FMT_19, FMT_16, eio%pacify)
  end if
  if (eio%writing) call dump (eio%unit)
  if (eio%screen) then
    call dump (output_unit)
    if (logfile_unit () > 0) call dump (logfile_unit ())
  end if
contains
  subroutine dump (u)
    integer, intent(in) :: u
    integer :: i
    call write_separator (u, 2)
    write (u, "(1x,A,I0)", advance="no") "Event"
    if (event%has_index ()) then
      write (u, "(1x,'#',I0)") event%get_index ()
    else
      write (u, *)
    end if
    call write_separator (u, 2)
    write (u, "(1x,A,1x,I0)") "count =", eio%count
    if (present (passed)) then
      write (u, "(1x,A,1x,L1)") "passed =", passed
    else
      write (u, "(1x,A)") "passed = [N/A]"
    end if
    write (u, "(1x,A,1x,I0)") "prc id =", i_prc
    if (eio%weights) then
      call write_separator (u)
      if (event%sqme_ref_known) then
        write (u, "(1x,A," // fmt // ")") "sqme (ref)  = ", &
          event%sqme_ref
      else
        write (u, "(1x,A)") "sqme (ref)  = [undefined]"
      end if
      if (event%sqme_prc_known) then
```

```

        write (u, "(1x,A," // fmt // ")") "sqme (prc) = ", &
            event%sqme_prc
    else
        write (u, "(1x,A)") "sqme (prc) = [undefined]"
    end if
    if (event%weight_ref_known) then
        write (u, "(1x,A," // fmt // ")") "weight (ref) = ", &
            event%weight_ref
    else
        write (u, "(1x,A)") "weight (ref) = [undefined]"
    end if
    if (event%weight_prc_known) then
        write (u, "(1x,A," // fmt // ")") "weight (prc) = ", &
            event%weight_prc
    else
        write (u, "(1x,A)") "weight (prc) = [undefined]"
    end if
    if (event%excess_prc_known) then
        write (u, "(1x,A," // fmt // ")") "excess (prc) = ", &
            event%excess_prc
    else
        write (u, "(1x,A)") "excess (prc) = [undefined]"
    end if
    do i = 1, event%n_alt
        if (event%sqme_ref_known) then
            write (u, "(1x,A,IO,A," // fmt // ")") "sqme (", i, ") = ", &
                event%sqme_prc
        else
            write (u, "(1x,A,IO,A)") "sqme (", i, ") = [undefined]"
        end if
        if (event%weight_prc_known) then
            write (u, "(1x,A,IO,A," // fmt // ")") "weight (", i, ") = ", &
                event%weight_prc
        else
            write (u, "(1x,A,IO,A)") "weight (", i, ") = [undefined]"
        end if
    end do
end if
call write_separator (u)
if (event%particle_set_is_valid) then
    call event%particle_set%write (unit = u, &
        summary = eio%summary, compressed = eio%compressed, &
        testflag = eio%pacify)
else
    write (u, "(1x,A)") "Particle set: [invalid]"
end if
end subroutine dump
end subroutine eio_dump_output

```

Input an event.

(EIO dump: eio dump: TBP)+≡

```

procedure :: input_i_prc => eio_dump_input_i_prc
procedure :: input_event => eio_dump_input_event

```

```

<EIO dump: procedures>+=
  subroutine eio_dump_input_i_prc (eio, i_prc, iostat)
    class(eio_dump_t), intent(inout) :: eio
    integer, intent(out) :: i_prc
    integer, intent(out) :: iostat
    call msg_bug ("Dump stream: event input not supported")
    i_prc = 0
    iostat = 1
  end subroutine eio_dump_input_i_prc

  subroutine eio_dump_input_event (eio, event, iostat, event_handle)
    class(eio_dump_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    call msg_bug ("Dump stream: event input not supported")
    iostat = 1
  end subroutine eio_dump_input_event

<EIO dump: eio dump: TBP>+=
  procedure :: skip => eio_dump_skip

<EIO dump: procedures>+=
  subroutine eio_dump_skip (eio, iostat)
    class(eio_dump_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    iostat = 0
  end subroutine eio_dump_skip

```

18.9.4 Unit tests

Test module, followed by the corresponding implementation module.

```

<eio_dump.ut.f90>≡
  <File header>

  module eio_dump_ut
    use unit_tests
    use eio_dump_uti

    <Standard module head>

    <EIO dump: public test>

    contains

    <EIO dump: test driver>

  end module eio_dump_ut

<eio_dump.uti.f90>≡
  <File header>

  module eio_dump_uti

```

```

    <Use kinds>
    <Use strings>
    use io_units
    use event_base
    use eio_data
    use eio_base

    use eio_dump

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO dump: test declarations>

contains

    <EIO dump: tests>

end module eio_dump_utl
API: driver for the unit tests below.
<EIO dump: public test>≡
    public :: eio_dump_test
<EIO dump: test driver>≡
    subroutine eio_dump_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <EIO dump: execute tests>
end subroutine eio_dump_test

```

Test I/O methods

We test the implementation of all I/O methods.

```

<EIO dump: execute tests>≡
    call test (eio_dump_1, "eio_dump_1", &
        "write event contents", &
        u, results)

<EIO dump: test declarations>≡
    public :: eio_dump_1

<EIO dump: tests>≡
    subroutine eio_dump_1 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        class(eio_t), allocatable :: eio
        integer :: i_prc
        integer :: u_file

        write (u, "(A)")  "* Test output: eio_dump_1"
        write (u, "(A)")  "* Purpose: generate events and write essentials to output"
        write (u, "(A)")
    end subroutine eio_dump_1

```

```

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

write (u, "(A)")
write (u, "(A)")  "* Generate and write three events (two passed)"
write (u, "(A)")

allocate (eio_dump_t :: eio)
select type (eio)
type is (eio_dump_t)
    call eio%set_parameters (unit = u, weights = .true., pacify = .true.)
end select

i_prc = 42

call eio%init_out (var_str (""))

call event%generate (1, [0._default, 0._default])
call eio%output (event, i_prc = i_prc)

call event%generate (1, [0.1_default, 0._default])
call event%set_index (99)
call eio%output (event, i_prc = i_prc, passed = .false.)

call event%generate (1, [0.2_default, 0._default])
call event%increment_index ()
call eio%output (event, i_prc = i_prc, passed = .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of eio_dump object"
write (u, "(A)")

call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

select type (eio)
type is (eio_dump_t)
    eio%writing = .false.
end select
call eio%final ()

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_dump_1"
end subroutine eio_dump_1

```

18.10 ASCII File Formats

Here, we implement several ASCII file formats. It is possible to switch between them using flags.

```
<eio_ascii.f90>≡  
  <File header>  
  
  module eio_ascii  
  
    <Use strings>  
    use io_units  
    use diagnostics  
    use event_base  
    use event_handles, only: event_handle_t  
    use eio_data  
    use eio_base  
    use hep_common  
    use hep_events  
  
    <Standard module head>  
  
    <EIO ascii: public>  
  
    <EIO ascii: types>  
  
    contains  
  
    <EIO ascii: procedures>  
  
  end module eio_ascii
```

18.10.1 Type

```
<EIO ascii: public>≡  
  public :: eio_ascii_t  
  
<EIO ascii: types>≡  
  type, abstract, extends (eio_t) :: eio_ascii_t  
    logical :: writing = .false.  
    integer :: unit = 0  
    logical :: keep_beams = .false.  
    logical :: keep_remnants = .true.  
    logical :: ensure_order = .false.  
    contains  
    <EIO ascii: eio ascii: TBP>  
  end type eio_ascii_t  
  
<EIO ascii: public>+≡  
  public :: eio_ascii_ascii_t  
  
<EIO ascii: types>+≡  
  type, extends (eio_ascii_t) :: eio_ascii_ascii_t  
  end type eio_ascii_ascii_t
```



```

<EIO ascii: public>+≡
    public :: eio_ascii_athena_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_athena_t
    end type eio_ascii_athena_t

```

The debug format has a few options that can be controlled by Sindarin variables.

```

<EIO ascii: public>+≡
    public :: eio_ascii_debug_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_debug_t
        logical :: show_process = .true.
        logical :: show_transforms = .true.
        logical :: show_decay = .true.
        logical :: verbose = .true.
    end type eio_ascii_debug_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_hepevt_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_hepevt_t
    end type eio_ascii_hepevt_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_hepevt_verb_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_hepevt_verb_t
    end type eio_ascii_hepevt_verb_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_lha_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_lha_t
    end type eio_ascii_lha_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_lha_verb_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_lha_verb_t
    end type eio_ascii_lha_verb_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_long_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_long_t
    end type eio_ascii_long_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_mokka_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_mokka_t
    end type eio_ascii_mokka_t

```

```

<EIO ascii: public>+≡
    public :: eio_ascii_short_t

<EIO ascii: types>+≡
    type, extends (eio_ascii_t) :: eio_ascii_short_t
    end type eio_ascii_short_t

```

18.10.2 Specific Methods

Set parameters that are specifically used with ASCII file formats. In particular, this is the file extension.

```

<EIO ascii: eio ascii: TBP>≡
    procedure :: set_parameters => eio_ascii_set_parameters

<EIO ascii: procedures>≡
    subroutine eio_ascii_set_parameters (eio, &
        keep_beams, keep_remnants, ensure_order, extension, &
        show_process, show_transforms, show_decay, verbose)
        class(eio_ascii_t), intent(inout) :: eio
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        logical, intent(in), optional :: ensure_order
        type(string_t), intent(in), optional :: extension
        logical, intent(in), optional :: show_process, show_transforms, show_decay
        logical, intent(in), optional :: verbose
        if (present (keep_beams)) eio%keep_beams = keep_beams
        if (present (keep_remnants)) eio%keep_remnants = keep_remnants
        if (present (ensure_order)) eio%ensure_order = ensure_order
        if (present (extension)) then
            eio%extension = extension
        else
            select type (eio)
            type is (eio_ascii_ascii_t)
                eio%extension = "evt"
            type is (eio_ascii_athena_t)
                eio%extension = "athena.evt"
            type is (eio_ascii_debug_t)
                eio%extension = "debug"
            type is (eio_ascii_hepevt_t)
                eio%extension = "hepevt"
            type is (eio_ascii_hepevt_verb_t)
                eio%extension = "hepevt.verb"
            type is (eio_ascii_lha_t)
                eio%extension = "lha"
            type is (eio_ascii_lha_verb_t)
                eio%extension = "lha.verb"
        end if
    end subroutine

```

```

        type is (eio_ascii_long_t)
            eio%extension = "long.evt"
        type is (eio_ascii_mokka_t)
            eio%extension = "mokka.evt"
        type is (eio_ascii_short_t)
            eio%extension = "short.evt"
    end select
end if
select type (eio)
type is (eio_ascii_debug_t)
    if (present (show_process)) eio%show_process = show_process
    if (present (show_transforms)) eio%show_transforms = show_transforms
    if (present (show_decay)) eio%show_decay = show_decay
    if (present (verbose)) eio%verbose = verbose
end select
end subroutine eio_ascii_set_parameters

```

18.10.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: write => eio_ascii_write

<EIO ascii: procedures>+≡
    subroutine eio_ascii_write (object, unit)
        class(eio_ascii_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        select type (object)
        type is (eio_ascii_ascii_t)
            write (u, "(1x,A)") "ASCII event stream (default format):"
        type is (eio_ascii_athena_t)
            write (u, "(1x,A)") "ASCII event stream (ATHENA format):"
        type is (eio_ascii_debug_t)
            write (u, "(1x,A)") "ASCII event stream (Debugging format):"
        type is (eio_ascii_hepevt_t)
            write (u, "(1x,A)") "ASCII event stream (HEPEVT format):"
        type is (eio_ascii_hepevt_verb_t)
            write (u, "(1x,A)") "ASCII event stream (verbose HEPEVT format):"
        type is (eio_ascii_lha_t)
            write (u, "(1x,A)") "ASCII event stream (LHA format):"
        type is (eio_ascii_lha_verb_t)
            write (u, "(1x,A)") "ASCII event stream (verbose LHA format):"
        type is (eio_ascii_long_t)
            write (u, "(1x,A)") "ASCII event stream (long format):"
        type is (eio_ascii_mokka_t)
            write (u, "(1x,A)") "ASCII event stream (MOKKA format):"
        type is (eio_ascii_short_t)
            write (u, "(1x,A)") "ASCII event stream (short format):"
        end select
    if (object%writing) then

```

```

        write (u, "(3x,A,A)") "Writing to file   = ", char (object%filename)
    else
        write (u, "(3x,A)") "[closed]"
    end if
    write (u, "(3x,A,L1)") "Keep beams       = ", object%keep_beams
    write (u, "(3x,A,L1)") "Keep remnants   = ", object%keep_remnants
    select type (object)
    type is (eio_ascii_debug_t)
        write (u, "(3x,A,L1)") "Show process     = ", object%show_process
        write (u, "(3x,A,L1)") "Show transforms  = ", object%show_transforms
        write (u, "(3x,A,L1)") "Show decay tree  = ", object%show_decay
        write (u, "(3x,A,L1)") "Verbose output   = ", object%verbose
    end select
end subroutine eio_ascii_write

```

Finalizer: close any open file.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: final => eio_ascii_final

<EIO ascii: procedures>+≡
    subroutine eio_ascii_final (object)
        class(eio_ascii_t), intent(inout) :: object
        if (object%writing) then
            write (msg_buffer, "(A,A,A)") "Events: closing ASCII file '", &
                char (object%filename), "'"
            call msg_message ()
            close (object%unit)
            object%writing = .false.
        end if
    end subroutine eio_ascii_final

```

Initialize event writing.

Check weight normalization. This applies to all ASCII-type files that use the HEPHUP common block. We can't allow normalization conventions that are not covered by the HEPHUP definition.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: init_out => eio_ascii_init_out

<EIO ascii: procedures>+≡
    subroutine eio_ascii_init_out (eio, sample, data, success, extension)
        class(eio_ascii_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        integer :: i
        if (.not. present (data)) &
            call msg_bug ("ASCII initialization: missing data")
        if (data%n_beam /= 2) &
            call msg_fatal ("ASCII: defined for scattering processes only")
        eio%sample = sample
        call eio%check_normalization (data)
        call eio%set_splitting (data)
        call eio%set_filename ()
    end subroutine eio_ascii_init_out

```

```

eio%unit = free_unit ()
write (msg_buffer, "(A,A,A)") "Events: writing to ASCII file '", &
    char (eio%filename), "'"
call msg_message ()
eio%writing = .true.
open (eio%unit, file = char (eio%filename), &
    action = "write", status = "replace")
select type (eio)
type is (eio_ascii_lha_t)
    call heprup_init( &
        data%pdg_beam, &
        data%energy_beam, &
        n_processes = data%n_proc, &
        unweighted = data%unweighted, &
        negative_weights = data%negative_weights)
    do i = 1, data%n_proc
        call heprup_set_process_parameters (i = i, &
            process_id = data%proc_num_id(i), &
            cross_section = data%cross_section(i), &
            error = data%error(i))
    end do
    call heprup_write_ascii (eio%unit)
type is (eio_ascii_lha_verb_t)
    call heprup_init( &
        data%pdg_beam, &
        data%energy_beam, &
        n_processes = data%n_proc, &
        unweighted = data%unweighted, &
        negative_weights = data%negative_weights)
    do i = 1, data%n_proc
        call heprup_set_process_parameters (i = i, &
            process_id = data%proc_num_id(i), &
            cross_section = data%cross_section(i), &
            error = data%error(i))
    end do
    call heprup_write_verbose (eio%unit)
end select
if (present (success)) success = .true.
end subroutine eio_ascii_init_out

```

Some event properties do not go well with some output formats. In particular, many formats require unweighted events.

<EIO ascii: eio ascii: TBP>+≡

```
procedure :: check_normalization => eio_ascii_check_normalization
```

<EIO ascii: procedures>+≡

```

subroutine eio_ascii_check_normalization (eio, data)
    class(eio_ascii_t), intent(in) :: eio
    type(event_sample_data_t), intent(in) :: data
    if (data%unweighted) then
    else
        select type (eio)
        type is (eio_ascii_athena_t); call msg_fatal &
            ("Event output (Athena format): events must be unweighted.")

```

```

type is (eio_ascii_hepevt_t); call msg_fatal &
    ("Event output (HEPEVT format): events must be unweighted.")
type is (eio_ascii_hepevt_verb_t); call msg_fatal &
    ("Event output (HEPEVT format): events must be unweighted.")
end select
select case (data%norm_mode)
case (NORM_SIGMA)
case default
    select type (eio)
    type is (eio_ascii_lha_t)
        call msg_fatal &
            ("Event output (LHA): normalization for weighted events &
            &must be 'sigma'")
    type is (eio_ascii_lha_verb_t)
        call msg_fatal &
            ("Event output (LHA): normalization for weighted events &
            &must be 'sigma'")
    end select
end select
end if
end subroutine eio_ascii_check_normalization

```

Initialize event reading.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: init_in => eio_ascii_init_in
<EIO ascii: procedures>+≡
    subroutine eio_ascii_init_in (eio, sample, data, success, extension)
        class(eio_ascii_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        call msg_bug ("ASCII: event input not supported")
        if (present (success)) success = .false.
    end subroutine eio_ascii_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: switch_inout => eio_ascii_switch_inout
<EIO ascii: procedures>+≡
    subroutine eio_ascii_switch_inout (eio, success)
        class(eio_ascii_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("ASCII: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_ascii_switch_inout

```

Split event file: increment the counter, close the current file, open a new one. If the file needs a header, repeat it for the new file. (We assume that the common block contents are still intact.)

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: split_out => eio_ascii_split_out

```

```

<EIO ascii: procedures>+=
subroutine eio_ascii_split_out (eio)
  class(eio_ascii_t), intent(inout) :: eio
  if (eio%split) then
    eio%split_index = eio%split_index + 1
    call eio%set_filename ()
    write (msg_buffer, "(A,A,A)") "Events: writing to ASCII file '", &
      char (eio%filename), "'"
    call msg_message ()
    close (eio%unit)
    open (eio%unit, file = char (eio%filename), &
      action = "write", status = "replace")
    select type (eio)
    type is (eio_ascii_lha_t)
      call heprup_write_ascii (eio%unit)
    type is (eio_ascii_lha_verb_t)
      call heprup_write_verbose (eio%unit)
    end select
  end if
end subroutine eio_ascii_split_out

```

Output an event. Write first the event indices, then weight and squared matrix element, then the particle set.

Events that did not pass the selection are skipped. The exceptions are the `ascii` and `debug` formats. These are the formats that contain the `passed` flag in their output, and should be most useful for debugging purposes.

```

<EIO ascii: eio ascii: TBP>+=
procedure :: output => eio_ascii_output

<EIO ascii: procedures>+=
subroutine eio_ascii_output &
  (eio, event, i_prc, reading, passed, pacify, event_handle)
  class(eio_ascii_t), intent(inout) :: eio
  class(generic_event_t), intent(in), target :: event
  integer, intent(in) :: i_prc
  logical, intent(in), optional :: reading, passed, pacify
  class(event_handle_t), intent(inout), optional :: event_handle
  if (present (passed)) then
    if (.not. passed) then
      select type (eio)
      type is (eio_ascii_debug_t)
      type is (eio_ascii_ascii_t)
      class default
        return
      end select
    end if
  end if
  if (eio%writing) then
    select type (eio)
    type is (eio_ascii_lha_t)
      call hepeup_from_event (event, &
        process_index = i_prc, &
        keep_beams = eio%keep_beams, &
        keep_remnants = eio%keep_remnants)

```

```

        call hepeup_write_lha (eio%unit)
type is (eio_ascii_lha_verb_t)
        call hepeup_from_event (event, &
            process_index = i_prc, &
            keep_beams = eio%keep_beams, &
            keep_remnants = eio%keep_remnants)
        call hepeup_write_verbose (eio%unit)
type is (eio_ascii_ascii_t)
        call event%write (eio%unit, &
            show_process = .false., &
            show_transforms = .false., &
            show_decay = .false., &
            verbose = .false., testflag = pacify)
type is (eio_ascii_athena_t)
        call hepevt_from_event (event, &
            keep_beams = eio%keep_beams, &
            keep_remnants = eio%keep_remnants, &
            ensure_order = eio%ensure_order)
        call hepevt_write_athena (eio%unit)
type is (eio_ascii_debug_t)
        call event%write (eio%unit, &
            show_process = eio%show_process, &
            show_transforms = eio%show_transforms, &
            show_decay = eio%show_decay, &
            verbose = eio%verbose, &
            testflag = pacify)
type is (eio_ascii_hepevt_t)
        call hepevt_from_event (event, &
            keep_beams = eio%keep_beams, &
            keep_remnants = eio%keep_remnants, &
            ensure_order = eio%ensure_order)
        call hepevt_write_hepevt (eio%unit)
type is (eio_ascii_hepevt_verb_t)
        call hepevt_from_event (event, &
            keep_beams = eio%keep_beams, &
            keep_remnants = eio%keep_remnants, &
            ensure_order = eio%ensure_order)
        call hepevt_write_verbose (eio%unit)
type is (eio_ascii_long_t)
        call hepevt_from_event (event, &
            keep_beams = eio%keep_beams, &
            keep_remnants = eio%keep_remnants, &
            ensure_order = eio%ensure_order)
        call hepevt_write_ascii (eio%unit, .true.)
type is (eio_ascii_mokka_t)
        call hepevt_from_event (event, &
            keep_beams = eio%keep_beams, &
            keep_remnants = eio%keep_remnants, &
            ensure_order = eio%ensure_order)
        call hepevt_write_mokka (eio%unit)
type is (eio_ascii_short_t)
        call hepevt_from_event (event, &
            keep_beams = eio%keep_beams, &
            keep_remnants = eio%keep_remnants, &

```



```

        ensure_order = eio%ensure_order)
    call hepevt_write_ascii (eio%unit, .false.)
end select
else
    call eio%write ()
    call msg_fatal ("ASCII file is not open for writing")
end if
end subroutine eio_ascii_output

```

Input an event.

```

<EIO ascii: eio ascii: TBP>+≡
    procedure :: input_i_prc => eio_ascii_input_i_prc
    procedure :: input_event => eio_ascii_input_event

<EIO ascii: procedures>+≡
    subroutine eio_ascii_input_i_prc (eio, i_prc, iostat)
        class(eio_ascii_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        call msg_bug ("ASCII: event input not supported")
        i_prc = 0
        iostat = 1
    end subroutine eio_ascii_input_i_prc

    subroutine eio_ascii_input_event (eio, event, iostat, event_handle)
        class(eio_ascii_t), intent(inout) :: eio
        class(generic_event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
        call msg_bug ("ASCII: event input not supported")
        iostat = 1
    end subroutine eio_ascii_input_event

<EIO ascii: eio ascii: TBP>+≡
    procedure :: skip => eio_ascii_skip

<EIO ascii: procedures>+≡
    subroutine eio_ascii_skip (eio, iostat)
        class(eio_ascii_t), intent(inout) :: eio
        integer, intent(out) :: iostat
        iostat = 0
    end subroutine eio_ascii_skip

```

18.10.4 Unit tests

Test module, followed by the corresponding implementation module.

```

<eio_ascii_ut.f90>≡
    <File header>

    module eio_ascii_ut
        use unit_tests
        use eio_ascii_ut

```

```

    <Standard module head>

    <EIO ascii: public test>

    contains

    <EIO ascii: test driver>

    end module eio_ascii_ut

    <eio_ascii_uti.f90>≡
    <File header>

    module eio_ascii_uti

    <Use kinds>
    <Use strings>
        use io_units
        use lorentz
        use model_data
        use event_base
        use particles
        use eio_data
        use eio_base

        use eio_ascii

        use eio_base_ut, only: eio_prepare_test, eio_cleanup_test

    <Standard module head>

    <EIO ascii: test declarations>

    contains

    <EIO ascii: tests>

    end module eio_ascii_uti
API: driver for the unit tests below.
    <EIO ascii: public test>≡
        public :: eio_ascii_test
    <EIO ascii: test driver>≡
        subroutine eio_ascii_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <EIO ascii: execute tests>
        end subroutine eio_ascii_test

```

Test I/O methods

We test the implementation of all I/O methods, method `ascii`:

```

<EIO ascii: execute tests>≡
  call test (eio_ascii_1, "eio_ascii_1", &
    "read and write event contents, format [ascii]", &
    u, results)

<EIO ascii: test declarations>≡
  public :: eio_ascii_1

<EIO ascii: tests>≡
  subroutine eio_ascii_1 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat
    character(80) :: buffer

    write (u, "(A)")  "* Test output: eio_ascii_1"
    write (u, "(A)")  "* Purpose: generate an event in ASCII ascii format"
    write (u, "(A)")  "* and write weight to file"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    call eio_prepare_test (event, unweighted = .false.)

    call data%init (1)
    data%n_evt = 1
    data%n_beam = 2
    data%pdg_beam = 25
    data%energy_beam = 500
    data%proc_num_id = [42]
    data%cross_section(1) = 100
    data%error(1) = 1
    data%total_cross_section = sum (data%cross_section)

    write (u, "(A)")
    write (u, "(A)")  "* Generate and write an event"
    write (u, "(A)")

    sample = "eio_ascii_1"

    allocate (eio_ascii_ascii_t :: eio)

    select type (eio)
    class is (eio_ascii_t); call eio%set_parameters ()
    end select
    call eio%init_out (sample, data)
    call event%generate (1, [0._default, 0._default])
    call event%set_index (42)
    call event%evaluate_expressions ()

    call eio%output (event, i_prc = 1)
    call eio%write (u)

```

```

call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_ascii_t :: eio)

select type (eio)
type is (eio_ascii_ascii_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_1"

end subroutine eio_ascii_1

```

We test the implementation of all I/O methods, method `athena`:

```

<EIO ascii: execute tests>+≡
  call test (eio_ascii_2, "eio_ascii_2", &
    "read and write event contents, format [athena]", &
    u, results)
<EIO ascii: test declarations>+≡
  public :: eio_ascii_2
<EIO ascii: tests>+≡
  subroutine eio_ascii_2 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio

```

```

type(string_t) :: sample
integer :: u_file, iostat
character(80) :: buffer

write (u, "(A)")  "* Test output: eio_ascii_2"
write (u, "(A)")  "*   Purpose: generate an event in ASCII athena format"
write (u, "(A)")  "*           and write weight to file"
write (u, "(A)")

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_2"

allocate (eio_ascii_athena_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (42)
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char(sample // ".athena.evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit

```

```

        write (u, "(A)") trim (buffer)
    end do
    close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Reset data"
    write (u, "(A)")

    deallocate (eio)
    allocate (eio_ascii_athena_t :: eio)

    select type (eio)
    type is (eio_ascii_athena_t)
        call eio%set_parameters (keep_beams = .true.)
    end select
    call eio%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_ascii_2"

end subroutine eio_ascii_2

```

We test the implementation of all I/O methods, method `debug`:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_3, "eio_ascii_3", &
        "read and write event contents, format [debug]", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_3

<EIO ascii: tests>+≡
    subroutine eio_ascii_3 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_ascii_3"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII debug format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

```

```

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_3"

allocate (eio_ascii_debug_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".debug"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_debug_t :: eio)

select type (eio)
type is (eio_ascii_debug_t)

```

```

        call eio%set_parameters (keep_beams = .true.)
    end select
    call eio%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_ascii_3"

end subroutine eio_ascii_3

```

We test the implementation of all I/O methods, method `hepevt`:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_4, "eio_ascii_4", &
        "read and write event contents, format [hepevt]", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_4

<EIO ascii: tests>+≡
    subroutine eio_ascii_4 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_ascii_4"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII hepevt format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

```



```

sample = "eio_ascii_4"

allocate (eio_ascii_hepevt_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".hepevt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_hepevt_t :: eio)

select type (eio)
type is (eio_ascii_hepevt_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_4"

end subroutine eio_ascii_4

```

We test the implementation of all I/O methods, method `lha` (old LHA):

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_5, "eio_ascii_5", &
        "read and write event contents, format [lha]", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_5

<EIO ascii: tests>+≡
    subroutine eio_ascii_5 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_ascii_5"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII LHA format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

        sample = "eio_ascii_5"

        allocate (eio_ascii_lha_t :: eio)

        select type (eio)
            class is (eio_ascii_t); call eio%set_parameters ()
        end select
        call eio%init_out (sample, data)
        call event%generate (1, [0._default, 0._default])
        call event%increment_index ()
        call event%evaluate_expressions ()

```

```

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".lha"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_lha_t :: eio)

select type (eio)
type is (eio_ascii_lha_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_5"

end subroutine eio_ascii_5

```

We test the implementation of all I/O methods, method long:

```

<EIO ascii: execute tests>+≡
  call test (eio_ascii_6, "eio_ascii_6", &
    "read and write event contents, format [long]", &
    u, results)
<EIO ascii: test declarations>+≡
  public :: eio_ascii_6
<EIO ascii: tests>+≡
  subroutine eio_ascii_6 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event

```

```

type(event_sample_data_t) :: data
class(eio_t), allocatable :: eio
type(string_t) :: sample
integer :: u_file, iostat
character(80) :: buffer

write (u, "(A)")  "* Test output: eio_ascii_6"
write (u, "(A)")  "* Purpose: generate an event in ASCII long format"
write (u, "(A)")  "*           and write weight to file"
write (u, "(A)")

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_6"

allocate (eio_ascii_long_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".long.evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer

```

```

        if (buffer(1:21) == " <generator_version>") buffer = "[...]"
        if (iostat /= 0) exit
        write (u, "(A)") trim (buffer)
    end do
    close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Reset data"
    write (u, "(A)")

    deallocate (eio)
    allocate (eio_ascii_long_t :: eio)

    select type (eio)
    type is (eio_ascii_long_t)
        call eio%set_parameters (keep_beams = .true.)
    end select
    call eio%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call eio_cleanup_test (event)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: eio_ascii_6"

end subroutine eio_ascii_6

```

We test the implementation of all I/O methods, method mokka:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_7, "eio_ascii_7", &
        "read and write event contents, format [mokka]", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_7

<EIO ascii: tests>+≡
    subroutine eio_ascii_7 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_ascii_7"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII mokka format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"
    end subroutine eio_ascii_7

```

```

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_7"

allocate (eio_ascii_mokka_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".mokka.evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_mokka_t :: eio)

```

```

select type (eio)
type is (eio_ascii_mokka_t)
    call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_7"

end subroutine eio_ascii_7

```

We test the implementation of all I/O methods, method `short`:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_8, "eio_ascii_8", &
        "read and write event contents, format [short]", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_8

<EIO ascii: tests>+≡
    subroutine eio_ascii_8 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_ascii_8"
        write (u, "(A)")  "*   Purpose: generate an event in ASCII short format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")

```

```

write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_8"

allocate (eio_ascii_short_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".short.evt"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_short_t :: eio)

select type (eio)
type is (eio_ascii_short_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_8"

```



```
end subroutine eio_ascii_8
```

We test the implementation of all I/O methods, method `lha` (old LHA) in verbose version:

```
<EIO ascii: execute tests>+≡
  call test (eio_ascii_9, "eio_ascii_9", &
    "read and write event contents, format [lha_verb]", &
    u, results)

<EIO ascii: test declarations>+≡
  public :: eio_ascii_9

<EIO ascii: tests>+≡
  subroutine eio_ascii_9 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat
    character(80) :: buffer

    write (u, "(A)")  "* Test output: eio_ascii_9"
    write (u, "(A)")  "* Purpose: generate an event in ASCII LHA verbose format"
    write (u, "(A)")  "* and write weight to file"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    call eio_prepare_test (event, unweighted = .false.)

    call data%init (1)
    data%n_evt = 1
    data%n_beam = 2
    data%pdg_beam = 25
    data%energy_beam = 500
    data%proc_num_id = [42]
    data%cross_section(1) = 100
    data%error(1) = 1
    data%total_cross_section = sum (data%cross_section)

    write (u, "(A)")
    write (u, "(A)")  "* Generate and write an event"
    write (u, "(A)")

    sample = "eio_ascii_9"

    allocate (eio_ascii_lha_verb_t :: eio)

    select type (eio)
    class is (eio_ascii_t); call eio%set_parameters ()
    end select
    call eio%init_out (sample, data)
    call event%generate (1, [0._default, 0._default])
```

```

call event%increment_index ()
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".lha.verb"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:21) == " <generator_version>") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_lha_verb_t :: eio)

select type (eio)
type is (eio_ascii_lha_verb_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_9"

end subroutine eio_ascii_9

```

We test the implementation of all I/O methods, method `hepevt_verb`:

```

<EIO ascii: execute tests>+≡
  call test (eio_ascii_10, "eio_ascii_10", &
    "read and write event contents, format [hepevt_verb]", &
    u, results)

<EIO ascii: test declarations>+≡
  public :: eio_ascii_10

<EIO ascii: tests>+≡

```

```

subroutine eio_ascii_10 (u)
  integer, intent(in) :: u
  class(generic_event_t), pointer :: event
  type(event_sample_data_t) :: data
  class(eio_t), allocatable :: eio
  type(string_t) :: sample
  integer :: u_file, iostat
  character(80) :: buffer

  write (u, "(A)")  "* Test output: eio_ascii_10"
  write (u, "(A)")  "*   Purpose: generate an event in ASCII hepevt verbose format"
  write (u, "(A)")  "*           and write weight to file"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize test process"

  call eio_prepare_test (event, unweighted = .false.)

  call data%init (1)
  data%n_evt = 1
  data%n_beam = 2
  data%pdg_beam = 25
  data%energy_beam = 500
  data%proc_num_id = [42]
  data%cross_section(1) = 100
  data%error(1) = 1
  data%total_cross_section = sum (data%cross_section)

  write (u, "(A)")
  write (u, "(A)")  "* Generate and write an event"
  write (u, "(A)")

  sample = "eio_ascii_10"

  allocate (eio_ascii_hepevt_verb_t :: eio)

  select type (eio)
  class is (eio_ascii_t); call eio%set_parameters ()
  end select
  call eio%init_out (sample, data)
  call event%generate (1, [0._default, 0._default])
  call event%increment_index ()
  call event%evaluate_expressions ()

  call eio%output (event, i_prc = 1)
  call eio%write (u)
  call eio%final ()

  write (u, "(A)")
  write (u, "(A)")  "* File contents:"
  write (u, "(A)")

  u_file = free_unit ()
  open (u_file, file = char (sample // ".hepevt.verb"), &

```

```

        action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (buffer(1:21) == " <generator_version>") buffer = "[...]"
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_ascii_hepevt_verb_t :: eio)

select type (eio)
type is (eio_ascii_hepevt_verb_t)
    call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_10"

end subroutine eio_ascii_10

```

We test the implementation of all I/O methods, method mokka:

```

<EIO ascii: execute tests>+≡
    call test (eio_ascii_11, "eio_ascii_11", &
        "read and write event contents, format [mokka], tiny value", &
        u, results)

<EIO ascii: test declarations>+≡
    public :: eio_ascii_11

<EIO ascii: tests>+≡
    subroutine eio_ascii_11 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(particle_set_t), pointer :: pset
        type(vector4_t) :: pnew
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(128) :: buffer
        real(default), parameter :: tval = 1.e-111_default

        write (u, "(A)")  "* Test output: eio_ascii_11"
    end subroutine eio_ascii_11

```

```

write (u, "(A)")  "*"   Purpose: generate an event in ASCII mokka format"
write (u, "(A)")  "*"       and write weight to file"
write (u, "(A)")  "*"       with low-value cutoff"
write (u, "(A)")

write (u, "(A)")  "*" Initialize test process"

call eio_prepare_test (event, unweighted = .false.)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "*" Generate and write an event"
write (u, "(A)")

sample = "eio_ascii_11"

allocate (eio_ascii_mokka_t :: eio)

select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()

! Manipulate values in the event record
pset => event%get_particle_set_ptr ()
call pset%set_momentum (3, &
    vector4_moving (-tval, vector3_moving ([-tval, -tval, -tval])), &
    -tval**2)
call pset%set_momentum (4, &
    vector4_moving (tval, vector3_moving ([tval, tval, tval])), &
    tval**2)

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "*" File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".mokka.evt"), &

```

```

        action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (buffer(1:21) == " <generator_version>")  buffer = "[...]"
  if (iostat /= 0)  exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_ascii_11"

end subroutine eio_ascii_11

```

18.11 HEP Common Blocks

Long ago, to transfer data between programs one had to set up a common block and link both programs as libraries to the main executable. The HEP community standardizes several of those common blocks.

The modern way of data exchange uses data files with standard formats. However, the LHEF standard data format derives from a common block (actually, two).

WHIZARD used to support those common blocks, and LHEF was implemented via writing/reading blocks. We still keep this convention, but intend to eliminate common blocks (or any other static storage) from the workflow in the future. This will gain flexibility towards concurrent running of program images.

We encapsulate everything here in a module. The module holds the variables which are part of the common block. To access the common block variables, we just have to **use** this module. (They are nevertheless in the common block, since external software may access it in this way.)

Note: This code is taken essentially unchanged from WHIZARD 2.1 and does not (yet) provide unit tests.

```

<hep_common.f90>≡
  <File header>

  module hep_common

    <Use kinds>
    use kinds, only: double
    use constants
    <Use strings>
    <Use debug>
    use io_units
    use diagnostics
    use numeric_utils

```

```

use format_utils, only: refmt_tiny
use physics_defs, only: HADRON_REMNANT
use physics_defs, only: HADRON_REMNANT_SINGLET
use physics_defs, only: HADRON_REMNANT_TRIPLET
use physics_defs, only: HADRON_REMNANT_OCTET
use physics_defs, only: pb_per_fb
use xml
use lorentz
use flavors
use colors
use polarizations
use model_data
use particles
use subevents, only: PRT_BEAM, PRT_INCOMING, PRT_OUTGOING
use subevents, only: PRT_UNDEFINED
use subevents, only: PRT_VIRTUAL, PRT_RESONANT, PRT_BEAM_REMNANT

<Standard module head>

<HEP common: public>

<HEP common: interfaces>

<HEP common: parameters>

<HEP common: variables>

<HEP common: common blocks>

contains

<HEP common: procedures>

end module hep_common

```

18.11.1 Event characteristics

The maximal number of particles in an event record.

<HEP common: parameters>≡
integer, parameter, public :: MAXNUP = 500

The number of particles in this event.

<HEP common: variables>≡
integer, public :: NUP

The process ID for this event.

<HEP common: variables>+≡
integer, public :: IDPRUP

The weight of this event (± 1 for unweighted events).

<HEP common: variables>+≡
double precision, public :: XWGTUP

The factorization scale that is used for PDF calculation (-1 if undefined).

<HEP common: variables>+≡
double precision, public :: SCALUP

The QED and QCD couplings α used for this event (-1 if undefined).

```
<HEP common: variables>+≡  
  double precision, public :: AQEDUP  
  double precision, public :: AQCDUP
```

18.11.2 Particle characteristics

The PDG code:

```
<HEP common: variables>+≡  
  integer, dimension(MAXNUP), public :: IDUP
```

The status code. Incoming: -1 , outgoing: $+1$. Intermediate t-channel propagator: -2 (currently not used by WHIZARD). Intermediate resonance whose mass should be preserved: 2 . Intermediate resonance for documentation: 3 (currently not used). Beam particles: -9 .

```
<HEP common: variables>+≡  
  integer, dimension(MAXNUP), public :: ISTUP
```

Index of first and last mother.

```
<HEP common: variables>+≡  
  integer, dimension(2,MAXNUP), public :: MOTHUP
```

Color line index of the color and anticolor entry for the particle. The standard recommends using large numbers; we start from MAXNUP+1.

```
<HEP common: variables>+≡  
  integer, dimension(2,MAXNUP), public :: ICOLUP
```

Momentum, energy, and invariant mass: (p_x, p_y, p_z, E, M) . For space-like particles, M is the negative square root of the absolute value of the invariant mass.

```
<HEP common: variables>+≡  
  double precision, dimension(5,MAXNUP), public :: PUP
```

Invariant lifetime (distance) from production to decay in mm.

```
<HEP common: variables>+≡  
  double precision, dimension(MAXNUP), public :: VTIMUP
```

Cosine of the angle between the spin-vector and a particle and the 3-momentum of its mother, given in the lab frame. If undefined/unpolarized: 9 .

```
<HEP common: variables>+≡  
  double precision, dimension(MAXNUP), public :: SPINUP
```

18.11.3 The HEPRUP common block

This common block is filled once per run.

Run characteristics

The maximal number of different processes.

```
<HEP common: parameters>+≡  
  integer, parameter, public :: MAXPUP = 100
```

The beam PDG codes.

```
<HEP common: variables>+≡  
  integer, dimension(2), public :: IDBMUP
```


The beam energies in GeV.

```
<HEP common: variables>+≡  
    double precision, dimension(2), public :: EBMUP
```

The PDF group and set for the two beams. (Undefined: use -1 ; LHAPDF: use group = 0).

```
<HEP common: variables>+≡  
    integer, dimension(2), public :: PDFGUP  
    integer, dimension(2), public :: PDFSUP
```

The (re)weighting model. 1: events are weighted, the shower generator (SHG) selects processes according to the maximum weight (in pb) and unweights events. 2: events are weighted, the SHG selects processes according to their cross section (in pb) and unweights events. 3: events are unweighted and simply run through the SHG. 4: events are weighted, and the SHG keeps the weight. Negative numbers: negative weights are allowed (and are reweighted to ± 1 by the SHG, if allowed).

WHIZARD only supports modes 3 and 4, as the SHG is not given control over process selection. This is consistent with writing events to file, for offline showering.

```
<HEP common: variables>+≡  
    integer, public :: IDWTUP
```

The number of different processes.

```
<HEP common: variables>+≡  
    integer, public :: NPRUP
```

Process characteristics

Cross section and error in pb. (Cross section is needed only for IDWTUP = 2, so here both values are given for informational purposes only.)

```
<HEP common: variables>+≡  
    double precision, dimension(MAXPUP), public :: XSECUP  
    double precision, dimension(MAXPUP), public :: XERRUP
```

Maximum weight, i.e., the maximum value that XWGTUP can take. Also unused for the supported weighting models. It is ± 1 for unweighted events.

```
<HEP common: variables>+≡  
    double precision, dimension(MAXPUP), public :: XMAXUP
```

Internal ID of the selected process, matches IDPRUP below.

```
<HEP common: variables>+≡  
    integer, dimension(MAXPUP), public :: LPRUP
```

The common block

```
<HEP common: common blocks>≡  
    common /HEPRUP/ &  
        IDBMUP, EBMUP, PDFGUP, PDFSUP, IDWTUP, NPRUP, &  
        XSECUP, XERRUP, XMAXUP, LPRUP  
    save /HEPRUP/
```

Fill the run characteristics of the common block. The initialization sets the beam properties, number of processes, and weighting model.

```

<HEP common: public>≡
    public :: heprup_init
<HEP common: procedures>≡
    subroutine heprup_init &
        (beam_pdg, beam_energy, n_processes, unweighted, negative_weights)
        integer, dimension(2), intent(in) :: beam_pdg
        real(default), dimension(2), intent(in) :: beam_energy
        integer, intent(in) :: n_processes
        logical, intent(in) :: unweighted
        logical, intent(in) :: negative_weights
        IDBMUP = beam_pdg
        EBMUP = beam_energy
        PDFGUP = -1
        PDFSUP = -1
        if (unweighted) then
            IDWTUP = 3
        else
            IDWTUP = 4
        end if
        if (negative_weights) IDWTUP = - IDWTUP
        NPRUP = n_processes
    end subroutine heprup_init

```

The HEPRUP (event) common block is needed for the interface to the shower. Filling of it is triggered by some output file formats. If these are not present, the common block is filled with some dummy information. Be generous with the number of processes in HEPRUP so that PYTHIA only rarely needs to be reinitialized in case events with higher process ids are generated.

```

<HEP common: public>+≡
    public :: assure_heprup
<HEP common: procedures>+≡
    subroutine assure_heprup (pset)
        type(particle_set_t), intent(in) :: pset
        integer :: i, num_id
        integer, parameter :: min_processes = 10
        num_id = 1
        if (LPRUP (num_id) /= 0) return
        call heprup_init ( &
            [pset%prt(1)%get_pdg (), pset%prt(2)%get_pdg ()] , &
            [pset%prt(1)%p%p(0), pset%prt(2)%p%p(0)], &
            num_id, .false., .false.)
        do i = 1, (num_id / min_processes + 1) * min_processes
            call heprup_set_process_parameters (i = i, process_id = &
                i, cross_section = 1._default, error = 1._default)
        end do
    end subroutine assure_heprup

```

Read in the LHE file opened in unit u and add the final particles to the `particle_set`, the outgoing particles of the existing `particle_set` are compared to the particles that are read in. When they are equal in flavor and

momenta, they are erased and their mother-daughter relations are transferred to the existing particles.

```

<HEP common: public>+≡
    public :: combine_lhef_with_particle_set

<HEP common: procedures>+≡
    subroutine combine_lhef_with_particle_set &
        (particle_set, u, model_in, model_hadrons)
        type(particle_set_t), intent(inout) :: particle_set
        integer, intent(in) :: u
        class(model_data_t), intent(in), target :: model_in
        class(model_data_t), intent(in), target :: model_hadrons
        type(flavor_t) :: flv
        type(color_t) :: col
        class(model_data_t), pointer :: model
        type(particle_t), dimension(:), allocatable :: prt_tmp, prt
        integer :: i, j
        type(vector4_t) :: mom, d_mom
        integer, PARAMETER :: MAXLEN=200
        character(len=maxlen) :: string
        integer :: ibeg, n_tot, n_entries
        integer, dimension(:), allocatable :: relations, mothers, tbd
        INTEGER :: NUP, IDPRUP, IDUP, ISTUP
        real(kind=double) :: XWGTUP, SCALUP, AQEDUP, AQCDUP, VTIMUP, SPINUP
        integer :: MOTHUP(1:2), ICOLUP(1:2)
        real(kind=double) :: PUP(1:5)
        real(kind=default) :: pup_dum(1:5)
        character(len=5) :: buffer
        character(len=6) :: strfmt
        logical :: not_found
        logical :: debug_lhef = .false.
        STRFMT='(A000)'
        WRITE (STRFMT(3:5), '(I3)') MAXLEN

        if (debug_lhef) call particle_set%write ()

        rewind (u)

        do
            read (u,*, END=501, ERR=502) STRING
            IBEG = 0
            do
                if (signal_is_pending ()) return
                IBEG = IBEG + 1
                ! Allow indentation.
                IF (STRING (IBEG:IBEG) .EQ. ' ' .and. IBEG < MAXLEN-6) cycle
                exit
            end do
            IF (string(IBEG:IBEG+6) /= '<event>' .and. &
                string(IBEG:IBEG+6) /= '<event ') cycle
            exit
        end do
        !!! Read first line of event info -> number of entries
        read (u, *, END=503, ERR=504) NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP

```

```

n_tot = particle_set%get_n_tot ()
allocate (prt_tmp (1:n_tot+NUP))
allocate (relations (1:NUP), mothers (1:NUP), tbd(1:NUP))
do i = 1, n_tot
    if (signal_is_pending ()) return
    prt_tmp (i) = particle_set%get_particle (i)
end do
!!! transfer particles from lhef to particle_set
!!!...Read NUP subsequent lines with information on each particle.
n_entries = 1
mothers = 0
relations = 0
PARTICLE_LOOP: do I = 1, NUP
    read (u,*, END=200, ERR=505) IDUP, ISTUP, MOTHUP(1), MOTHUP(2), &
        ICOLUP(1), ICOLUP(2), (PUP (J),J=1,5), VTIMUP, SPINUP
    if (model_in%test_field (IDUP)) then
        model => model_in
    else if (model_hadrons%test_field (IDUP)) then
        model => model_hadrons
    else
        write (buffer, "(I5)") IDUP
        call msg_error ("Parton " // buffer // &
            " found neither in given model file nor in SM_hadrons")
        return
    end if
    if (debug_lhef) then
        print *, "IDUP, ISTUP, MOTHUP, PUP = ", IDUP, ISTUP, MOTHUP(1), &
            MOTHUP(2), PUP
    end if
    call flv%init (IDUP, model)
    if (IABS(IDUP) == 2212 .or. IABS(IDUP) == 2112) then
        ! PYTHIA sometimes sets color indices for protons and neutrons (?)
        ICOLUP (1) = 0
        ICOLUP (2) = 0
    end if
    call col%init_col_acl (ICOLUP (1), ICOLUP (2))
    !!! Settings for unpolarized particles
    ! particle_set%prt (oldsize+i)%hel = ??
    ! particle_set%prt (oldsize+i)%pol = ??
    if (MOTHUP(1) /= 0) then
        mothers(i) = MOTHUP(1)
    end if
    pup_dum = PUP
    if (pup_dum(4) < 1E-10_default) cycle
    mom = vector4_moving (pup_dum (4), &
        vector3_moving ([pup_dum (1), pup_dum (2), pup_dum (3)]))
    not_found = .true.
SCAN_PARTICLES: do j = 1, n_tot
    d_mom = prt_tmp(j)%get_momentum ()
    if (all (nearly_equal &
        (mom%p, d_mom%p, abs_smallness = 1.E-4_default)) .and. &
        (prt_tmp(j)%get_pdg () == IDUP)) then
        if (.not. prt_tmp(j)%get_status () == PRT_BEAM .or. &
            .not. prt_tmp(j)%get_status () == PRT_BEAM_REMNANT) &

```

```

        relations(i) = j
        not_found = .false.
    end if
end do SCAN_PARTICLES
if (not_found) then
    if (debug_lhef) &
        print *, "Not found: adding particle"
    call prt_tmp(n_tot+n_entries)%set_flavor (flv)
    call prt_tmp(n_tot+n_entries)%set_color (col)
    call prt_tmp(n_tot+n_entries)%set_momentum (mom)
    if (MOTHUP(1) /= 0) then
        if (relations(MOTHUP(1)) /= 0) then
            call prt_tmp(n_tot+n_entries)%set_parents &
                ([relations(MOTHUP(1))])
            call prt_tmp(relations(MOTHUP(1)))%add_child (n_tot+n_entries)
            if (prt_tmp(relations(MOTHUP(1)))%get_status () &
                == PRT_OUTGOING) &
                call prt_tmp(relations(MOTHUP(1)))%reset_status &
                    (PRT_VIRTUAL)
        end if
    end if
    call prt_tmp(n_tot+n_entries)%set_status (PRT_OUTGOING)
    if (debug_lhef) call prt_tmp(n_tot+n_entries)%write ()
    n_entries = n_entries + 1
end if
end do PARTICLE_LOOP
do i = 1, n_tot
    if (prt_tmp(i)%get_status () == PRT_OUTGOING .and. &
        prt_tmp(i)%get_n_children () /= 0) then
        call prt_tmp(i)%reset_status (PRT_VIRTUAL)
    end if
end do

allocate (prt (1:n_tot+n_entries-1))
prt = prt_tmp (1:n_tot+n_entries-1)
! transfer to particle_set
call particle_set%replace (prt)
deallocate (prt, prt_tmp)

if (debug_lhef) then
    call particle_set%write ()
    print *, "combine_lhef_with_particle_set"
    ! stop
end if

200 continue
return

501 write(*,*) "READING LHEF failed 501"
return
502 write(*,*) "READING LHEF failed 502"
return
503 write(*,*) "READING LHEF failed 503"
return

```

```

504 write(*,*) "READING LHEF failed 504"
    return
505 write(*,*) "READING LHEF failed 505"
    return
end subroutine combine_lhef_with_particle_set

<HEP common: public>+≡
    public :: w2p_write_lhef_event

<HEP common: procedures>+≡
    subroutine w2p_write_lhef_event (unit)
        integer, intent(in) :: unit
        type(xml_tag_t), allocatable :: tag_lhef, tag_head, tag_init, &
            tag_event, tag_gen_n, tag_gen_v
        if (debug_on) call msg_debug (D_EVENTS, "w2p_write_lhef_event")
        allocate (tag_lhef, tag_head, tag_init, tag_event, &
            tag_gen_n, tag_gen_v)
        call tag_lhef%init (var_str ("LesHouchesEvents"), &
            [xml_attribute (var_str ("version"), var_str ("1.0"))], .true.)
        call tag_head%init (var_str ("header"), .true.)
        call tag_init%init (var_str ("init"), .true.)
        call tag_event%init (var_str ("event"), .true.)
        call tag_gen_n%init (var_str ("generator_name"), .true.)
        call tag_gen_v%init (var_str ("generator_version"), .true.)
        call tag_lhef%write (unit); write (unit, *)
        call tag_head%write (unit); write (unit, *)
        write (unit, "(2x)", advance = "no")
        call tag_gen_n%write (var_str ("WHIZARD"), unit)
        write (unit, *)
        write (unit, "(2x)", advance = "no")
        call tag_gen_v%write (var_str ("<Version>"), unit)
        write (unit, *)
        call tag_head%close (unit); write (unit, *)
        call tag_init%write (unit); write (unit, *)
        call heprup_write_lhef (unit)
        call tag_init%close (unit); write (unit, *)
        call tag_event%write (unit); write (unit, *)
        call hepeup_write_lhef (unit)
        call tag_event%close (unit); write (unit, *)
        call tag_lhef%close (unit); write (unit, *)
        deallocate (tag_lhef, tag_head, tag_init, tag_event, &
            tag_gen_n, tag_gen_v)
    end subroutine w2p_write_lhef_event

```

Extract parameters from the common block. We leave it to the caller to specify which parameters it actually needs.

PDFGUP and PDFSUP are not extracted. IDWTUP=1,2 are not supported by WHIZARD, but correspond to weighted events.

```

<HEP common: public>+≡
    public :: heprup_get_run_parameters

<HEP common: procedures>+≡
    subroutine heprup_get_run_parameters &
        (beam_pdg, beam_energy, n_processes, unweighted, negative_weights)

```

```

integer, dimension(2), intent(out), optional :: beam_pdg
real(default), dimension(2), intent(out), optional :: beam_energy
integer, intent(out), optional :: n_processes
logical, intent(out), optional :: unweighted
logical, intent(out), optional :: negative_weights
if (present (beam_pdg)) beam_pdg = IDBMUP
if (present (beam_energy)) beam_energy = EBMUP
if (present (n_processes)) n_processes = NPRUP
if (present (unweighted)) then
  select case (abs (IDWTUP))
    case (3)
      unweighted = .true.
    case (4)
      unweighted = .false.
    case (1,2) !!! not supported by WHIZARD
      unweighted = .false.
    case default
      call msg_fatal ("HEPRUP: unsupported IDWTUP value")
  end select
end if
if (present (negative_weights)) then
  negative_weights = IDWTUP < 0
end if
end subroutine heprup_get_run_parameters

```

Specify PDF set info. Since we support only LHAPDF, the group entry is zero.

```

<HEP common: public>+≡
  public :: heprup_set_lhapdf_id

<HEP common: procedures>+≡
  subroutine heprup_set_lhapdf_id (i_beam, pdf_id)
    integer, intent(in) :: i_beam, pdf_id
    PDFGUP(i_beam) = 0
    PDFSUP(i_beam) = pdf_id
  end subroutine heprup_set_lhapdf_id

```

Fill the characteristics for a particular process. Only the process ID is mandatory. Note that WHIZARD computes cross sections in fb, so we have to rescale to pb. The maximum weight is meaningless for unweighted events.

```

<HEP common: public>+≡
  public :: heprup_set_process_parameters

<HEP common: procedures>+≡
  subroutine heprup_set_process_parameters &
    (i, process_id, cross_section, error, max_weight)
    integer, intent(in) :: i, process_id
    real(default), intent(in), optional :: cross_section, error, max_weight
    LPRUP(i) = process_id
    if (present (cross_section)) then
      XSECUP(i) = cross_section * pb_per_fb
    else
      XSECUP(i) = 0
    end if
    if (present (error)) then

```

```

        XERRUP(i) = error * pb_per_fb
    else
        XERRUP(i) = 0
    end if
    select case (IDWTUP)
    case (3); XMAXUP(i) = 1
    case (4)
        if (present (max_weight)) then
            XMAXUP(i) = max_weight * pb_per_fb
        else
            XMAXUP(i) = 0
        end if
    end select
end subroutine heprup_set_process_parameters

```

Extract the process parameters, as far as needed.

```

<HEP common: public>+≡
    public :: heprup_get_process_parameters

<HEP common: procedures>+≡
    subroutine heprup_get_process_parameters &
        (i, process_id, cross_section, error, max_weight)
        integer, intent(in) :: i
        integer, intent(out), optional :: process_id
        real(default), intent(out), optional :: cross_section, error, max_weight
        if (present (process_id)) process_id = LPRUP(i)
        if (present (cross_section)) then
            cross_section = XSECUP(i) / pb_per_fb
        end if
        if (present (error)) then
            error = XERRUP(i) / pb_per_fb
        end if
        if (present (max_weight)) then
            select case (IDWTUP)
            case (3)
                max_weight = 1
            case (4)
                max_weight = XMAXUP(i) / pb_per_fb
            case (1,2) !!! not supported by WHIZARD
                max_weight = 0
            case default
                call msg_fatal ("HEPRUP: unsupported IDWTUP value")
            end select
        end if
    end subroutine heprup_get_process_parameters

```

18.11.4 Run parameter output (verbose)

This is a verbose output of the HEPRUP block.

```

<HEP common: public>+≡
    public :: heprup_write_verbose

```



```

<HEP common: procedures>+≡
subroutine heprup_write_verbose (unit)
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(A)") "HEPRUP Common Block"
  write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "IDBMUP", IDBMUP, &
    "PDG code of beams"
  write (u, "(3x,A6,' = ',G12.5,1x,G12.5,8x,A)") "EBMUP ", EBMUP, &
    "Energy of beams in GeV"
  write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "PDFGUP", PDFGUP, &
    "PDF author group [-1 = undefined]"
  write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "PDFSUP", PDFSUP, &
    "PDF set ID [-1 = undefined]"
  write (u, "(3x,A6,' = ',I9,3x,1x,9x,3x,8x,A)") "IDWTUP", IDWTUP, &
    "LHA code for event weight mode"
  write (u, "(3x,A6,' = ',I9,3x,1x,9x,3x,8x,A)") "NPRUP ", NPRUP, &
    "Number of user subprocesses"
  do i = 1, NPRUP
    write (u, "(1x,A,I0)") "Subprocess #", i
    write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "XSECUP", XSECUP(i), &
      "Cross section in pb"
    write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "XERRUP", XERRUP(i), &
      "Cross section error in pb"
    write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "XMAXUP", XMAXUP(i), &
      "Maximum event weight (cf. IDWTUP)"
    write (u, "(3x,A6,' = ',I9,3x,1x,12x,8x,A)") "LPRUP ", LPRUP(i), &
      "Subprocess ID"
  end do
end subroutine heprup_write_verbose

```

18.11.5 Run parameter output (other formats)

This routine writes the initialization block according to the LHEF standard. It uses the current contents of the HEPRUP block.

```

<HEP common: public>+≡
  public :: heprup_write_lhef

<HEP common: procedures>+≡
subroutine heprup_write_lhef (unit)
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(2(1x,I0),2(1x,ES17.10),6(1x,I0))") &
    IDBMUP, EBMUP, PDFGUP, PDFSUP, IDWTUP, NPRUP
  do i = 1, NPRUP
    write (u, "(3(1x,ES17.10),1x,I0)") &
      XSECUP(i), XERRUP(i), XMAXUP(i), LPRUP(i)
  end do
end subroutine heprup_write_lhef

```

This routine is a complete dummy at the moment. It uses the current contents of the HEPUP block. At the end, it should depend on certain input flags for the different ASCII event formats.

```

<HEP common: public>+≡
  public :: heprup_write_ascii

<HEP common: procedures>+≡
  subroutine heprup_write_ascii (unit)
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(2(1x,I0),2(1x,ES17.10),6(1x,I0))") &
      IDBMUP, EBMUP, PDFGUP, PDFSUP, IDWTUP, NPRUP
    do i = 1, NPRUP
      write (u, "(3(1x,ES17.10),1x,I0)") &
        XSECUP(i), XERRUP(i), XMAXUP(i), LPRUP(i)
    end do
  end subroutine heprup_write_ascii

```

Run parameter input (LHEF)

In a LHEF file, the parameters are written in correct order on separate lines, but we should not count on the precise format. List-directed input should just work.

```

<HEP common: public>+≡
  public :: heprup_read_lhef

<HEP common: procedures>+≡
  subroutine heprup_read_lhef (u)
    integer, intent(in) :: u
    integer :: i
    read (u, *) &
      IDBMUP, EBMUP, PDFGUP, PDFSUP, IDWTUP, NPRUP
    do i = 1, NPRUP
      read (u, *) &
        XSECUP(i), XERRUP(i), XMAXUP(i), LPRUP(i)
    end do
  end subroutine heprup_read_lhef

```

18.11.6 The HEPEUP common block

```

<HEP common: common blocks>+≡
  common /HEPEUP/ &
    NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP, &
    IDUP, ISTUP, MOTHUP, ICOLUP, PUP, VTIMUP, SPINUP
  save /HEPEUP/

```

Initialization

Fill the event characteristics of the common block. The initialization sets only the number of particles and initializes the rest with default values. The other routine sets the optional parameters.

```
<HEP common: public>+≡
  public :: hepeup_init
  public :: hepeup_set_event_parameters

<HEP common: procedures>+≡
  subroutine hepeup_init (n_tot)
    integer, intent(in) :: n_tot
    NUP = n_tot
    IDPRUP = 0
    XWGTUP = 1
    SCALUP = -1
    AQEDUP = -1
    AQCDUP = -1
  end subroutine hepeup_init

  subroutine hepeup_set_event_parameters &
    (proc_id, weight, scale, alpha_qed, alpha_qcd)
    integer, intent(in), optional :: proc_id
    real(default), intent(in), optional :: weight, scale, alpha_qed, alpha_qcd
    if (present (proc_id)) IDPRUP = proc_id
    if (present (weight)) XWGTUP = weight
    if (present (scale)) SCALUP = scale
    if (present (alpha_qed)) AQEDUP = alpha_qed
    if (present (alpha_qcd)) AQCDUP = alpha_qcd
  end subroutine hepeup_set_event_parameters
```

Extract event information. The caller determines the parameters.

```
<HEP common: public>+≡
  public :: hepeup_get_event_parameters

<HEP common: procedures>+≡
  subroutine hepeup_get_event_parameters &
    (proc_id, weight, scale, alpha_qed, alpha_qcd)
    integer, intent(out), optional :: proc_id
    real(default), intent(out), optional :: weight, scale, alpha_qed, alpha_qcd
    if (present (proc_id)) proc_id = IDPRUP
    if (present (weight)) weight = XWGTUP
    if (present (scale)) scale = SCALUP
    if (present (alpha_qed)) alpha_qed = AQEDUP
    if (present (alpha_qcd)) alpha_qcd = AQCDUP
  end subroutine hepeup_get_event_parameters
```

Particle data

Below we need the particle status codes which are actually defined in the subevents module.

Set the entry for a specific particle. All parameters are set with the exception of lifetime and spin, where default values are stored.

```

<HEP common: public>+≡
    public :: hepeup_set_particle

<HEP common: procedures>+≡
    subroutine hepeup_set_particle (i, pdg, status, parent, col, p, m2)
        integer, intent(in) :: i
        integer, intent(in) :: pdg, status
        integer, dimension(:), intent(in) :: parent
        type(vector4_t), intent(in) :: p
        integer, dimension(2), intent(in) :: col
        real(default), intent(in) :: m2
        if (i > MAXNUP) then
            call msg_error (arr=[ &
                var_str ("Too many particles in HEPEUP common block. " // &
                    "If this happened "), &
                var_str ("during event output, your events will be " // &
                    "invalid; please consider "), &
                var_str ("switching to a modern event format like HEPMC. " // &
                    "If you are not "), &
                var_str ("using an old, HEPEUP based format and " // &
                    "nevertheless get this error,"), &
                var_str ("please notify the WHIZARD developers,") ])
            return
        end if
        IDUP(i) = pdg
        select case (status)
            case (PRT_BEAM);          ISTUP(i) = -9
            case (PRT_INCOMING);      ISTUP(i) = -1
            case (PRT_BEAM_REMNANT);  ISTUP(i) = 3
            case (PRT_OUTGOING);      ISTUP(i) = 1
            case (PRT_RESONANT);      ISTUP(i) = 2
            case (PRT_VIRTUAL);       ISTUP(i) = 3
            case default;             ISTUP(i) = 0
        end select
        select case (size (parent))
            case (0);      MOTHUP(:,i) = 0
            case (1);      MOTHUP(1,i) = parent(1); MOTHUP(2,i) = 0
            case default;  MOTHUP(:,i) = [ parent(1), parent(size (parent)) ]
        end select
        if (col(1) > 0) then
            ICOLUP(1,i) = 500 + col(1)
        else
            ICOLUP(1,i) = 0
        end if
        if (col(2) > 0) then
            ICOLUP(2,i) = 500 + col(2)
        else
            ICOLUP(2,i) = 0
        end if
        PUP(1:3,i) = refmt_tiny (vector3_get_components (space_part (p)))
        PUP(4,i) = refmt_tiny (energy (p))
        PUP(5,i) = refmt_tiny (sign (sqrt (abs (m2)), m2))
    end subroutine

```

```

      VTIMUP(i) = 0
      SPINUP(i) = 9
end subroutine hepeup_set_particle

```

Set the lifetime, actually $c\tau$ measured in mm, where τ is the invariant lifetime.

```

<HEP common: public>+≡
  public :: hepeup_set_particle_lifetime

<HEP common: procedures>+≡
  subroutine hepeup_set_particle_lifetime (i, lifetime)
    integer, intent(in) :: i
    real(default), intent(in) :: lifetime
    VTIMUP(i) = lifetime
  end subroutine hepeup_set_particle_lifetime

```

Set the particle spin entry. We need the cosine of the angle of the spin axis with respect to the three-momentum of the parent particle.

If the particle has a full polarization density matrix given, we need the particle momentum and polarization as well as the mother-particle momentum. The polarization is transformed into a spin vector (which is sensible only for spin-1/2 or massless particles), which then is transformed into the lab frame (by a rotation of the 3-axis to the particle momentum axis). Finally, we compute the scalar product of this vector with the mother-particle three-momentum.

This puts severe restrictions on the applicability of this definition, and Lorentz invariance is lost. Unfortunately, the Les Houches Accord requires this computation.

```

<HEP common: public>+≡
  public :: hepeup_set_particle_spin

<HEP common: interfaces>≡
  interface hepeup_set_particle_spin
    module procedure hepeup_set_particle_spin_pol
  end interface

<HEP common: procedures>+≡
  subroutine hepeup_set_particle_spin_pol (i, p, pol, p_mother)
    integer, intent(in) :: i
    type(vector4_t), intent(in) :: p
    type(polarization_t), intent(in) :: pol
    type(vector4_t), intent(in) :: p_mother
    type(vector3_t) :: s3, p3
    type(vector4_t) :: s4
    s3 = vector3_moving (pol%get_axis ())
    p3 = space_part (p)
    s4 = rotation_to_2nd (3, p3) * vector4_moving (0._default, s3)
    SPINUP(i) = enclosed_angle_ct (s4, p_mother)
  end subroutine hepeup_set_particle_spin_pol

```

Extract particle data. The caller decides which ones to retrieve.

Status codes: beam remnants share the status code with virtual particles. However, for the purpose of WHIZARD we should identify them. We use the PDG code for this.

```

<HEP common: public>+≡

```

```

public :: hepeup_get_particle
<HEP common: procedures>+≡
subroutine hepeup_get_particle (i, pdg, status, parent, col, p, m2)
  integer, intent(in) :: i
  integer, intent(out), optional :: pdg, status
  integer, dimension(:), intent(out), optional :: parent
  type(vector4_t), intent(out), optional :: p
  integer, dimension(2), intent(out), optional :: col
  real(default), dimension(5,MAXNUP) :: pup_def
  real(default), intent(out), optional :: m2
  if (present (pdg)) pdg = IDUP(i)
  if (present (status)) then
    select case (ISTUP(i))
    case (-9); status = PRT_BEAM
    case (-1); status = PRT_INCOMING
    case (1); status = PRT_OUTGOING
    case (2); status = PRT_RESONANT
    case (3);
      select case (abs (IDUP(i)))
      case (HADRON_REMNANT, HADRON_REMNANT_SINGLET, &
            HADRON_REMNANT_TRIPLET, HADRON_REMNANT_OCTET)
        status = PRT_BEAM_REMNANT
      case default
        status = PRT_VIRTUAL
      end select
    case default
      status = PRT_UNDEFINED
    end select
  end if
  if (present (parent)) then
    select case (size (parent))
    case (0)
    case (1); parent(1) = MOTHUP(1,i)
    case (2); parent = MOTHUP(:,i)
    end select
  end if
  if (present (col)) then
    col = ICOLUP(:,i)
  end if
  if (present (p)) then
    pup_def = PUP
    p = vector4_moving (pup_def(4,i), vector3_moving (pup_def(1:3,i)))
  end if
  if (present (m2)) then
    m2 = sign (PUP(5,i) ** 2, PUP(5,i))
  end if
end subroutine hepeup_get_particle

```

18.11.7 The HEPEVT and HEPEV4 common block

For the LEP Monte Carlos, a standard common block has been proposed in AKV89. We strongly recommend its use. (The description is an abbreviated

transcription of AKV89, Vol. 3, pp. 327-330).

NMXHEP is the maximum number of entries:

```
<HEP common: variables>+≡  
integer, parameter :: NMXHEP = 4000
```

NEVHEP is normally the event number, but may take special values as follows:

0 the program does not keep track of event numbers. -1 a special initialization record. -2 a special final record.

```
<HEP common: variables>+≡  
integer :: NEVHEP
```

NHEP holds the number of entries for this event.

```
<HEP common: variables>+≡  
integer, public :: NHEP
```

The entry ISTHEP(N) gives the status code for the Nth entry, with the following semantics: 0 a null entry. 1 an existing entry, which has not decayed or fragmented. 2 a decayed or fragmented entry, which is retained for event history information. 3 documentation line. 4- 10 reserved for future standards. 11-200 at the disposal of each model builder. 201- at the disposal of users.

```
<HEP common: variables>+≡  
integer, dimension(NMXHEP), public :: ISTHEP
```

The Particle Data Group has proposed standard particle codes, which are to be stored in IDHEP(N).

```
<HEP common: variables>+≡  
integer, dimension(NMXHEP), public :: IDHEP
```

JMOHEP(1,N) points to the mother of the Nth entry, if any. It is set to zero for initial entries. JMOHEP(2,N) points to the second mother, if any.

```
<HEP common: variables>+≡  
integer, dimension(2, NMXHEP), public :: JMOHEP
```

JDAHEP(1,N) and JDAHEP(2,N) point to the first and last daughter of the Nth entry, if any. These are zero for entries which have not yet decayed. The other daughters are stored in between these two.

```
<HEP common: variables>+≡  
integer, dimension(2, NMXHEP), public :: JDAHEP
```

In PHEP we store the momentum of the particle, more specifically this means that PHEP(1,N), PHEP(2,N), and PHEP(3,N) contain the momentum in the x , y , and z direction (as defined by the machine people), measured in GeV/c. PHEP(4,N) contains the energy in GeV and PHEP(5,N) the mass in GeV/ c^2 . The latter may be negative for spacelike partons.

```
<HEP common: variables>+≡  
double precision, dimension(5, NMXHEP), public :: PHEP
```

Finally VHEP is the place to store the position of the production vertex. VHEP(1,N), VHEP(2,N), and VHEP(3,N) contain the x , y , and z coordinate (as defined by the machine people), measured in mm. VHEP(4,N) contains the production time in mm/c.

```
<HEP common: variables>+≡
  double precision, dimension(4, NMXHEP) :: VHEP
```

As an amendment to the proposed standard common block HEPEVT, we also have a polarisation common block HEPSPN, as described in AKV89. SHEP(1,N), SHEP(2,N), and SHEP(3,N) give the x , y , and z component of the spinvector s of a fermion in the fermions restframe.

Furthermore, we add the polarization of the corresponding outgoing particles:

```
<HEP common: variables>+≡
  integer, dimension(NMXHEP) :: hepevt_pol
```

By this variable the identity of the current process is given, defined via the LPRUP codes.

```
<HEP common: variables>+≡
  integer, public :: idruplh
```

This is the event weight, i.e. the cross section divided by the total number of generated events for the output of the parton shower programs.

```
<HEP common: variables>+≡
  double precision, public :: eventweightlh
```

There are the values for the electromagnetic and the strong coupling constants, α_{em} and α_s .

```
<HEP common: variables>+≡
  double precision, public :: alphasqedlh, alphasqcdlh
```

This is the squared scale Q of the event.

```
<HEP common: variables>+≡
  double precision, dimension(10), public :: scalelh
```

Finally, these variables contain the spin information and the color/anticolor flow of the particles.

```
<HEP common: variables>+≡
  double precision, dimension (3,NMXHEP), public :: spinlh
  integer, dimension (2,NMXHEP), public :: icolorflowlh
```

By convention, SHEP(4,N) is always 1. All this is taken from StdHep 4.06 manual and written using Fortran90 conventions.

```
<HEP common: common blocks>+≡
  common /HEPEVT/ &
    NEVHEP, NHEP, ISTHEP, IDHEP, &
    JMOHEP, JDAHEP, PHEP, VHEP
  save /HEPEVT/
```


Here we store HEPEVT parameters of the WHIZARD 1 realization which are not part of the HEPEVT common block.

```
<HEP common: variables>+≡
  integer :: hepevt_n_out, hepevt_n_remnants
```

```
<HEP common: variables>+≡
  double precision :: hepevt_weight, hepevt_function_value
  double precision :: hepevt_function_ratio
```

The HEPEV4 common block is an extension of the HEPEVT common block to allow for partonic colored events, including especially the color flow etc.

```
<HEP common: common blocks>+≡
  common /HEPEV4/ &
    eventweightlh, alphaqedlh, alphaqcdlh, scalelh, &
    spinlh, icolorflowlh, idruplh
  save /HEPEV4/
```

Filling HEPEVT: If the event count is not provided, set `NEVHEP` to zero. If the event count is `-1` or `-2`, the record corresponds to initialization and finalization, and the event is irrelevant.

Note that the event count may be larger than 2^{31} (2 GEvents). In that case, cut off the upper bits since `NEVHEP` is probably limited to default integer.

For the HEPEV4 common block, it is unclear why the `scalelh` variable is 10-dimensional. We choose to only set the first value of the array.

```
<HEP common: public>+≡
  public :: hepevt_init
  public :: hepevt_set_event_parameters

<HEP common: procedures>+≡
  subroutine hepevt_init (n_tot, n_out)
    integer, intent(in) :: n_tot, n_out
    NHEP                = n_tot
    NEVHEP              = 0
    idruplh             = 0
    hepevt_n_out        = n_out
    hepevt_n_remnants   = 0
    hepevt_weight       = 1
    eventweightlh       = 1
    hepevt_function_value = 0
    hepevt_function_ratio = 1
    alphaqcdlh          = -1
    alphaqedlh          = -1
    scalelh             = -1
  end subroutine hepevt_init

  subroutine hepevt_set_event_parameters &
    (proc_id, weight, function_value, function_ratio, &
    alpha_qcd, alpha_qed, scale, i_evt)
    integer, intent(in), optional :: proc_id
    integer, intent(in), optional :: i_evt
    real(default), intent(in), optional :: weight, function_value, &
    function_ratio, alpha_qcd, alpha_qed, scale
```

```

if (present (proc_id)) idruplh = proc_id
if (present (i_evt)) NEVHEP = i_evt
if (present (weight)) then
    hepevt_weight = weight
    eventweightlh = weight
end if
if (present (function_value)) hepevt_function_value = &
    function_value
if (present (function_ratio)) hepevt_function_ratio = &
    function_ratio
if (present (alpha_qcd)) alphaqcdlh = alpha_qcd
if (present (alpha_qed)) alphaqedlh = alpha_qed
if (present (scale)) scalelh(1) = scale
if (present (i_evt)) NEVHEP = i_evt
end subroutine hepevt_set_event_parameters

```

Set the entry for a specific particle. All parameters are set with the exception of lifetime and spin, where default values are stored.

```

<HEP common: public>+≡
    public :: hepevt_set_particle

<HEP common: procedures>+≡
    subroutine hepevt_set_particle &
        (i, pdg, status, parent, child, p, m2, hel, vtx, &
         col, pol_status, pol, fill_hepev4)
        integer, intent(in) :: i
        integer, intent(in) :: pdg, status
        integer, dimension(:), intent(in) :: parent
        integer, dimension(:), intent(in) :: child
        logical, intent(in), optional :: fill_hepev4
        type(vector4_t), intent(in) :: p
        real(default), intent(in) :: m2
        integer, dimension(2), intent(in) :: col
        integer, intent(in) :: pol_status
        integer, intent(in) :: hel
        type(polarization_t), intent(in), optional :: pol
        type(vector4_t), intent(in) :: vtx
        logical :: hepev4
        hepev4 = .false.; if (present (fill_hepev4)) hepev4 = fill_hepev4
        IDHEP(i) = pdg
        select case (status)
            case (PRT_BEAM);      ISTHEP(i) = 2
            case (PRT_INCOMING);  ISTHEP(i) = 2
            case (PRT_OUTGOING);  ISTHEP(i) = 1
            case (PRT_VIRTUAL);   ISTHEP(i) = 2
            case (PRT_RESONANT);  ISTHEP(i) = 2
            case default;         ISTHEP(i) = 0
        end select
        select case (size (parent))
            case (0);      JMOHEP(:,i) = 0
            case (1);      JMOHEP(1,i) = parent(1); JMOHEP(2,i) = 0
            case default;   JMOHEP(:,i) = [ parent(1), parent(size (parent)) ]
        end select
        select case (size (child))

```

```

case (0);      JDAHEP(:,i) = 0
case (1);      JDAHEP(:,i) = child(1)
case default;  JDAHEP(:,i) = [ child(1), child(size (child)) ]
end select
PHEP(1:3,i) = refmt_tiny (vector3_get_components (space_part (p)))
PHEP(4,i) = refmt_tiny (energy (p))
PHEP(5,i) = refmt_tiny (sign (sqrt (abs (m2))), m2))
VHEP(1:3,i) = vtx%p(1:3)
VHEP(4,i) = vtx%p(0)
hepevt_pol(i) = hel
if (hepev4) then
  if (col(1) > 0) then
    icolorflowlh(1,i) = 500 + col(1)
  else
    icolorflowlh(1,i) = 0
  end if
  if (col(2) > 0) then
    icolorflowlh(2,i) = 500 + col(2)
  else
    icolorflowlh(2,i) = 0
  end if
  if (present (pol) .and. &
      pol_status == PRT_GENERIC_POLARIZATION) then
    if (pol%is_polarized ()) &
        spinlh(:,i) = pol%get_axis ()
  else
    spinlh(:,i) = zero
    spinlh(3,i) = hel
  end if
end if
end subroutine hepevt_set_particle

```

18.11.8 Event output

This is a verbose output of the HEPEVT block.

(HEP common: public)+≡

```
public :: hepevt_write_verbose
```

(HEP common: procedures)+≡

```

subroutine hepevt_write_verbose (unit)
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(A)") "HEPEVT Common Block"
  write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "NEVHEP", NEVHEP, &
    "Event number"
  write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "NHEP ", NHEP, &
    "Number of particles in event"
  do i = 1, NHEP
    write (u, "(1x,A,I0)") "Particle #", i
    write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)", advance="no") &
      "ISTHEP", ISTHEP(i), "Status code: "
    select case (ISTHEP(i))

```

```

case ( 0); write (u, "(A)") "null entry"
case ( 1); write (u, "(A)") "outgoing"
case ( 2); write (u, "(A)") "decayed"
case ( 3); write (u, "(A)") "documentation"
case (4:10); write (u, "(A)") "[unspecified]"
case (11:200); write (u, "(A)") "[model-specific]"
case (201:); write (u, "(A)") "[user-defined]"
case default; write (u, "(A)") "[undefined]"
end select
write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "IDHEP ", IDHEP(i), &
"PDG code of particle"
write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "JMOHEP", JMOHEP(:,i), &
"Index of first/second mother"
write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "JDAHEP", JDAHEP(:,i), &
"Index of first/last daughter"
write (u, "(3x,A6,' = ',ES12.5,1x,ES12.5,8x,A)") "PHEP12", &
PHEP(1:2,i), "Transversal momentum (x/y) in GeV"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PHEP3 ", PHEP(3,i), &
"Longitudinal momentum (z) in GeV"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PHEP4 ", PHEP(4,i), &
"Energy in GeV"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PHEP5 ", PHEP(5,i), &
"Invariant mass in GeV"
write (u, "(3x,A6,' = ',ES12.5,1x,ES12.5,8x,A)") "VHEP12", VHEP(1:2,i), &
"Transversal displacement (xy) in mm"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "VHEP3 ", VHEP(3,i), &
"Longitudinal displacement (z) in mm"
write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "VHEP4 ", VHEP(4,i), &
"Production time in mm"
end do
end subroutine hepevt_write_verbose

```

This is a verbose output of the HEPEUP block.

```

<HEP common: public>+≡
public :: hepeup_write_verbose

<HEP common: procedures>+≡
subroutine hepeup_write_verbose (unit)
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit); if (u < 0) return
write (u, "(A)") "HEPEUP Common Block"
write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "NUP ", NUP, &
"Number of particles in event"
write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "IDPRUP", IDPRUP, &
"Subprocess ID"
write (u, "(3x,A6,' = ',ES12.5,1x,20x,A)") "XWGTUP", XWGTUP, &
"Event weight"
write (u, "(3x,A6,' = ',ES12.5,1x,20x,A)") "SCALUP", SCALUP, &
"Event energy scale in GeV"
write (u, "(3x,A6,' = ',ES12.5,1x,20x,A)") "AQEDUP", AQEDUP, &
"QED coupling [-1 = undefined]"
write (u, "(3x,A6,' = ',ES12.5,1x,20x,A)") "AQCDUP", AQCDUP, &
"QCD coupling [-1 = undefined]"

```

```

do i = 1, NUP
  write (u, "(1x,A,I0)") "Particle #", i
  write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)") "IDUP ", IDUP(i), &
    "PDG code of particle"
  write (u, "(3x,A6,' = ',I9,3x,1x,20x,A)", advance="no") &
    "ISTUP ", ISTUP(i), "Status code: "
  select case (ISTUP(i))
  case (-1); write (u, "(A)") "incoming"
  case ( 1); write (u, "(A)") "outgoing"
  case (-2); write (u, "(A)") "spacelike"
  case ( 2); write (u, "(A)") "resonance"
  case ( 3); write (u, "(A)") "resonance (doc)"
  case (-9); write (u, "(A)") "beam"
  case default; write (u, "(A)") "[undefined]"
  end select
  write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "MOTHUP", MOTHUP(:,i), &
    "Index of first/last mother"
  write (u, "(3x,A6,' = ',I9,3x,1x,I9,3x,8x,A)") "ICOLUP", ICOLUP(:,i), &
    "Color/anticolor flow index"
  write (u, "(3x,A6,' = ',ES12.5,1x,ES12.5,8x,A)") "PUP1/2", PUP(1:2,i), &
    "Transversal momentum (x/y) in GeV"
  write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PUP3 ", PUP(3,i), &
    "Longitudinal momentum (z) in GeV"
  write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PUP4 ", PUP(4,i), &
    "Energy in GeV"
  write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "PUP5 ", PUP(5,i), &
    "Invariant mass in GeV"
  write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "VTIMUP", VTIMUP(i), &
    "Invariant lifetime in mm"
  write (u, "(3x,A6,' = ',ES12.5,1x,12x,8x,A)") "SPINUP", SPINUP(i), &
    "cos(spin angle) [9 = undefined]"
end do
end subroutine hepeup_write_verbose

```

18.11.9 Event output in various formats

This routine writes event output according to the LHEF standard. It uses the current contents of the HEPEUP block.

```

<HEP common: public>+≡
  public :: hepeup_write_lhef
  public :: hepeup_write_lha

<HEP common: procedures>+≡
  subroutine hepeup_write_lhef (unit)
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    if (debug_on) call msg_debug (D_EVENTS, "hepeup_write_lhef")
    if (debug_on) call msg_debug2 (D_EVENTS, "ID IST MOTH ICOL P VTIM SPIN")
    write (u, "(2(1x,I0),4(1x,ES17.10))") &
      NUP, IDPRUP, XWGTUP, SCALUP, AQCDUP, AQCDUP
    do i = 1, NUP
      write (u, "(6(1x,I0),7(1x,ES17.10))") &

```

```

        IDUP(i), ISTUP(i), MOTHUP(:,i), ICOLUP(:,i), &
        PUP(:,i), VTIMUP(i), SPINUP(i)
    if (debug2_active (D_EVENTS)) then
        write (msg_buffer, "(6(1x,I0),7(1x,ES17.10))") &
            IDUP(i), ISTUP(i), MOTHUP(:,i), ICOLUP(:,i), &
            PUP(:,i), VTIMUP(i), SPINUP(i)
        call msg_message ()
    end if
end do
end subroutine hepeup_write_lhef

subroutine hepeup_write_lha (unit)
    integer, intent(in), optional :: unit
    integer :: u, i
    integer, dimension(MAXNUP) :: spin_up
    spin_up = int(SPINUP)
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(2(1x,I5),1x,ES17.10,3(1x,ES13.6))") &
        NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP
    write (u, "(500(1x,I5))") IDUP(:NUP)
    write (u, "(500(1x,I5))") MOTHUP(1,:NUP)
    write (u, "(500(1x,I5))") MOTHUP(2,:NUP)
    write (u, "(500(1x,I5))") ICOLUP(1,:NUP)
    write (u, "(500(1x,I5))") ICOLUP(2,:NUP)
    write (u, "(500(1x,I5))") ISTUP(:NUP)
    write (u, "(500(1x,I5))") spin_up(:NUP)
    do i = 1, NUP
        write (u, "(1x,I5,4(1x,ES17.10))") i, PUP([ 4,1,2,3 ], i)
    end do
end subroutine hepeup_write_lha

```

This routine writes event output according to the HEPEVT standard. It uses the current contents of the HEPEVT block and some additional parameters according to the standard in WHIZARD 1. For the long ASCII format, the value of the sample function (i.e. the product of squared matrix element, structure functions and phase space factor is printed out). The option of reweighting matrix elements with respect to some reference cross section is not implemented in WHIZARD 2 for this event format, therefore the second entry in the long ASCII format (the function ratio) is always one. The ATHENA format is an implementation of the HEPEVT format that is readable by the ATLAS ATHENA software framework. It is very similar to the WHIZARD 1 HEPEVT format, except that it contains an event counter, a particle counter inside the event, and has the HEPEVT ISTHEP status before the PDG code. The MOKKA format is a special ASCII format that contains the information to be parsed to the MOKKA LC fast simulation software.

```

<HEP common: public>+≡
    public :: hepevt_write_hepevt
    public :: hepevt_write_ascii
    public :: hepevt_write_athena
    public :: hepevt_write_mokka
<HEP common: procedures>+≡

```

```

subroutine hepevt_write_hepevt (unit)
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(3(1x,I0),(1x,ES17.10))") &
    NHEP, hepevt_n_out, hepevt_n_remnants, hepevt_weight
  do i = 1, NHEP
    write (u, "(7(1x,I0))") &
      ISTHEP(i), IDHEP(i), JMOHEP(:,i), JDAHEP(:,i), hepevt_pol(i)
    write (u, "(5(1x,ES17.10))") PHEP(:,i)
    write (u, "(5(1x,ES17.10))") VHEP(:,i), 0.d0
  end do
end subroutine hepevt_write_hepevt

subroutine hepevt_write_ascii (unit, long)
  integer, intent(in), optional :: unit
  logical, intent(in) :: long
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(3(1x,I0),(1x,ES17.10))") &
    NHEP, hepevt_n_out, hepevt_n_remnants, hepevt_weight
  do i = 1, NHEP
    if (ISTHEP(i) /= 1) cycle
    write (u, "(2(1x,I0))") IDHEP(i), hepevt_pol(i)
    write (u, "(5(1x,ES17.10))") PHEP(:,i)
  end do
  if (long) then
    write (u, "(2(1x,ES17.10))") &
      hepevt_function_value, hepevt_function_ratio
  end if
end subroutine hepevt_write_ascii

subroutine hepevt_write_athena (unit)
  integer, intent(in), optional :: unit
  integer :: u, i, num_event
  num_event = 0
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(2(1x,I0))") NEVHEP, NHEP
  do i = 1, NHEP
    write (u, "(7(1x,I0))") &
      i, ISTHEP(i), IDHEP(i), JMOHEP(:,i), JDAHEP(:,i)
    write (u, "(5(1x,ES17.10))") PHEP(:,i)
    write (u, "(5(1x,ES17.10))") VHEP(1:4,i)
  end do
end subroutine hepevt_write_athena

subroutine hepevt_write_mokka (unit)
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(3(1x,I0),(1x,ES17.10))") &
    NHEP, hepevt_n_out, hepevt_n_remnants, hepevt_weight
  do i = 1, NHEP
    write (u, "(4(1x,I0),4(1x,ES17.10))") &

```

```

        ISTHEP(i), IDHEP(i), JDAHEP(1,i), JDAHEP(2,i), &
        PHEP(1:3,i), PHEP(5,i)
    end do
end subroutine hepevt_write_mokka

```

18.11.10 Event input in various formats

This routine writes event output according to the LHEF standard. It uses the current contents of the HEPEUP block.

```

<HEP common: public>+≡
    public :: hepeup_read_lhef

<HEP common: procedures>+≡
    subroutine hepeup_read_lhef (u)
        integer, intent(in) :: u
        integer :: i
        read (u, *) &
            NUP, IDPRUP, XWGTUP, SCALUP, AQEDUP, AQCDUP
        do i = 1, NUP
            read (u, *) &
                IDUP(i), ISTUP(i), MOTHUP(:,i), ICOLUP(:,i), &
                PUP(:,i), VTIMUP(i), SPINUP(i)
        end do
    end subroutine hepeup_read_lhef

```

18.11.11 Data Transfer: particle sets

The WHIZARD format for handling particle data in events is `particle_set_t`. We have to interface this to the common blocks.

We first create a new particle set that contains only the particles that are supported by the LHEF format. These are: beam, incoming, resonant, outgoing. We drop particles with unknown, virtual or beam-remnant status.

From this set we fill the common block. Event information such as process ID and weight is not transferred here; this has to be done by the caller. The spin information is set only if the particle has a unique mother, and if its polarization is fully defined.

We use this routine also to hand over information to Pythia which lets Tauola access SPINUP. Tauola expects in SPINUP the helicity and not the LHA convention. We switch to this mode with `tauola_convention`.

```

<HEP common: public>+≡
    public :: hepeup_from_particle_set

<HEP common: procedures>+≡
    subroutine hepeup_from_particle_set (pset_in, &
        keep_beams, keep_remnants, tauola_convention)
        type(particle_set_t), intent(in) :: pset_in
        type(particle_set_t), target :: pset
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        logical, intent(in), optional :: tauola_convention

```



```

integer :: i, n_parents, status, n_tot
integer, dimension(1) :: i_mother
logical :: kr, tc
kr = .true.; if (present (keep_remnants)) kr = keep_remnants
tc = .false.; if (present (tauola_convention)) tc = tauola_convention
call pset_in%filter_particles (pset, real_parents = .true. , &
    keep_beams = keep_beams, keep_virtuals = .false.)
n_tot = pset%get_n_tot ()
call hepeup_init (n_tot)
do i = 1, n_tot
    associate (prt => pset%prt(i))
        status = prt%get_status ()
        if (kr .and. status == PRT_BEAM_REMNANT &
            .and. prt%get_n_children () == 0) &
            status = PRT_OUTGOING
        call hepeup_set_particle (i, &
            prt%get_pdg (), &
            status, &
            prt%get_parents (), &
            prt%get_color (), &
            prt%get_momentum (), &
            prt%get_p2 ())
        n_parents = prt%get_n_parents ()
        call hepeup_set_particle_lifetime (i, &
            prt%get_lifetime ())
        if (.not. tc) then
            if (n_parents == 1) then
                i_mother = prt%get_parents ()
                select case (prt%get_polarization_status ())
                case (PRT_GENERIC_POLARIZATION)
                    call hepeup_set_particle_spin (i, &
                        prt%get_momentum (), &
                        prt%get_polarization (), &
                        pset%prt(i_mother(1))%get_momentum ())
                end select
            end if
        else
            select case (prt%get_polarization_status ())
            case (PRT_DEFINITE_HELICITY)
                SPINUP(i) = prt%get_helicity()
            end select
        end if
    end associate
end do
end subroutine hepeup_from_particle_set

```

Input. The particle set should be allocated properly, but we replace the particle contents.

If there are no beam particles in the event, we try to reconstruct beam particles and beam remnants. We assume for simplicity that the beam particles, if any, are the first two particles. If they are absent, the first two particles should be the incoming partons.

(HEP common: public)+=

```

public :: hepeup_to_particle_set
<HEP common: procedures>+≡
subroutine hepeup_to_particle_set &
    (particle_set, recover_beams, model, alt_model)
    type(particle_set_t), intent(inout), target :: particle_set
    logical, intent(in), optional :: recover_beams
    class(model_data_t), intent(in), target :: model, alt_model
    type(particle_t), dimension(:), allocatable :: prt
    integer, dimension(2) :: parent
    integer, dimension(:), allocatable :: child
    integer :: i, j, k, pdg, status
    type(flavor_t) :: flv
    type(color_t) :: col
    integer, dimension(2) :: c
    type(vector4_t) :: p
    real(default) :: p2
    logical :: reconstruct
    integer :: off
    if (present (recover_beams)) then
        reconstruct = recover_beams .and. .not. all (ISTUP(1:2) == PRT_BEAM)
    else
        reconstruct = .false.
    end if
    if (reconstruct) then
        off = 4
    else
        off = 0
    end if
    allocate (prt (NUP + off), child (NUP + off))
    do i = 1, NUP
        k = i + off
        call hepeup_get_particle (i, pdg, status, col = c, p = p, m2 = p2)
        call flv%init (pdg, model, alt_model)
        call prt(k)%set_flavor (flv)
        call prt(k)%reset_status (status)
        call col%init (c)
        call prt(k)%set_color (col)
        call prt(k)%set_momentum (p, p2)
        where (MOTHUP(:,i) /= 0)
            parent = MOTHUP(:,i) + off
        elsewhere
            parent = 0
        end where
        call prt(k)%set_parents (parent)
        child = [(j, j = 1 + off, NUP + off)]
        where (MOTHUP(1,:NUP) /= i .and. MOTHUP(2,:NUP) /= i) child = 0
        call prt(k)%set_children (child)
    end do
    if (reconstruct) then
        do k = 1, 2
            call prt(k)%reset_status (PRT_BEAM)
            call prt(k)%set_children ([k+2,k+4])
        end do
        do k = 3, 4

```

```

        call prt(k)%reset_status (PRT_BEAM_REMNANT)
        call prt(k)%set_parents ([k-2])
    end do
    do k = 5, 6
        call prt(k)%set_parents ([k-4])
    end do
end if
call particle_set%replace (prt)
end subroutine hepeup_to_particle_set

```

The HEPEVT common block is quite similar, but does contain less information, e.g. no color flows (it was LEP time). The spin information is set only if the particle has a unique mother, and if its polarization is fully defined.

```

<HEP common: public>+≡
    public :: hepevt_from_particle_set

<HEP common: procedures>+≡
    subroutine hepevt_from_particle_set &
        (particle_set, keep_beams, keep_remnants, ensure_order, fill_hepev4)
        type(particle_set_t), intent(in) :: particle_set
        type(particle_set_t), target :: pset_hepevt, pset_tmp
        logical, intent(in), optional :: keep_beams
        logical, intent(in), optional :: keep_remnants
        logical, intent(in), optional :: ensure_order
        logical, intent(in), optional :: fill_hepev4
        integer :: i, status, n_tot
        logical :: activate_remnants, ensure
        activate_remnants = .true.
        if (present (keep_remnants)) activate_remnants = keep_remnants
        ensure = .false.
        if (present (ensure_order)) ensure = ensure_order
        call particle_set%filter_particles (pset_tmp, real_parents = .true., &
            keep_virtualls = .false., keep_beams = keep_beams)
        if (ensure) then
            call pset_tmp%to_hepevt_form (pset_hepevt)
        else
            pset_hepevt = pset_tmp
        end if
        n_tot = pset_hepevt%get_n_tot ()
        call hepevt_init (n_tot, pset_hepevt%get_n_out ())
        do i = 1, n_tot
            associate (prt => pset_hepevt%prt(i))
                status = prt%get_status ()
                if (activate_remnants &
                    .and. status == PRT_BEAM_REMNANT &
                    .and. prt%get_n_children () == 0) &
                    status = PRT_OUTGOING
                select case (prt%get_polarization_status ())
                case (PRT_GENERIC_POLARIZATION)
                    call hepevt_set_particle (i, &
                        prt%get_pdg (), status, &
                        prt%get_parents (), &
                        prt%get_children (), &
                        prt%get_momentum (), &

```

```

        prt%get_p2 (), &
        prt%get_helicity (), &
        prt%get_vertex (), &
        prt%get_color (), &
        prt%get_polarization_status (), &
        pol = prt%get_polarization (), &
        fill_hepev4 = fill_hepev4)
    case default
        call hepevt_set_particle (i, &
            prt%get_pdg (), status, &
            prt%get_parents (), &
            prt%get_children (), &
            prt%get_momentum (), &
            prt%get_p2 (), &
            prt%get_helicity (), &
            prt%get_vertex (), &
            prt%get_color (), &
            prt%get_polarization_status (), &
            fill_hepev4 = fill_hepev4)
    end select
end associate
end do
call pset_hepevt%final ()
end subroutine hepevt_from_particle_set

```

18.12 HepMC events

This section provides the interface to the HepMC C++ library for handling Monte-Carlo events.

Each C++ class of HepMC that we use is mirrored by a Fortran type, which contains as its only component the C pointer to the C++ object.

Each C++ method of HepMC that we use has a C wrapper function. This function takes a pointer to the host object as its first argument. Further arguments are either C pointers, or in the case of simple types (integer, real), interoperable C/Fortran objects.

The C wrapper functions have explicit interfaces in the Fortran module. They are called by Fortran wrapper procedures. These are treated as methods of the corresponding Fortran type.

(hepmc_interface.f90)≡
⟨File header⟩

```

module hepmc_interface

    use, intrinsic :: iso_c_binding !NODEP!

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use constants, only: PI
    use physics_defs, only: pb_per_fb
    use system_dependencies, only: HEPMC2_AVAILABLE
    use system_dependencies, only: HEPMC3_AVAILABLE

```

```

    use diagnostics
    use lorentz
    use flavors
    use colors
    use helicities
    use polarizations
    use event_handles, only: event_handle_t

    <Standard module head>

    <HepMC interface: public>

    <HepMC interface: types>

    <HepMC interface: parameters>

    <HepMC interface: interfaces>

    contains

    <HepMC interface: procedures>

    end module hepmc_interface

```

18.12.1 Interface check

This function can be called in order to verify that we are using the actual HepMC library, and not the dummy version.

```

<HepMC interface: interfaces>≡
    interface
        logical(c_bool) function hepmc_available () bind(C)
            import
        end function hepmc_available
    end interface

<HepMC interface: public>≡
    public :: hepmc_is_available

<HepMC interface: procedures>≡
    function hepmc_is_available () result (flag)
        logical :: flag
        flag = hepmc_available ()
    end function hepmc_is_available

```

18.12.2 FourVector

The C version of four-vectors is often transferred by value, and the associated procedures are all inlined. The wrapper needs to transfer by reference, so we create FourVector objects on the heap which have to be deleted explicitly. The input is a `vector4_t` or `vector3_t` object from the `lorentz` module.

```

<HepMC interface: public>+≡
    public :: hepmc_four_vector_t

```

```

<HepMC interface: types>≡
  type :: hepmc_four_vector_t
  private
  type(c_ptr) :: obj
  end type hepmc_four_vector_t

```

In the C constructor, the zero-component (fourth argument) is optional; if missing, it is set to zero. The Fortran version has initializer form and takes either a three-vector or a four-vector. A further version extracts the four-vector from a HepMC particle object.

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_four_vector_xyz (x, y, z) bind(C)
    import
    real(c_double), value :: x, y, z
    end function new_four_vector_xyz
  end interface
  interface
    type(c_ptr) function new_four_vector_xyz_t (x, y, z, t) bind(C)
    import
    real(c_double), value :: x, y, z, t
    end function new_four_vector_xyz_t
  end interface

<HepMC interface: public>+≡
  public :: hepmc_four_vector_init

<HepMC interface: interfaces>+≡
  interface hepmc_four_vector_init
    module procedure hepmc_four_vector_init_v4
    module procedure hepmc_four_vector_init_v3
    module procedure hepmc_four_vector_init_hepmc_ptr
  end interface

<HepMC interface: procedures>+≡
  subroutine hepmc_four_vector_init_v4 (pp, p)
    type(hepmc_four_vector_t), intent(out) :: pp
    type(vector4_t), intent(in) :: p
    real(default), dimension(0:3) :: pa
    pa = vector4_get_components (p)
    pp%obj = new_four_vector_xyz_t &
      (real (pa(1), c_double), &
       real (pa(2), c_double), &
       real (pa(3), c_double), &
       real (pa(0), c_double))
  end subroutine hepmc_four_vector_init_v4

  subroutine hepmc_four_vector_init_v3 (pp, p)
    type(hepmc_four_vector_t), intent(out) :: pp
    type(vector3_t), intent(in) :: p
    real(default), dimension(3) :: pa
    pa = vector3_get_components (p)
    pp%obj = new_four_vector_xyz &
      (real (pa(1), c_double), &
       real (pa(2), c_double), &

```

```

        real (pa(3), c_double))
end subroutine hepmc_four_vector_init_v3

subroutine hepmc_four_vector_init_hepmc_prt (pp, prt)
    type(hepmc_four_vector_t), intent(out) :: pp
    type(hepmc_particle_t), intent(in) :: prt
    pp%obj = gen_particle_momentum (prt%obj)
end subroutine hepmc_four_vector_init_hepmc_prt

```

Here, the destructor is explicitly needed.

```

<HepMC interface: interfaces>+≡
    interface
        subroutine four_vector_delete (p_obj) bind(C)
            import
            type(c_ptr), value :: p_obj
        end subroutine four_vector_delete
    end interface

<HepMC interface: public>+≡
    public :: hepmc_four_vector_final

<HepMC interface: procedures>+≡
    subroutine hepmc_four_vector_final (p)
        type(hepmc_four_vector_t), intent(inout) :: p
        call four_vector_delete (p%obj)
    end subroutine hepmc_four_vector_final

```

Convert to a Lorentz vector.

```

<HepMC interface: interfaces>+≡
    interface
        function four_vector_px (p_obj) result (px) bind(C)
            import
            real(c_double) :: px
            type(c_ptr), value :: p_obj
        end function four_vector_px
    end interface

    interface
        function four_vector_py (p_obj) result (py) bind(C)
            import
            real(c_double) :: py
            type(c_ptr), value :: p_obj
        end function four_vector_py
    end interface

    interface
        function four_vector_pz (p_obj) result (pz) bind(C)
            import
            real(c_double) :: pz
            type(c_ptr), value :: p_obj
        end function four_vector_pz
    end interface

    interface
        function four_vector_e (p_obj) result (e) bind(C)
            import
            real(c_double) :: e

```

```

        type(c_ptr), value :: p_obj
    end function four_vector_e
end interface
<HepMC interface: public>+≡
    public :: hepmc_four_vector_to_vector4
<HepMC interface: procedures>+≡
    subroutine hepmc_four_vector_to_vector4 (pp, p)
        type(hepmc_four_vector_t), intent(in) :: pp
        type(vector4_t), intent(out) :: p
        real(default) :: E
        real(default), dimension(3) :: p3
        E = four_vector_e (pp%obj)
        p3(1) = four_vector_px (pp%obj)
        p3(2) = four_vector_py (pp%obj)
        p3(3) = four_vector_pz (pp%obj)
        p = vector4_moving (E, vector3_moving (p3))
    end subroutine hepmc_four_vector_to_vector4

```

18.12.3 Polarization

Polarization objects are temporarily used for assigning particle polarization. We add a flag `polarized`. If this is false, the polarization is not set and should not be transferred to `hepmc_particle` objects.

```

<HepMC interface: public>+≡
    public :: hepmc_polarization_t
<HepMC interface: types>+≡
    type :: hepmc_polarization_t
    private
    logical :: polarized = .false.
    type(c_ptr) :: obj
end type hepmc_polarization_t

```

Constructor. The C wrapper takes polar and azimuthal angle as arguments. The Fortran version allows for either a complete polarization density matrix, or for a definite (diagonal) helicity.

HepMC does not allow to specify the degree of polarization, therefore we have to map it to either 0 or 1. We choose 0 for polarization less than 0.5 and 1 for polarization greater than 0.5. Even this simplification works only for spin-1/2 and for massless particles; massive vector bosons cannot be treated this way. In particular, zero helicity is always translated as unpolarized.

For massive vector bosons, we arbitrarily choose the convention that the longitudinal (zero) helicity state is mapped to the theta angle $\pi/2$. This works under the condition that helicity is projected onto one of the basis states.

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function new_polarization (theta, phi) bind(C)
            import
            real(c_double), value :: theta, phi
        end function new_polarization
    end interface

```



```

<HepMC interface: public>+≡
    public :: hepmc_polarization_init

<HepMC interface: interfaces>+≡
    interface hepmc_polarization_init
        module procedure hepmc_polarization_init_pol
        module procedure hepmc_polarization_init_hel
        module procedure hepmc_polarization_init_int
    end interface

<HepMC interface: procedures>+≡
    subroutine hepmc_polarization_init_pol (hpol, pol)
        type(hepmc_polarization_t), intent(out) :: hpol
        type(polarization_t), intent(in) :: pol
        real(default) :: r, theta, phi
        if (pol%is_polarized ()) then
            call pol%to_angles (r, theta, phi)
            if (r >= 0.5) then
                hpol%polarized = .true.
                hpol%obj = new_polarization &
                    (real (theta, c_double), real (phi, c_double))
            end if
        end if
    end subroutine hepmc_polarization_init_pol

    subroutine hepmc_polarization_init_hel (hpol, hel)
        type(hepmc_polarization_t), intent(out) :: hpol
        type(helicity_t), intent(in) :: hel
        integer, dimension(2) :: h
        if (hel%is_defined ()) then
            h = hel%to_pair ()
            select case (h(1))
            case (1:)
                hpol%polarized = .true.
                hpol%obj = new_polarization (0._c_double, 0._c_double)
            case (-1)
                hpol%polarized = .true.
                hpol%obj = new_polarization (real (pi, c_double), 0._c_double)
            case (0)
                hpol%polarized = .true.
                hpol%obj = new_polarization (real (pi/2, c_double), 0._c_double)
            end select
        end if
    end subroutine hepmc_polarization_init_hel

    subroutine hepmc_polarization_init_int (hpol, hel)
        type(hepmc_polarization_t), intent(out) :: hpol
        integer, intent(in) :: hel
        select case (hel)
        case (1:)
            hpol%polarized = .true.
            hpol%obj = new_polarization (0._c_double, 0._c_double)
        case (-1)
            hpol%polarized = .true.
            hpol%obj = new_polarization (real (pi, c_double), 0._c_double)
        end select
    end subroutine hepmc_polarization_init_int

```

```

    case (0)
        hpol%polarized = .true.
        hpol%obj = new_polarization (real (pi/2, c_double), 0._c_double)
    end select
end subroutine hepmc_polarization_init_int

```

Destructor. The C object is deallocated only if the polarized flag is set.

```

<HepMC interface: interfaces>+≡
    interface
        subroutine polarization_delete (pol_obj) bind(C)
            import
            type(c_ptr), value :: pol_obj
        end subroutine polarization_delete
    end interface
<HepMC interface: public>+≡
    public :: hepmc_polarization_final
<HepMC interface: procedures>+≡
    subroutine hepmc_polarization_final (hpol)
        type(hepmc_polarization_t), intent(inout) :: hpol
        if (hpol%polarized) call polarization_delete (hpol%obj)
    end subroutine hepmc_polarization_final

```

Recover polarization from HepMC polarization object (with the abovementioned deficiencies).

```

<HepMC interface: interfaces>+≡
    interface
        function polarization_theta (pol_obj) result (theta) bind(C)
            import
            real(c_double) :: theta
            type(c_ptr), value :: pol_obj
        end function polarization_theta
    end interface
    interface
        function polarization_phi (pol_obj) result (phi) bind(C)
            import
            real(c_double) :: phi
            type(c_ptr), value :: pol_obj
        end function polarization_phi
    end interface
<HepMC interface: public>+≡
    public :: hepmc_polarization_to_pol
<HepMC interface: procedures>+≡
    subroutine hepmc_polarization_to_pol (hpol, flv, pol)
        type(hepmc_polarization_t), intent(in) :: hpol
        type(flavor_t), intent(in) :: flv
        type(polarization_t), intent(out) :: pol
        real(default) :: theta, phi
        theta = polarization_theta (hpol%obj)
        phi = polarization_phi (hpol%obj)
        call pol%init_angles (flv, 1._default, theta, phi)
    end subroutine hepmc_polarization_to_pol

```

Recover helicity. Here, ϕ is ignored and only the sign of $\cos \theta$ is relevant, mapped to positive/negative helicity.

```

<HepMC interface: public>+≡
    public :: hepmc_polarization_to_hel

<HepMC interface: procedures>+≡
    subroutine hepmc_polarization_to_hel (hpol, flv, hel)
        type(hepmc_polarization_t), intent(in) :: hpol
        type(flavor_t), intent(in) :: flv
        type(helicity_t), intent(out) :: hel
        real(default) :: theta
        integer :: hmax
        theta = polarization_theta (hpol%obj)
        hmax = flv%get_spin_type () / 2
        call hel%init (sign (hmax, nint (cos (theta))))
    end subroutine hepmc_polarization_to_hel

```

18.12.4 GenParticle

Particle objects have the obvious meaning.

```

<HepMC interface: public>+≡
    public :: hepmc_particle_t

<HepMC interface: types>+≡
    type :: hepmc_particle_t
    private
    type(c_ptr) :: obj
    end type hepmc_particle_t

```

Constructor. The C version takes a FourVector object, which in the Fortran wrapper is created on the fly from a `vector4` Lorentz vector.

No destructor is needed as long as all particles are entered into vertex containers.

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function new_gen_particle (prt_obj, pdg_id, status) bind(C)
            import
            type(c_ptr), value :: prt_obj
            integer(c_int), value :: pdg_id, status
        end function new_gen_particle
    end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_init

<HepMC interface: procedures>+≡
    subroutine hepmc_particle_init (prt, p, pdg, status)
        type(hepmc_particle_t), intent(out) :: prt
        type(vector4_t), intent(in) :: p
        integer, intent(in) :: pdg, status
        type(hepmc_four_vector_t) :: pp
        call hepmc_four_vector_init (pp, p)
        prt%obj = new_gen_particle (pp%obj, int (pdg, c_int), int (status, c_int))
    end subroutine hepmc_particle_init

```

```

    call hepmc_four_vector_final (pp)
end subroutine hepmc_particle_init

```

Set the particle color flow.

<HepMC interface: interfaces>+≡

```

interface
  subroutine gen_particle_set_flow (prt_obj, code_index, code) bind(C)
  import
    type(c_ptr), value :: prt_obj
    integer(c_int), value :: code_index, code
  end subroutine gen_particle_set_flow
end interface

```

Set the particle color. Either from a `color_t` object or directly from a pair of integers.

<HepMC interface: interfaces>+≡

```

interface hepmc_particle_set_color
  module procedure hepmc_particle_set_color_col
  module procedure hepmc_particle_set_color_int
end interface hepmc_particle_set_color

```

<HepMC interface: public>+≡

```

public :: hepmc_particle_set_color

```

<HepMC interface: procedures>+≡

```

subroutine hepmc_particle_set_color_col (prt, col)
  type(hepmc_particle_t), intent(inout) :: prt
  type(color_t), intent(in) :: col
  integer(c_int) :: c
  c = col%get_col ()
  if (c /= 0) call gen_particle_set_flow (prt%obj, 1_c_int, c)
  c = col%get_acl ()
  if (c /= 0) call gen_particle_set_flow (prt%obj, 2_c_int, c)
end subroutine hepmc_particle_set_color_col

subroutine hepmc_particle_set_color_int (prt, col)
  type(hepmc_particle_t), intent(inout) :: prt
  integer, dimension(2), intent(in) :: col
  integer(c_int) :: c
  c = col(1)
  if (c /= 0) call gen_particle_set_flow (prt%obj, 1_c_int, c)
  c = col(2)
  if (c /= 0) call gen_particle_set_flow (prt%obj, 2_c_int, c)
end subroutine hepmc_particle_set_color_int

```

Set the particle polarization. For the restrictions on particle polarization in HepMC, see above `hepmc_polarization_init`.

<HepMC interface: interfaces>+≡

```

interface
  subroutine gen_particle_set_polarization (prt_obj, pol_obj) bind(C)
  import
    type(c_ptr), value :: prt_obj, pol_obj
  end subroutine gen_particle_set_polarization
end interface

```

```

<HepMC interface: public>+≡
    public :: hepmc_particle_set_polarization

<HepMC interface: interfaces>+≡
    interface hepmc_particle_set_polarization
        module procedure hepmc_particle_set_polarization_pol
        module procedure hepmc_particle_set_polarization_hel
        module procedure hepmc_particle_set_polarization_int
    end interface

<HepMC interface: procedures>+≡
    subroutine hepmc_particle_set_polarization_pol (prt, pol)
        type(hepmc_particle_t), intent(inout) :: prt
        type(polarization_t), intent(in) :: pol
        type(hepmc_polarization_t) :: hpol
        call hepmc_polarization_init (hpol, pol)
        if (hpol%polarized) call gen_particle_set_polarization (prt%obj, hpol%obj)
        call hepmc_polarization_final (hpol)
    end subroutine hepmc_particle_set_polarization_pol

    subroutine hepmc_particle_set_polarization_hel (prt, hel)
        type(hepmc_particle_t), intent(inout) :: prt
        type(helicity_t), intent(in) :: hel
        type(hepmc_polarization_t) :: hpol
        call hepmc_polarization_init (hpol, hel)
        if (hpol%polarized) call gen_particle_set_polarization (prt%obj, hpol%obj)
        call hepmc_polarization_final (hpol)
    end subroutine hepmc_particle_set_polarization_hel

    subroutine hepmc_particle_set_polarization_int (prt, hel)
        type(hepmc_particle_t), intent(inout) :: prt
        integer, intent(in) :: hel
        type(hepmc_polarization_t) :: hpol
        call hepmc_polarization_init (hpol, hel)
        if (hpol%polarized) call gen_particle_set_polarization (prt%obj, hpol%obj)
        call hepmc_polarization_final (hpol)
    end subroutine hepmc_particle_set_polarization_int

```

Return the HepMC barcode (unique integer ID) of the particle.

```

<HepMC interface: interfaces>+≡
    interface
        function gen_particle_barcode (prt_obj) result (barcode) bind(C)
            import
            integer(c_int) :: barcode
            type(c_ptr), value :: prt_obj
        end function gen_particle_barcode
    end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_get_barcode

<HepMC interface: procedures>+≡
    function hepmc_particle_get_barcode (prt) result (barcode)
        integer :: barcode
        type(hepmc_particle_t), intent(in) :: prt
        barcode = gen_particle_barcode (prt%obj)
    end function

```

```
end function hepmc_particle_get_barcode
```

Return the four-vector component of the particle object as a `vector4_t` Lorentz vector.

```
<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function gen_particle_momentum (prt_obj) bind(C)
    import
    type(c_ptr), value :: prt_obj
    end function gen_particle_momentum
  end interface

<HepMC interface: public>+≡
  public :: hepmc_particle_get_momentum

<HepMC interface: procedures>+≡
  function hepmc_particle_get_momentum (prt) result (p)
    type(vector4_t) :: p
    type(hepmc_particle_t), intent(in) :: prt
    type(hepmc_four_vector_t) :: pp
    call hepmc_four_vector_init (pp, prt)
    call hepmc_four_vector_to_vector4 (pp, p)
    call hepmc_four_vector_final (pp)
  end function hepmc_particle_get_momentum
```

Return the invariant mass squared of the particle object. HepMC stores the signed invariant mass (no squaring).

```
<HepMC interface: interfaces>+≡
  interface
    function gen_particle_generated_mass (prt_obj) result (mass) bind(C)
    import
    real(c_double) :: mass
    type(c_ptr), value :: prt_obj
    end function gen_particle_generated_mass
  end interface

<HepMC interface: public>+≡
  public :: hepmc_particle_get_mass_squared

<HepMC interface: procedures>+≡
  function hepmc_particle_get_mass_squared (prt) result (m2)
    real(default) :: m2
    type(hepmc_particle_t), intent(in) :: prt
    real(default) :: m
    m = gen_particle_generated_mass (prt%obj)
    m2 = sign (m**2, m)
  end function hepmc_particle_get_mass_squared
```

Return the PDG ID:

```
<HepMC interface: interfaces>+≡
  interface
    function gen_particle_pdg_id (prt_obj) result (pdg_id) bind(C)
    import
    integer(c_int) :: pdg_id
```

```

        type(c_ptr), value :: prt_obj
    end function gen_particle_pdg_id
end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_get_pdg

<HepMC interface: procedures>+≡
    function hepmc_particle_get_pdg (prt) result (pdg)
        integer :: pdg
        type(hepmc_particle_t), intent(in) :: prt
        pdg = gen_particle_pdg_id (prt%obj)
    end function hepmc_particle_get_pdg

Return the status code:

<HepMC interface: interfaces>+≡
    interface
        function gen_particle_status (prt_obj) result (status) bind(C)
            import
            integer(c_int) :: status
            type(c_ptr), value :: prt_obj
        end function gen_particle_status
    end interface

<HepMC interface: public>+≡
    public :: hepmc_particle_get_status

<HepMC interface: procedures>+≡
    function hepmc_particle_get_status (prt) result (status)
        integer :: status
        type(hepmc_particle_t), intent(in) :: prt
        status = gen_particle_status (prt%obj)
    end function hepmc_particle_get_status

<HepMC interface: interfaces>+≡
    interface
        function gen_particle_is_beam (prt_obj) result (is_beam) bind(C)
            import
            logical(c_bool) :: is_beam
            type(c_ptr), value :: prt_obj
        end function gen_particle_is_beam
    end interface

Determine whether a particle is a beam particle.

<HepMC interface: public>+≡
    public :: hepmc_particle_is_beam

<HepMC interface: procedures>+≡
    function hepmc_particle_is_beam (prt) result (is_beam)
        logical :: is_beam
        type(hepmc_particle_t), intent(in) :: prt
        is_beam = gen_particle_is_beam (prt%obj)
    end function hepmc_particle_is_beam

```

Return the production/decay vertex (as a pointer, no finalization necessary).

(HepMC interface: interfaces)+≡

```
interface
  type(c_ptr) function gen_particle_production_vertex (prt_obj) bind(C)
  import
  type(c_ptr), value :: prt_obj
  end function gen_particle_production_vertex
end interface
interface
  type(c_ptr) function gen_particle_end_vertex (prt_obj) bind(C)
  import
  type(c_ptr), value :: prt_obj
  end function gen_particle_end_vertex
end interface
```

(HepMC interface: public)+≡

```
public :: hepmc_particle_get_production_vertex
public :: hepmc_particle_get_decay_vertex
```

(HepMC interface: procedures)+≡

```
function hepmc_particle_get_production_vertex (prt) result (v)
  type(hepmc_vertex_t) :: v
  type(hepmc_particle_t), intent(in) :: prt
  v%obj = gen_particle_production_vertex (prt%obj)
end function hepmc_particle_get_production_vertex

function hepmc_particle_get_decay_vertex (prt) result (v)
  type(hepmc_vertex_t) :: v
  type(hepmc_particle_t), intent(in) :: prt
  v%obj = gen_particle_end_vertex (prt%obj)
end function hepmc_particle_get_decay_vertex
```

Convenience function: Return the array of parent particles for a given HepMC particle. The contents are HepMC barcodes that still have to be mapped to the particle indices.

(HepMC interface: public)+≡

```
public :: hepmc_particle_get_parent_barcodes
public :: hepmc_particle_get_child_barcodes
```

(HepMC interface: procedures)+≡

```
function hepmc_particle_get_parent_barcodes (prt) result (parent_barcode)
  type(hepmc_particle_t), intent(in) :: prt
  integer, dimension(:), allocatable :: parent_barcode
  type(hepmc_vertex_t) :: v
  type(hepmc_vertex_particle_in_iterator_t) :: it
  integer :: i
  v = hepmc_particle_get_production_vertex (prt)
  if (hepmc_vertex_is_valid (v)) then
    allocate (parent_barcode (hepmc_vertex_get_n_in (v)))
    if (size (parent_barcode) /= 0) then
      if (HEPMC2_AVAILABLE) then
        call hepmc_vertex_particle_in_iterator_init (it, v)
        do i = 1, size (parent_barcode)
          parent_barcode(i) = hepmc_particle_get_barcode &
            (hepmc_vertex_particle_in_iterator_get (it))
        end do
      else
        ! Fallback to manual iteration
        do i = 1, size (parent_barcode)
          parent_barcode(i) = hepmc_particle_get_barcode (v%obj, i)
        end do
      end if
    end if
  end if
end function
```



```

        call hepmc_vertex_particle_in_iterator_advance (it)
    end do
    call hepmc_vertex_particle_in_iterator_final (it)
else if (HEPMC3_AVAILABLE) then
    do i = 1, size (parent_barcode)
        parent_barcode(i) = hepmc_particle_get_barcode &
            (hepmc_vertex_get_nth_particle_in (v, i))
    end do
end if
end if
else
    allocate (parent_barcode (0))
end if
end function hepmc_particle_get_parent_barcodes

function hepmc_particle_get_child_barcodes (prt) result (child_barcode)
    type(hepmc_particle_t), intent(in) :: prt
    integer, dimension(:), allocatable :: child_barcode
    type(hepmc_vertex_t) :: v
    type(hepmc_vertex_particle_out_iterator_t) :: it
    integer :: i
    v = hepmc_particle_get_decay_vertex (prt)
    if (hepmc_vertex_is_valid (v)) then
        allocate (child_barcode (hepmc_vertex_get_n_out (v)))
        if (size (child_barcode) /= 0) then
            if (HEPMC2_AVAILABLE) then
                call hepmc_vertex_particle_out_iterator_init (it, v)
                do i = 1, size (child_barcode)
                    child_barcode(i) = hepmc_particle_get_barcode &
                        (hepmc_vertex_particle_out_iterator_get (it))
                    call hepmc_vertex_particle_out_iterator_advance (it)
                end do
                call hepmc_vertex_particle_out_iterator_final (it)
            else if (HEPMC3_AVAILABLE) then
                do i = 1, size (child_barcode)
                    child_barcode(i) = hepmc_particle_get_barcode &
                        (hepmc_vertex_get_nth_particle_out (v, i))
                end do
            end if
        end if
    end if
else
    allocate (child_barcode (0))
end if
end function hepmc_particle_get_child_barcodes

```

Return the polarization (assuming that the particle is completely polarized).
 Note that the generated polarization object needs finalization.

(*HepMC interface: interfaces*)+≡

```

interface
    type(c_ptr) function gen_particle_polarization (prt_obj) bind(C)
    import
    type(c_ptr), value :: prt_obj
end function gen_particle_polarization

```

```

end interface

<HepMC interface: public>+≡
  public :: hepmc_particle_get_polarization

<HepMC interface: procedures>+≡
  function hepmc_particle_get_polarization (prt) result (pol)
    type(hepmc_polarization_t) :: pol
    type(hepmc_particle_t), intent(in) :: prt
    pol%obj = gen_particle_polarization (prt%obj)
  end function hepmc_particle_get_polarization

Return the particle color as a two-dimensional array (color, anticolor).

<HepMC interface: interfaces>+≡
  interface
    function gen_particle_flow (prt_obj, code_index) result (code) bind(C)
      import
      integer(c_int) :: code
      type(c_ptr), value :: prt_obj
      integer(c_int), value :: code_index
    end function gen_particle_flow
  end interface

<HepMC interface: public>+≡
  public :: hepmc_particle_get_color

<HepMC interface: procedures>+≡
  function hepmc_particle_get_color (prt) result (col)
    integer, dimension(2) :: col
    type(hepmc_particle_t), intent(in) :: prt
    col(1) = gen_particle_flow (prt%obj, 1)
    col(2) = - gen_particle_flow (prt%obj, 2)
  end function hepmc_particle_get_color

<HepMC interface: interfaces>+≡
  interface
    function gen_vertex_pos_x (v_obj) result (x) bind(C)
      import
      type(c_ptr), value :: v_obj
      real(c_double) :: x
    end function gen_vertex_pos_x
  end interface
  interface
    function gen_vertex_pos_y (v_obj) result (y) bind(C)
      import
      type(c_ptr), value :: v_obj
      real(c_double) :: y
    end function gen_vertex_pos_y
  end interface
  interface
    function gen_vertex_pos_z (v_obj) result (z) bind(C)
      import
      type(c_ptr), value :: v_obj
      real(c_double) :: z
    end function gen_vertex_pos_z
  end interface

```

```

end interface
interface
  function gen_vertex_time (v_obj) result (t) bind(C)
    import
    type(c_ptr), value :: v_obj
    real(c_double) :: t
  end function gen_vertex_time
end interface

<HepMC interface: public>+≡
  public :: hepmc_vertex_to_vertex

<HepMC interface: procedures>+≡
  function hepmc_vertex_to_vertex (vtx) result (v)
    type(hepmc_vertex_t), intent(in) :: vtx
    type(vector4_t) :: v
    real(default) :: t, vx, vy, vz
    if (hepmc_vertex_is_valid (vtx)) then
      t = gen_vertex_time (vtx%obj)
      vx = gen_vertex_pos_x (vtx%obj)
      vy = gen_vertex_pos_y (vtx%obj)
      vz = gen_vertex_pos_z (vtx%obj)
      v = vector4_moving (t, &
        vector3_moving ([vx, vy, vz]))
    end if
  end function hepmc_vertex_to_vertex

```

18.12.5 GenVertex

Vertices are made of particles (incoming and outgoing).

```

<HepMC interface: public>+≡
  public :: hepmc_vertex_t

<HepMC interface: types>+≡
  type :: hepmc_vertex_t
  private
  type(c_ptr) :: obj
  end type hepmc_vertex_t

```

Constructor. Two versions, one plain, one with the position in space and time (measured in mm) as argument. The Fortran version has initializer form, and the vertex position is an optional argument.

A destructor is unnecessary as long as all vertices are entered into an event container.

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_gen_vertex () bind(C)
      import
    end function new_gen_vertex
  end interface
  interface
    type(c_ptr) function new_gen_vertex_pos (prt_obj) bind(C)
      import
    end function new_gen_vertex_pos
  end interface

```

```

        type(c_ptr), value :: prt_obj
    end function new_gen_vertex_pos
end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_init

<HepMC interface: procedures>+≡
    subroutine hepmc_vertex_init (v, x)
        type(hepmc_vertex_t), intent(out) :: v
        type(vector4_t), intent(in), optional :: x
        type(hepmc_four_vector_t) :: pos
        if (present (x)) then
            call hepmc_four_vector_init (pos, x)
            v%obj = new_gen_vertex_pos (pos%obj)
            call hepmc_four_vector_final (pos)
        else
            v%obj = new_gen_vertex ()
        end if
    end subroutine hepmc_vertex_init

```

Return true if the vertex pointer is non-null:

```

<HepMC interface: interfaces>+≡
    interface
        function gen_vertex_is_valid (v_obj) result (flag) bind(C)
            import
            logical(c_bool) :: flag
            type(c_ptr), value :: v_obj
        end function gen_vertex_is_valid
    end interface

    <HepMC interface: public>+≡
        public :: hepmc_vertex_is_valid

    <HepMC interface: procedures>+≡
        function hepmc_vertex_is_valid (v) result (flag)
            logical :: flag
            type(hepmc_vertex_t), intent(in) :: v
            flag = gen_vertex_is_valid (v%obj)
        end function hepmc_vertex_is_valid

```

Add a particle to a vertex, incoming or outgoing.

```

<HepMC interface: interfaces>+≡
    interface
        subroutine gen_vertex_add_particle_in (v_obj, prt_obj) bind(C)
            import
            type(c_ptr), value :: v_obj, prt_obj
        end subroutine gen_vertex_add_particle_in
    end interface

    interface
        subroutine gen_vertex_add_particle_out (v_obj, prt_obj) bind(C)
            import
            type(c_ptr), value :: v_obj, prt_obj
        end subroutine gen_vertex_add_particle_out
    end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_vertex_add_particle_in
  public :: hepmc_vertex_add_particle_out

<HepMC interface: procedures>+≡
  subroutine hepmc_vertex_add_particle_in (v, prt)
    type(hepmc_vertex_t), intent(inout) :: v
    type(hepmc_particle_t), intent(in) :: prt
    call gen_vertex_add_particle_in (v%obj, prt%obj)
  end subroutine hepmc_vertex_add_particle_in

  subroutine hepmc_vertex_add_particle_out (v, prt)
    type(hepmc_vertex_t), intent(inout) :: v
    type(hepmc_particle_t), intent(in) :: prt
    call gen_vertex_add_particle_out (v%obj, prt%obj)
  end subroutine hepmc_vertex_add_particle_out

```

Return the number of incoming/outgoing particles.

```

<HepMC interface: interfaces>+≡
  interface
    function gen_vertex_particles_in_size (v_obj) result (size) bind(C)
      import
      integer(c_int) :: size
      type(c_ptr), value :: v_obj
    end function gen_vertex_particles_in_size
  end interface

  interface
    function gen_vertex_particles_out_size (v_obj) result (size) bind(C)
      import
      integer(c_int) :: size
      type(c_ptr), value :: v_obj
    end function gen_vertex_particles_out_size
  end interface

  interface
    function gen_particle_get_n_parents (p_obj) result (size) bind(C)
      import
      integer(c_int) :: size
      type(c_ptr), value :: p_obj
    end function gen_particle_get_n_parents
  end interface

  interface
    function gen_particle_get_n_children (p_obj) result (size) bind(C)
      import
      integer(c_int) :: size
      type(c_ptr), value :: p_obj
    end function gen_particle_get_n_children
  end interface

<HepMC interface: public>+≡
  public :: hepmc_vertex_get_n_in
  public :: hepmc_vertex_get_n_out
  public :: hepmc_particle_get_parents
  public :: hepmc_particle_get_children

<HepMC interface: procedures>+≡

```

```

function hepmc_vertex_get_n_in (v) result (n_in)
  integer :: n_in
  type(hepmc_vertex_t), intent(in) :: v
  n_in = gen_vertex_particles_in_size (v%obj)
end function hepmc_vertex_get_n_in

function hepmc_vertex_get_n_out (v) result (n_out)
  integer :: n_out
  type(hepmc_vertex_t), intent(in) :: v
  n_out = gen_vertex_particles_out_size (v%obj)
end function hepmc_vertex_get_n_out

function hepmc_particle_get_parents (p) result (n_p)
  integer :: n_p
  type(hepmc_particle_t), intent(in) :: p
  n_p = gen_particle_get_n_parents (p%obj)
end function hepmc_particle_get_parents

function hepmc_particle_get_children (p) result (n_ch)
  integer :: n_ch
  type(hepmc_particle_t), intent(in) :: p
  n_ch = gen_particle_get_n_children (p%obj)
end function hepmc_particle_get_children

```

Return the number of parents/children.

<HepMC interface: public>+≡

```

public :: hepmc_particle_get_n_parents
public :: hepmc_particle_get_n_children

```

<HepMC interface: procedures>+≡

```

function hepmc_particle_get_n_parents (prt) result (n_parents)
  integer :: n_parents
  type(hepmc_particle_t), intent(in) :: prt
  type(hepmc_vertex_t) :: v
  if (HEPMC2_AVAILABLE) then
    v = hepmc_particle_get_production_vertex (prt)
    if (hepmc_vertex_is_valid (v)) then
      n_parents = hepmc_vertex_get_n_in (v)
    else
      n_parents = 0
    end if
  else if (HEPMC3_AVAILABLE) then
    n_parents = hepmc_particle_get_parents (prt)
  end if
end function hepmc_particle_get_n_parents

function hepmc_particle_get_n_children (prt) result (n_children)
  integer :: n_children
  type(hepmc_particle_t), intent(in) :: prt
  type(hepmc_vertex_t) :: v
  if (HEPMC2_AVAILABLE) then
    v = hepmc_particle_get_decay_vertex (prt)
    if (hepmc_vertex_is_valid (v)) then
      n_children = hepmc_vertex_get_n_out (v)
    end if
  end if
end function hepmc_particle_get_n_children

```

```

        else
            n_children = 0
        end if
    else if (HEPMC3_AVAILABLE) then
        n_children = hePMC_particle_get_children (prt)
    end if
end function hePMC_particle_get_n_children

```

18.12.6 Vertex-particle-in iterator

This iterator iterates over all incoming particles in an vertex. We store a pointer to the vertex in addition to the iterator. This allows for simple end checking.

The iterator is actually a constant iterator; it can only read.

```

<HepMC interface: public>+≡
    public :: hePMC_vertex_particle_in_iterator_t

<HepMC interface: types>+≡
    type :: hePMC_vertex_particle_in_iterator_t
    private
        type(c_ptr) :: obj
        type(c_ptr) :: v_obj
    end type hePMC_vertex_particle_in_iterator_t

```

Constructor. The iterator is initialized at the first particle in the vertex.

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function &
            new_vertex_particles_in_const_iterator (v_obj) bind(C)
        import
            type(c_ptr), value :: v_obj
        end function new_vertex_particles_in_const_iterator
    end interface

<HepMC interface: public>+≡
    public :: hePMC_vertex_particle_in_iterator_init

<HepMC interface: procedures>+≡
    subroutine hePMC_vertex_particle_in_iterator_init (it, v)
        type(hePMC_vertex_particle_in_iterator_t), intent(out) :: it
        type(hePMC_vertex_t), intent(in) :: v
        it%obj = new_vertex_particles_in_const_iterator (v%obj)
        it%v_obj = v%obj
    end subroutine hePMC_vertex_particle_in_iterator_init

```

Destructor. Necessary because the iterator is allocated on the heap.

```

<HepMC interface: interfaces>+≡
    interface
        subroutine vertex_particles_in_const_iterator_delete (it_obj) bind(C)
        import
            type(c_ptr), value :: it_obj
        end subroutine vertex_particles_in_const_iterator_delete
    end interface

```

```

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_final
<HepMC interface: procedures>+≡
    subroutine hepmc_vertex_particle_in_iterator_final (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
        call vertex_particles_in_const_iterator_delete (it%obj)
    end subroutine hepmc_vertex_particle_in_iterator_final

```

Increment

```

<HepMC interface: interfaces>+≡
    interface
        subroutine vertex_particles_in_const_iterator_advance (it_obj) bind(C)
            import
            type(c_ptr), value :: it_obj
        end subroutine vertex_particles_in_const_iterator_advance
    end interface
<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_advance
<HepMC interface: procedures>+≡
    subroutine hepmc_vertex_particle_in_iterator_advance (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
        call vertex_particles_in_const_iterator_advance (it%obj)
    end subroutine hepmc_vertex_particle_in_iterator_advance

```

Reset to the beginning

```

<HepMC interface: interfaces>+≡
    interface
        subroutine vertex_particles_in_const_iterator_reset &
            (it_obj, v_obj) bind(C)
            import
            type(c_ptr), value :: it_obj, v_obj
        end subroutine vertex_particles_in_const_iterator_reset
    end interface
<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_reset
<HepMC interface: procedures>+≡
    subroutine hepmc_vertex_particle_in_iterator_reset (it)
        type(hepmc_vertex_particle_in_iterator_t), intent(inout) :: it
        call vertex_particles_in_const_iterator_reset (it%obj, it%v_obj)
    end subroutine hepmc_vertex_particle_in_iterator_reset

```

Test: return true as long as we are not past the end.

```

<HepMC interface: interfaces>+≡
    interface
        function vertex_particles_in_const_iterator_is_valid &
            (it_obj, v_obj) result (flag) bind(C)
            import
            logical(c_bool) :: flag
            type(c_ptr), value :: it_obj, v_obj
        end function vertex_particles_in_const_iterator_is_valid
    end interface

```



```

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_is_valid

<HepMC interface: procedures>+≡
    function hepmc_vertex_particle_in_iterator_is_valid (it) result (flag)
        logical :: flag
        type(hepmc_vertex_particle_in_iterator_t), intent(in) :: it
        flag = vertex_particles_in_const_iterator_is_valid (it%obj, it%v_obj)
    end function hepmc_vertex_particle_in_iterator_is_valid

```

Return the particle pointed to by the iterator. (The particle object should not be finalized, since it contains merely a pointer to the particle which is owned by the vertex.)

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function &
            vertex_particles_in_const_iterator_get (it_obj) bind(C)
        import
        type(c_ptr), value :: it_obj
        end function vertex_particles_in_const_iterator_get
    end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_in_iterator_get

<HepMC interface: procedures>+≡
    function hepmc_vertex_particle_in_iterator_get (it) result (prt)
        type(hepmc_particle_t) :: prt
        type(hepmc_vertex_particle_in_iterator_t), intent(in) :: it
        prt%obj = vertex_particles_in_const_iterator_get (it%obj)
    end function hepmc_vertex_particle_in_iterator_get

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function vertex_get_nth_particle_in (vtx_obj, n) bind(C)
        import
        type(c_ptr), value :: vtx_obj
        integer(c_int), value :: n
        end function vertex_get_nth_particle_in
    end interface
    interface
        type(c_ptr) function vertex_get_nth_particle_out (vtx_obj, n) bind(C)
        import
        type(c_ptr), value :: vtx_obj
        integer(c_int), value :: n
        end function vertex_get_nth_particle_out
    end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_get_nth_particle_in
    public :: hepmc_vertex_get_nth_particle_out

<HepMC interface: procedures>+≡
    function hepmc_vertex_get_nth_particle_in (vtx, n) result (prt)
        type(hepmc_particle_t) :: prt

```

```

    type(hepmc_vertex_t), intent(in) :: vtx
    integer, intent(in) :: n
    integer(c_int) :: nth
    nth = n
    prt%obj = vertex_get_nth_particle_in (vtx%obj, nth)
end function hepmc_vertex_get_nth_particle_in

function hepmc_vertex_get_nth_particle_out (vtx, n) result (prt)
    type(hepmc_particle_t) :: prt
    type(hepmc_vertex_t), intent(in) :: vtx
    integer, intent(in) :: n
    integer(c_int) :: nth
    nth = n
    prt%obj = vertex_get_nth_particle_out (vtx%obj, nth)
end function hepmc_vertex_get_nth_particle_out

```

18.12.7 Vertex-particle-out iterator

This iterator iterates over all incoming particles in an vertex. We store a pointer to the vertex in addition to the iterator. This allows for simple end checking.

The iterator is actually a constant iterator; it can only read.

```

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_out_iterator_t

<HepMC interface: types>+≡
    type :: hepmc_vertex_particle_out_iterator_t
    private
    type(c_ptr) :: obj
    type(c_ptr) :: v_obj
end type hepmc_vertex_particle_out_iterator_t

```

Constructor. The iterator is initialized at the first particle in the vertex.

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function &
            new_vertex_particles_out_const_iterator (v_obj) bind(C)
        import
        type(c_ptr), value :: v_obj
        end function new_vertex_particles_out_const_iterator
    end interface

<HepMC interface: public>+≡
    public :: hepmc_vertex_particle_out_iterator_init

<HepMC interface: procedures>+≡
    subroutine hepmc_vertex_particle_out_iterator_init (it, v)
        type(hepmc_vertex_particle_out_iterator_t), intent(out) :: it
        type(hepmc_vertex_t), intent(in) :: v
        it%obj = new_vertex_particles_out_const_iterator (v%obj)
        it%v_obj = v%obj
    end subroutine hepmc_vertex_particle_out_iterator_init

```

Destructor. Necessary because the iterator is allocated on the heap.

```
<HepMC interface: interfaces>+≡  
  interface  
    subroutine vertex_particles_out_const_iterator_delete (it_obj) bind(C)  
      import  
      type(c_ptr), value :: it_obj  
    end subroutine vertex_particles_out_const_iterator_delete  
  end interface  
  
<HepMC interface: public>+≡  
  public :: hepmc_vertex_particle_out_iterator_final  
  
<HepMC interface: procedures>+≡  
  subroutine hepmc_vertex_particle_out_iterator_final (it)  
    type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it  
    call vertex_particles_out_const_iterator_delete (it%obj)  
  end subroutine hepmc_vertex_particle_out_iterator_final
```

Increment

```
<HepMC interface: interfaces>+≡  
  interface  
    subroutine vertex_particles_out_const_iterator_advance (it_obj) bind(C)  
      import  
      type(c_ptr), value :: it_obj  
    end subroutine vertex_particles_out_const_iterator_advance  
  end interface  
  
<HepMC interface: public>+≡  
  public :: hepmc_vertex_particle_out_iterator_advance  
  
<HepMC interface: procedures>+≡  
  subroutine hepmc_vertex_particle_out_iterator_advance (it)  
    type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it  
    call vertex_particles_out_const_iterator_advance (it%obj)  
  end subroutine hepmc_vertex_particle_out_iterator_advance
```

Reset to the beginning

```
<HepMC interface: interfaces>+≡  
  interface  
    subroutine vertex_particles_out_const_iterator_reset &  
      (it_obj, v_obj) bind(C)  
      import  
      type(c_ptr), value :: it_obj, v_obj  
    end subroutine vertex_particles_out_const_iterator_reset  
  end interface  
  
<HepMC interface: public>+≡  
  public :: hepmc_vertex_particle_out_iterator_reset  
  
<HepMC interface: procedures>+≡  
  subroutine hepmc_vertex_particle_out_iterator_reset (it)  
    type(hepmc_vertex_particle_out_iterator_t), intent(inout) :: it  
    call vertex_particles_out_const_iterator_reset (it%obj, it%v_obj)  
  end subroutine hepmc_vertex_particle_out_iterator_reset
```

Test: return true as long as we are not past the end.

```

<HepMC interface: interfaces>+≡
  interface
    function vertex_particles_out_const_iterator_is_valid &
      (it_obj, v_obj) result (flag) bind(C)
    import
      logical(c_bool) :: flag
      type(c_ptr), value :: it_obj, v_obj
    end function vertex_particles_out_const_iterator_is_valid
  end interface

<HepMC interface: public>+≡
  public :: hepmc_vertex_particle_out_iterator_is_valid

<HepMC interface: procedures>+≡
  function hepmc_vertex_particle_out_iterator_is_valid (it) result (flag)
    logical :: flag
    type(hepmc_vertex_particle_out_iterator_t), intent(in) :: it
    flag = vertex_particles_out_const_iterator_is_valid (it%obj, it%v_obj)
  end function hepmc_vertex_particle_out_iterator_is_valid

```

Return the particle pointed to by the iterator. (The particle object should not be finalized, since it contains merely a pointer to the particle which is owned by the vertex.)

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function &
      vertex_particles_out_const_iterator_get (it_obj) bind(C)
    import
      type(c_ptr), value :: it_obj
    end function vertex_particles_out_const_iterator_get
  end interface

<HepMC interface: public>+≡
  public :: hepmc_vertex_particle_out_iterator_get

<HepMC interface: procedures>+≡
  function hepmc_vertex_particle_out_iterator_get (it) result (prt)
    type(hepmc_particle_t) :: prt
    type(hepmc_vertex_particle_out_iterator_t), intent(in) :: it
    prt%obj = vertex_particles_out_const_iterator_get (it%obj)
  end function hepmc_vertex_particle_out_iterator_get

```

18.12.8 GenEvent

The main object of HepMC is a GenEvent. The object is filled by GenVertex objects, which in turn contain GenParticle objects.

This is an extension of the abstract `event_handle_t`, so we can use the according communicator features.

```

<HepMC interface: public>+≡
  public :: hepmc_event_t

```

```

<HepMC interface: types>+≡
  type, extends (event_handle_t) :: hepmc_event_t
  private
  type(c_ptr) :: obj = c_null_ptr
end type hepmc_event_t

```

Constructor. Arguments are process ID (integer) and event ID (integer).
The Fortran version has initializer form.

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_gen_event (proc_id, event_id) bind(C)
    import
    integer(c_int), value :: proc_id, event_id
    end function new_gen_event
  end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_event_init

```

```

<HepMC interface: procedures>+≡
  subroutine hepmc_event_init (evt, proc_id, event_id)
    type(hepmc_event_t), intent(out) :: evt
    integer, intent(in), optional :: proc_id, event_id
    integer(c_int) :: pid, eid
    pid = 0; if (present (proc_id)) pid = proc_id
    eid = 0; if (present (event_id)) eid = event_id
    evt%obj = new_gen_event (pid, eid)
  end subroutine hepmc_event_init

```

Destructor.

```

<HepMC interface: interfaces>+≡
  interface
    subroutine gen_event_delete (evt_obj) bind(C)
    import
    type(c_ptr), value :: evt_obj
    end subroutine gen_event_delete
  end interface

```

Finalize: use the HepMC destructor. Also nullify the pointer explicitly, to be on the safe side.

```

<HepMC interface: public>+≡
  public :: hepmc_event_final

<HepMC interface: procedures>+≡
  subroutine hepmc_event_final (evt)
    type(hepmc_event_t), intent(inout) :: evt
    if (c_associated (evt%obj)) then
      call gen_event_delete (evt%obj)
      evt%obj = c_null_ptr
    end if
  end subroutine hepmc_event_final

```

Nullify: do not call the destructor, just nullify the C pointer. There should be another pointer associated with the object.

```

<HepMC interface: public>+≡
    public :: hepmc_event_nullify

<HepMC interface: procedures>+≡
    subroutine hepmc_event_nullify (evt)
        type(hepmc_event_t), intent(inout) :: evt
        evt%obj = c_null_ptr
    end subroutine hepmc_event_nullify

```

Return the actual object as a C pointer. For use in the native C++ interface only.

```

<HepMC interface: public>+≡
    public :: hepmc_event_get_c_ptr

<HepMC interface: procedures>+≡
    function hepmc_event_get_c_ptr (evt) result (p)
        type(hepmc_event_t), intent(in) :: evt
        type(c_ptr) :: p
        p = evt%obj
    end function hepmc_event_get_c_ptr

```

Screen output. Printing to file is possible in principle (using a C++ output channel), by allowing an argument. Printing to an open Fortran unit is obviously not possible.

```

<HepMC interface: interfaces>+≡
    interface
        subroutine gen_event_print (evt_obj) bind(C)
            import
            type(c_ptr), value :: evt_obj
        end subroutine gen_event_print
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_print

<HepMC interface: procedures>+≡
    subroutine hepmc_event_print (evt)
        type(hepmc_event_t), intent(in) :: evt
        call gen_event_print (evt%obj)
    end subroutine hepmc_event_print

```

Get the event number.

```

<HepMC interface: interfaces>+≡
    interface
        integer(c_int) function gen_event_event_number (evt_obj) bind(C)
            use iso_c_binding !NODEP!
            type(c_ptr), value :: evt_obj
        end function gen_event_event_number
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_get_event_index

```

```

<HepMC interface: procedures>+≡
function hepmc_event_get_event_index (evt) result (i_proc)
integer :: i_proc
type(hepmc_event_t), intent(in) :: evt
i_proc = gen_event_event_number (evt%obj)
end function hepmc_event_get_event_index

```

```

<HepMC interface: interfaces>+≡
interface
integer(c_int) function gen_event_get_n_particles &
(evt_obj) bind(C)
import
type(c_ptr), value :: evt_obj
end function gen_event_get_n_particles
end interface
interface
integer(c_int) function gen_event_get_n_beams &
(evt_obj) bind(C)
import
type(c_ptr), value :: evt_obj
end function gen_event_get_n_beams
end interface

```

```

<HepMC interface: public>+≡
public :: hepmc_event_get_n_particles
public :: hepmc_event_get_n_beams

```

```

<HepMC interface: procedures>+≡
function hepmc_event_get_n_particles (evt) result (n_tot)
integer :: n_tot
type(hepmc_event_t), intent(in) :: evt
n_tot = gen_event_get_n_particles (evt%obj)
end function hepmc_event_get_n_particles

function hepmc_event_get_n_beams (evt) result (n_tot)
integer :: n_tot
type(hepmc_event_t), intent(in) :: evt
n_tot = gen_event_get_n_beams (evt%obj)
end function hepmc_event_get_n_beams

```

Set the numeric signal process ID

```

<HepMC interface: interfaces>+≡
interface
subroutine gen_event_set_signal_process_id (evt_obj, proc_id) bind(C)
import
type(c_ptr), value :: evt_obj
integer(c_int), value :: proc_id
end subroutine gen_event_set_signal_process_id
end interface

<HepMC interface: public>+≡
public :: hepmc_event_set_process_id

<HepMC interface: procedures>+≡
subroutine hepmc_event_set_process_id (evt, proc)

```

```

    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in) :: proc
    integer(c_int) :: i_proc
    i_proc = proc
    call gen_event_set_signal_process_id (evt%obj, i_proc)
end subroutine hepmc_event_set_process_id

```

Get the numeric signal process ID

```

<HepMC interface: interfaces>+≡
    interface
        integer(c_int) function gen_event_signal_process_id (evt_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj
    end function gen_event_signal_process_id
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_get_process_id

<HepMC interface: procedures>+≡
    function hepmc_event_get_process_id (evt) result (i_proc)
        integer :: i_proc
        type(hepmc_event_t), intent(in) :: evt
        i_proc = gen_event_signal_process_id (evt%obj)
    end function hepmc_event_get_process_id

```

Set the event energy scale

```

<HepMC interface: interfaces>+≡
    interface
        subroutine gen_event_set_event_scale (evt_obj, scale) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: scale
    end subroutine gen_event_set_event_scale
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_set_scale

<HepMC interface: procedures>+≡
    subroutine hepmc_event_set_scale (evt, scale)
        type(hepmc_event_t), intent(in) :: evt
        real(default), intent(in) :: scale
        real(c_double) :: cscale
        cscale = scale
        call gen_event_set_event_scale (evt%obj, cscale)
    end subroutine hepmc_event_set_scale

```

Get the event energy scale

```

<HepMC interface: interfaces>+≡
    interface
        real(c_double) function gen_event_event_scale (evt_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj
    end function gen_event_event_scale
    end interface

```



```

        end function gen_event_event_scale
    end interface

    <HepMC interface: public>+≡
        public :: hepmc_event_get_scale

    <HepMC interface: procedures>+≡
        function hepmc_event_get_scale (evt) result (scale)
            real(default) :: scale
            type(hepmc_event_t), intent(in) :: evt
            scale = gen_event_event_scale (evt%obj)
        end function hepmc_event_get_scale

```

Set the value of α_{QCD} .

```

    <HepMC interface: interfaces>+≡
        interface
            subroutine gen_event_set_alpha_qcd (evt_obj, a) bind(C)
                import
                type(c_ptr), value :: evt_obj
                real(c_double), value :: a
            end subroutine gen_event_set_alpha_qcd
        end interface

    <HepMC interface: public>+≡
        public :: hepmc_event_set_alpha_qcd

    <HepMC interface: procedures>+≡
        subroutine hepmc_event_set_alpha_qcd (evt, alpha)
            type(hepmc_event_t), intent(in) :: evt
            real(default), intent(in) :: alpha
            real(c_double) :: a
            a = alpha
            call gen_event_set_alpha_qcd (evt%obj, a)
        end subroutine hepmc_event_set_alpha_qcd

```

Get the value of α_{QCD} .

```

    <HepMC interface: interfaces>+≡
        interface
            real(c_double) function gen_event_alpha_qcd (evt_obj) bind(C)
                import
                type(c_ptr), value :: evt_obj
            end function gen_event_alpha_qcd
        end interface

    <HepMC interface: public>+≡
        public :: hepmc_event_get_alpha_qcd

    <HepMC interface: procedures>+≡
        function hepmc_event_get_alpha_qcd (evt) result (alpha)
            real(default) :: alpha
            type(hepmc_event_t), intent(in) :: evt
            alpha = gen_event_alpha_qcd (evt%obj)
        end function hepmc_event_get_alpha_qcd

```

Set the value of α_{QED} .

```

<HepMC interface: interfaces>+≡
  interface
    subroutine gen_event_set_alpha_qed (evt_obj, a) bind(C)
      import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: a
    end subroutine gen_event_set_alpha_qed
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_set_alpha_qed

<HepMC interface: procedures>+≡
  subroutine hepmc_event_set_alpha_qed (evt, alpha)
    type(hepmc_event_t), intent(in) :: evt
    real(default), intent(in) :: alpha
    real(c_double) :: a
    a = alpha
    call gen_event_set_alpha_qed (evt%obj, a)
  end subroutine hepmc_event_set_alpha_qed

```

Get the value of α_{QED} .

```

<HepMC interface: interfaces>+≡
  interface
    real(c_double) function gen_event_alpha_qed (evt_obj) bind(C)
      import
        type(c_ptr), value :: evt_obj
    end function gen_event_alpha_qed
  end interface

<HepMC interface: public>+≡
  public :: hepmc_event_get_alpha_qed

<HepMC interface: procedures>+≡
  function hepmc_event_get_alpha_qed (evt) result (alpha)
    real(default) :: alpha
    type(hepmc_event_t), intent(in) :: evt
    alpha = gen_event_alpha_qed (evt%obj)
  end function hepmc_event_get_alpha_qed

```

Clear a weight value to the end of the weight container.

```

<HepMC interface: interfaces>+≡
  interface
    subroutine gen_event_clear_weights (evt_obj) bind(C)
      use iso_c_binding !NODEP!
      type(c_ptr), value :: evt_obj
    end subroutine gen_event_clear_weights
  end interface

```

The HepMC weights are measured in pb.

```

<HepMC interface: parameters>≡
  integer, parameter, public :: HEPMC3_MODE_HEPMC2 = 1
  integer, parameter, public :: HEPMC3_MODE_HEPMC3 = 2
  integer, parameter, public :: HEPMC3_MODE_ROOT = 3

```

```

integer, parameter, public :: HEPMC3_MODE_ROOTTREE = 4
integer, parameter, public :: HEPMC3_MODE_HEPEVT = 5

<HepMC interface: public>+≡
public :: hepmc_event_clear_weights

<HepMC interface: procedures>+≡
subroutine hepmc_event_clear_weights (evt)
  type(hepmc_event_t), intent(in) :: evt
  call gen_event_clear_weights (evt%obj)
end subroutine hepmc_event_clear_weights

```

Add a weight value to the end of the weight container.

```

<HepMC interface: interfaces>+≡
interface
  subroutine gen_event_add_weight (evt_obj, w) bind(C)
    use iso_c_binding !NODEP!
    type(c_ptr), value :: evt_obj
    real(c_double), value :: w
  end subroutine gen_event_add_weight
end interface

<HepMC interface: public>+≡
public :: hepmc_event_add_weight

<HepMC interface: procedures>+≡
subroutine hepmc_event_add_weight (evt, weight, rescale)
  type(hepmc_event_t), intent(in) :: evt
  real(default), intent(in) :: weight
  logical, intent(in) :: rescale
  real(c_double) :: w
  if (rescale) then
    w = weight * pb_per_fb
  else
    w = weight
  end if
  call gen_event_add_weight (evt%obj, w)
end subroutine hepmc_event_add_weight

```

Get the size of the weight container (the number of valid elements).

```

<HepMC interface: interfaces>+≡
interface
  integer(c_int) function gen_event_weights_size (evt_obj) bind(C)
    use iso_c_binding !NODEP!
    type(c_ptr), value :: evt_obj
  end function gen_event_weights_size
end interface

<HepMC interface: public>+≡
public :: hepmc_event_get_weights_size

<HepMC interface: procedures>+≡
function hepmc_event_get_weights_size (evt) result (n)
  integer :: n
  type(hepmc_event_t), intent(in) :: evt
  n = gen_event_weights_size (evt%obj)
end function

```

```
end function hepmc_event_get_weights_size
```

Get the value of the weight with index i. (Count from 1, while C counts from zero.)

```
<HepMC interface: interfaces>+≡
```

```
interface
  real(c_double) function gen_event_weight (evt_obj, i) bind(C)
  use iso_c_binding !NODEP!
  type(c_ptr), value :: evt_obj
  integer(c_int), value :: i
  end function gen_event_weight
end interface
```

```
<HepMC interface: public>+≡
```

```
public :: hepmc_event_get_weight
```

```
<HepMC interface: procedures>+≡
```

```
function hepmc_event_get_weight (evt, index, rescale) result (weight)
  real(default) :: weight
  type(hepmc_event_t), intent(in) :: evt
  integer, intent(in) :: index
  logical, intent(in) :: rescale
  integer(c_int) :: i
  i = index - 1
  if (rescale) then
    weight = gen_event_weight (evt%obj, i) / pb_per_fb
  else
    weight = gen_event_weight (evt%obj, i)
  end if
end function hepmc_event_get_weight
```

Add a vertex to the event container.

```
<HepMC interface: interfaces>+≡
```

```
interface
  subroutine gen_event_add_vertex (evt_obj, v_obj) bind(C)
  import
  type(c_ptr), value :: evt_obj
  type(c_ptr), value :: v_obj
  end subroutine gen_event_add_vertex
end interface
```

```
<HepMC interface: public>+≡
```

```
public :: hepmc_event_add_vertex
```

```
<HepMC interface: procedures>+≡
```

```
subroutine hepmc_event_add_vertex (evt, v)
  type(hepmc_event_t), intent(inout) :: evt
  type(hepmc_vertex_t), intent(in) :: v
  call gen_event_add_vertex (evt%obj, v%obj)
end subroutine hepmc_event_add_vertex
```

Mark a particular vertex as the signal process (hard interaction).

```
<HepMC interface: interfaces>+≡
```

```
interface
```

```

        subroutine gen_event_set_signal_process_vertex (evt_obj, v_obj) bind(C)
            import
            type(c_ptr), value :: evt_obj
            type(c_ptr), value :: v_obj
        end subroutine gen_event_set_signal_process_vertex
    end interface
    <HepMC interface: public>+≡
        public :: hepmc_event_set_signal_process_vertex
    <HepMC interface: procedures>+≡
        subroutine hepmc_event_set_signal_process_vertex (evt, v)
            type(hepmc_event_t), intent(inout) :: evt
            type(hepmc_vertex_t), intent(in) :: v
            call gen_event_set_signal_process_vertex (evt%obj, v%obj)
        end subroutine hepmc_event_set_signal_process_vertex

```

Return the the signal process (hard interaction).

```

    <HepMC interface: interfaces>+≡
        interface
            function gen_event_get_signal_process_vertex (evt_obj) &
                result (v_obj) bind(C)
            import
            type(c_ptr), value :: evt_obj
            type(c_ptr) :: v_obj
        end function gen_event_get_signal_process_vertex
    end interface
    <HepMC interface: public>+≡
        public :: hepmc_event_get_signal_process_vertex
    <HepMC interface: procedures>+≡
        function hepmc_event_get_signal_process_vertex (evt) result (v)
            type(hepmc_event_t), intent(in) :: evt
            type(hepmc_vertex_t) :: v
            v%obj = gen_event_get_signal_process_vertex (evt%obj)
        end function hepmc_event_get_signal_process_vertex

```

Set the beam particles explicitly.

```

    <HepMC interface: public>+≡
        public :: hepmc_event_set_beam_particles
    <HepMC interface: procedures>+≡
        subroutine hepmc_event_set_beam_particles (evt, prt1, prt2)
            type(hepmc_event_t), intent(inout) :: evt
            type(hepmc_particle_t), intent(in) :: prt1, prt2
            logical(c_bool) :: flag
            flag = gen_event_set_beam_particles (evt%obj, prt1%obj, prt2%obj)
        end subroutine hepmc_event_set_beam_particles

```

The C function returns a boolean which we do not use.

```

    <HepMC interface: interfaces>+≡
        interface
            logical(c_bool) function gen_event_set_beam_particles &
                (evt_obj, prt1_obj, prt2_obj) bind(C)

```

```

import
  type(c_ptr), value :: evt_obj, prt1_obj, prt2_obj
end function gen_event_set_beam_particles
end interface

```

Set the cross section and error explicitly. Note that HepMC uses pb, while WHIZARD uses fb.

```

<HepMC interface: public>+≡
  public :: hepmc_event_set_cross_section

<HepMC interface: procedures>+≡
  subroutine hepmc_event_set_cross_section (evt, xsec, xsec_err)
    type(hepmc_event_t), intent(inout) :: evt
    real(default), intent(in) :: xsec, xsec_err
    call gen_event_set_cross_section &
      (evt%obj, &
        real(xsec * 1e-3_default, c_double), &
        real(xsec_err * 1e-3_default, c_double))
  end subroutine hepmc_event_set_cross_section

```

The C function returns a boolean which we do not use.

```

<HepMC interface: interfaces>+≡
  interface
    subroutine gen_event_set_cross_section (evt_obj, xs, xs_err) bind(C)
      import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: xs, xs_err
    end subroutine gen_event_set_cross_section
  end interface

```

18.12.9 Event-particle iterator

This iterator iterates over all particles in an event. We store a pointer to the event in addition to the iterator. This allows for simple end checking.

The iterator is actually a constant iterator; it can only read.

```

<HepMC interface: public>+≡
  public :: hepmc_event_particle_iterator_t

<HepMC interface: types>+≡
  type :: hepmc_event_particle_iterator_t
  private
    type(c_ptr) :: obj
    type(c_ptr) :: evt_obj
  end type hepmc_event_particle_iterator_t

```

Constructor. The iterator is initialized at the first particle in the event.

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_event_particle_const_iterator (evt_obj) bind(C)
      import
        type(c_ptr), value :: evt_obj
    end function new_event_particle_const_iterator
  end interface

```

```

        end function new_event_particle_const_iterator
    end interface

    <HepMC interface: public>+≡
        public :: hepmc_event_particle_iterator_init

    <HepMC interface: procedures>+≡
        subroutine hepmc_event_particle_iterator_init (it, evt)
            type(hepmc_event_particle_iterator_t), intent(out) :: it
            type(hepmc_event_t), intent(in) :: evt
            it%obj = new_event_particle_const_iterator (evt%obj)
            it%evt_obj = evt%obj
        end subroutine hepmc_event_particle_iterator_init

```

Destructor. Necessary because the iterator is allocated on the heap.

```

    <HepMC interface: interfaces>+≡
        interface
            subroutine event_particle_const_iterator_delete (it_obj) bind(C)
                import
                type(c_ptr), value :: it_obj
            end subroutine event_particle_const_iterator_delete
        end interface

    <HepMC interface: public>+≡
        public :: hepmc_event_particle_iterator_final

    <HepMC interface: procedures>+≡
        subroutine hepmc_event_particle_iterator_final (it)
            type(hepmc_event_particle_iterator_t), intent(inout) :: it
            call event_particle_const_iterator_delete (it%obj)
        end subroutine hepmc_event_particle_iterator_final

```

Increment

```

    <HepMC interface: interfaces>+≡
        interface
            subroutine event_particle_const_iterator_advance (it_obj) bind(C)
                import
                type(c_ptr), value :: it_obj
            end subroutine event_particle_const_iterator_advance
        end interface

    <HepMC interface: public>+≡
        public :: hepmc_event_particle_iterator_advance

    <HepMC interface: procedures>+≡
        subroutine hepmc_event_particle_iterator_advance (it)
            type(hepmc_event_particle_iterator_t), intent(inout) :: it
            call event_particle_const_iterator_advance (it%obj)
        end subroutine hepmc_event_particle_iterator_advance

```

Reset to the beginning

```

    <HepMC interface: interfaces>+≡
        interface
            subroutine event_particle_const_iterator_reset (it_obj, evt_obj) bind(C)
                import

```

```

        type(c_ptr), value :: it_obj, evt_obj
    end subroutine event_particle_const_iterator_reset
end interface

<HepMC interface: public>+≡
    public :: hepmc_event_particle_iterator_reset

<HepMC interface: procedures>+≡
    subroutine hepmc_event_particle_iterator_reset (it)
        type(hepmc_event_particle_iterator_t), intent(inout) :: it
        call event_particle_const_iterator_reset (it%obj, it%evt_obj)
    end subroutine hepmc_event_particle_iterator_reset

```

Test: return true as long as we are not past the end.

```

<HepMC interface: interfaces>+≡
    interface
        function event_particle_const_iterator_is_valid &
            (it_obj, evt_obj) result (flag) bind(C)
        import
        logical(c_bool) :: flag
        type(c_ptr), value :: it_obj, evt_obj
    end function event_particle_const_iterator_is_valid
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_particle_iterator_is_valid

<HepMC interface: procedures>+≡
    function hepmc_event_particle_iterator_is_valid (it) result (flag)
        logical :: flag
        type(hepmc_event_particle_iterator_t), intent(in) :: it
        flag = event_particle_const_iterator_is_valid (it%obj, it%evt_obj)
    end function hepmc_event_particle_iterator_is_valid

```

Return the particle pointed to by the iterator. (The particle object should not be finalized, since it contains merely a pointer to the particle which is owned by the vertex.)

```

<HepMC interface: interfaces>+≡
    interface
        type(c_ptr) function event_particle_const_iterator_get (it_obj) bind(C)
        import
        type(c_ptr), value :: it_obj
    end function event_particle_const_iterator_get
    end interface

<HepMC interface: public>+≡
    public :: hepmc_event_particle_iterator_get

<HepMC interface: procedures>+≡
    function hepmc_event_particle_iterator_get (it) result (prt)
        type(hepmc_particle_t) :: prt
        type(hepmc_event_particle_iterator_t), intent(in) :: it
        prt%obj = event_particle_const_iterator_get (it%obj)
    end function hepmc_event_particle_iterator_get

```



```

<HepMC interface: interfaces>+≡
interface
    type(c_ptr) function gen_event_get_nth_particle (evt_obj, n) bind(C)
    import
        type(c_ptr), value :: evt_obj
        integer(c_int), value :: n
    end function gen_event_get_nth_particle
end interface
interface
    integer(c_int) function gen_event_get_nth_beam (evt_obj, n) bind(C)
    import
        type(c_ptr), value :: evt_obj
        integer(c_int), value :: n
    end function gen_event_get_nth_beam
end interface

<HepMC interface: public>+≡
public :: hepmc_event_get_nth_particle
public :: hepmc_event_get_nth_beam

<HepMC interface: procedures>+≡
function hepmc_event_get_nth_particle (evt, n) result (prt)
    type(hepmc_particle_t) :: prt
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in) :: n
    integer :: n_tot
    integer(c_int) :: nth
    nth = n
    n_tot = gen_event_get_n_particles (evt%obj)
    if (n > n_tot .or. n < 1) then
        prt%obj = c_null_ptr
        call msg_error ("HepMC interface called for wrong particle ID.")
    else
        prt%obj = gen_event_get_nth_particle (evt%obj, nth)
    end if
end function hepmc_event_get_nth_particle

function hepmc_event_get_nth_beam (evt, n) result (beam_barcode)
    integer :: beam_barcode
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in) :: n
    integer(c_int) :: bc
    bc = gen_event_get_nth_beam (evt%obj, n)
    beam_barcode = bc
end function hepmc_event_get_nth_beam

```

18.12.10 I/O streams

There is a specific I/O stream type for handling the output of GenEvent objects (i.e., Monte Carlo event samples) to file. Opening the file is done by the constructor, closing by the destructor.

```

<HepMC interface: public>+≡
public :: hepmc_iostream_t

```

```

<HepMC interface: types>+≡
  type :: hepmc_iostream_t
  private
  type(c_ptr) :: obj
end type hepmc_iostream_t

```

Constructor for an output stream associated to a file.

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_io_gen_event_out (hepmc3_mode, filename) bind(C)
    import
    integer(c_int), intent(in) :: hepmc3_mode
    character(c_char), dimension(*), intent(in) :: filename
  end function new_io_gen_event_out
  end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_iostream_open_out

```

```

<HepMC interface: procedures>+≡
  subroutine hepmc_iostream_open_out (iostream, filename, hepmc3_mode)
    type(hepmc_iostream_t), intent(out) :: iostream
    type(string_t), intent(in) :: filename
    integer, intent(in) :: hepmc3_mode
    integer(c_int) :: mode
    mode = hepmc3_mode
    iostream%obj = &
      new_io_gen_event_out (mode, char (filename) // c_null_char)
  end subroutine hepmc_iostream_open_out

```

Constructor for an input stream associated to a file.

```

<HepMC interface: interfaces>+≡
  interface
    type(c_ptr) function new_io_gen_event_in (hepmc3_mode, filename) bind(C)
    import
    integer(c_int), intent(in) :: hepmc3_mode
    character(c_char), dimension(*), intent(in) :: filename
  end function new_io_gen_event_in
  end interface

```

```

<HepMC interface: public>+≡
  public :: hepmc_iostream_open_in

```

```

<HepMC interface: procedures>+≡
  subroutine hepmc_iostream_open_in (iostream, filename, hepmc3_mode)
    type(hepmc_iostream_t), intent(out) :: iostream
    type(string_t), intent(in) :: filename
    integer, intent(in) :: hepmc3_mode
    integer(c_int) :: mode
    mode = hepmc3_mode
    iostream%obj = &
      new_io_gen_event_in (mode, char (filename) // c_null_char)
  end subroutine hepmc_iostream_open_in

```

Destructor:

```
<HepMC interface: interfaces>+≡
  interface
    subroutine io_gen_event_delete (io_obj) bind(C)
      import
      type(c_ptr), value :: io_obj
    end subroutine io_gen_event_delete
  end interface

<HepMC interface: public>+≡
  public :: hepmc_iostream_close

<HepMC interface: procedures>+≡
  subroutine hepmc_iostream_close (iostream)
    type(hepmc_iostream_t), intent(inout) :: iostream
    call io_gen_event_delete (iostream%obj)
  end subroutine hepmc_iostream_close
```

Write a single event to the I/O stream.

```
<HepMC interface: interfaces>+≡
  interface
    subroutine io_gen_event_write_event (io_obj, evt_obj) bind(C)
      import
      type(c_ptr), value :: io_obj, evt_obj
    end subroutine io_gen_event_write_event
  end interface
  interface
    subroutine io_gen_event_write_event_hepmc2 (io_obj, evt_obj) bind(C)
      import
      type(c_ptr), value :: io_obj, evt_obj
    end subroutine io_gen_event_write_event_hepmc2
  end interface

<HepMC interface: public>+≡
  public :: hepmc_iostream_write_event

<HepMC interface: procedures>+≡
  subroutine hepmc_iostream_write_event (iostream, evt, hepmc3_mode)
    type(hepmc_iostream_t), intent(inout) :: iostream
    type(hepmc_event_t), intent(in) :: evt
    integer, intent(in), optional :: hepmc3_mode
    integer :: mode
    mode = HEPMC3_MODE_HEPMC3
    if (present (hepmc3_mode)) mode = hepmc3_mode
    call io_gen_event_write_event (iostream%obj, evt%obj)
  end subroutine hepmc_iostream_write_event
```

Read a single event from the I/O stream. Return true if successful.

```
<HepMC interface: interfaces>+≡
  interface
    logical(c_bool) function io_gen_event_read_event (io_obj, evt_obj) bind(C)
      import
      type(c_ptr), value :: io_obj, evt_obj
    end function io_gen_event_read_event
  end interface
```

```

<HepMC interface: public>+≡
    public :: hepmc_iostream_read_event

<HepMC interface: procedures>+≡
    subroutine hepmc_iostream_read_event (iostream, evt, ok)
        type(hepmc_iostream_t), intent(inout) :: iostream
        type(hepmc_event_t), intent(inout) :: evt
        logical, intent(out) :: ok
        ok = io_gen_event_read_event (iostream%obj, evt%obj)
    end subroutine hepmc_iostream_read_event

```

18.12.11 Unit tests

Test module, followed by the corresponding implementation module.

```

<hepmc_interface_ut.f90>≡
    <File header>

    module hepmc_interface_ut
        use unit_tests
        use system_dependencies, only: HEPMC2_AVAILABLE
        use system_dependencies, only: HEPMC3_AVAILABLE
        use hepmc_interface_util

        <Standard module head>

        <HepMC interface: public test>

        contains

        <HepMC interface: test driver>

    end module hepmc_interface_ut

<hepmc_interface_util.f90>≡
    <File header>

    module hepmc_interface_util

        <Use kinds>
        <Use strings>
        use io_units
        use lorentz
        use flavors
        use colors
        use polarizations

        use hepmc_interface

        <Standard module head>

        <HepMC interface: test declarations>

        contains

```

<HepMC interface: tests>

end module hepmc_interface_util

API: driver for the unit tests below.

<HepMC interface: public test>≡

public :: hepmc_interface_test

<HepMC interface: test driver>≡

```
subroutine hepmc_interface_test (u, results)
  integer, intent(in) :: u
  type(test_results_t), intent(inout) :: results
<HepMC interface: execute tests>
end subroutine hepmc_interface_test
```

This test example is an abridged version from the build-from-scratch example in the HepMC distribution. We create two vertices for $p \rightarrow q$ PDF splitting, then a vertex for a $qq \rightarrow W^- g$ hard-interaction process, and finally a vertex for $W^- \rightarrow qq$ decay. The setup is for LHC kinematics.

Extending the original example, we set color flow for the incoming quarks and polarization for the outgoing photon. For the latter, we have to define a particle-data object for the photon, so a flavor object can be correctly initialized.

<HepMC interface: execute tests>≡

```
if (HEPMC2_AVAILABLE) then
  call test (hepmc_interface_1, "hepmc2_interface_1", &
    "check HepMC2 interface", &
    u, results)
else if (HEPMC3_AVAILABLE) then
  call test (hepmc_interface_1, "hepmc3_interface_1", &
    "check HepMC3 interface", &
    u, results)
end if
```

<HepMC interface: test declarations>≡

public :: hepmc_interface_1

<HepMC interface: tests>≡

```
subroutine hepmc_interface_1 (u)
  use physics_defs, only: VECTOR
  use model_data, only: field_data_t
  integer, intent(in) :: u
  integer :: u_file, iostat
  type(hepmc_event_t) :: evt
  type(hepmc_vertex_t) :: v1, v2, v3, v4
  type(hepmc_particle_t) :: prt1, prt2, prt3, prt4, prt5, prt6, prt7, prt8
  type(hepmc_iostream_t) :: iostream
  type(flavor_t) :: flv
  type(color_t) :: col
  type(polarization_t) :: pol
  type(field_data_t), target :: photon_data
  character(80) :: buffer

  write (u, "(A)")  "* Test output: HepMC interface"
  write (u, "(A)")  "* Purpose: test HepMC interface"
```

```

write (u, "(A)")

write (u, "(A)")  "* Initialization"
write (u, "(A)")

! Initialize a photon flavor object and some polarization
call photon_data%init (var_str ("PHOTON"), 22)
call photon_data%set (spin_type=VECTOR)
call photon_data%freeze ()
call flv%init (photon_data)
call pol%init_angles &
      (flv, 0.6_default, 1._default, 0.5_default)

! Event initialization
call hepmc_event_init (evt, 20, 1)

write (u, "(A)")  "* p -> q splitting"
write (u, "(A)")

! $p\to q$ splittings
call hepmc_vertex_init (v1)
call hepmc_event_add_vertex (evt, v1)
call hepmc_vertex_init (v2)
call hepmc_event_add_vertex (evt, v2)
call particle_init (prt1, &
      0._default, 0._default, 7000._default, 7000._default, &
      2212, 3)
call hepmc_vertex_add_particle_in (v1, prt1)
call particle_init (prt2, &
      0._default, 0._default, -7000._default, 7000._default, &
      2212, 3)
call hepmc_vertex_add_particle_in (v2, prt2)
call particle_init (prt3, &
      .750_default, -1.569_default, 32.191_default, 32.238_default, &
      1, 3)
call color_init_from_array (col, [501])
call hepmc_particle_set_color (prt3, col)
call hepmc_vertex_add_particle_out (v1, prt3)
call particle_init (prt4, &
      -3.047_default, -19._default, -54.629_default, 57.920_default, &
      -2, 3)
call color_init_from_array (col, [-501])
call hepmc_particle_set_color (prt4, col)
call hepmc_vertex_add_particle_out (v2, prt4)

write (u, "(A)")  "* Hard interaction"
write (u, "(A)")

! Hard interaction
call hepmc_vertex_init (v3)
call hepmc_event_add_vertex (evt, v3)
call hepmc_vertex_add_particle_in (v3, prt3)
call hepmc_vertex_add_particle_in (v3, prt4)
call particle_init (prt6, &

```

```

-3.813_default, 0.113_default, -1.833_default, 4.233_default, &
22, 1)
call hepmc_particle_set_polarization (prt6, pol)
call hepmc_vertex_add_particle_out (v3, prt6)
call particle_init (prt5, &
1.517_default, -20.68_default, -20.605_default, 85.925_default, &
-24, 3)
call hepmc_vertex_add_particle_out (v3, prt5)
call hepmc_event_set_signal_process_vertex (evt, v3)

! $W^-$ decay
call vertex_init_pos (v4, &
0.12_default, -0.3_default, 0.05_default, 0.004_default)
call hepmc_event_add_vertex (evt, v4)
call hepmc_vertex_add_particle_in (v4, prt5)
call particle_init (prt7, &
-2.445_default, 28.816_default, 6.082_default, 29.552_default, &
1, 1)
call hepmc_vertex_add_particle_out (v4, prt7)
call particle_init (prt8, &
3.962_default, -49.498_default, -26.687_default, 56.373_default, &
-2, 1)
call hepmc_vertex_add_particle_out (v4, prt8)

! Event output
call hepmc_event_print (evt)
write (u, "(A)") "Writing to file 'hepmc_test.hepmc'"
write (u, "(A)")

call hepmc_iostream_open_out (iostream, var_str ("hepmc_test.hepmc"), 2)
call hepmc_iostream_write_event (iostream, evt)
call hepmc_iostream_close (iostream)

write (u, "(A)") "Writing completed"

write (u, "(A)")
write (u, "(A)") "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "hepmc_test.hepmc", &
action = "read", status = "old")
do
read (u_file, "(A)", iostat = iostat) buffer
if (buffer(1:14) == "HepMC::Version") buffer = "[...]"
if (iostat /= 0) exit
write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)") "* Cleanup"
write (u, "(A)")

```

```

! Wrapup
! call pol%final ()
call hepmc_event_final (evt)

write (u, "(A)")
write (u, "(A)")  "* Test output end: hepmc_interface_1"

contains

subroutine vertex_init_pos (v, x, y, z, t)
  type(hepmc_vertex_t), intent(out) :: v
  real(default), intent(in) :: x, y, z, t
  type(vector4_t) :: xx
  xx = vector4_moving (t, vector3_moving ([x, y, z]))
  call hepmc_vertex_init (v, xx)
end subroutine vertex_init_pos

subroutine particle_init (prt, px, py, pz, E, pdg, status)
  type(hepmc_particle_t), intent(out) :: prt
  real(default), intent(in) :: px, py, pz, E
  integer, intent(in) :: pdg, status
  type(vector4_t) :: p
  p = vector4_moving (E, vector3_moving ([px, py, pz]))
  call hepmc_particle_init (prt, p, pdg, status)
end subroutine particle_init

end subroutine hepmc_interface_1

```

18.13 LCIO events

This section provides the interface to the LCIO C++ library for handling Monte-Carlo events.

Each C++ class of LCIO that we use is mirrored by a Fortran type, which contains as its only component the C pointer to the C++ object.

Each C++ method of LCIO that we use has a C wrapper function. This function takes a pointer to the host object as its first argument. Further arguments are either C pointers, or in the case of simple types (integer, real), interoperable C/Fortran objects.

The C wrapper functions have explicit interfaces in the Fortran module. They are called by Fortran wrapper procedures. These are treated as methods of the corresponding Fortran type.

```

<lcio_interface.f90>≡
  <File header>

```

```

module lcio_interface

  use, intrinsic :: iso_c_binding !NODEP!

  <Use kinds>
  <Use strings>
  use constants, only: PI

```



```

    use physics_defs, only: ns_per_mm
    use diagnostics
    use lorentz
    use flavors
    use colors
    use helicities
    use polarizations
    use event_handles, only: event_handle_t

    <Standard module head>

    <LCIO interface: public>

    <LCIO interface: types>

    <LCIO interface: interfaces>

contains

    <LCIO interface: procedures>

end module lcio_interface

```

18.13.1 Interface check

This function can be called in order to verify that we are using the actual LCIO library, and not the dummy version.

```

<LCIO interface: interfaces>≡
    interface
        logical(c_bool) function lcio_available () bind(C)
            import
        end function lcio_available
    end interface

<LCIO interface: public>≡
    public :: lcio_is_available

<LCIO interface: procedures>≡
    function lcio_is_available () result (flag)
        logical :: flag
        flag = lcio_available ()
    end function lcio_is_available

```

18.13.2 LCIO Run Header

This is a type for the run header of the LCIO file.

```

<LCIO interface: public>+≡
    public :: lcio_run_header_t

<LCIO interface: types>≡
    type :: lcio_run_header_t
    private
    type(c_ptr) :: obj

```

```
end type lcio_run_header_t
```

The Fortran version has initializer form.

<LCIO interface: interfaces>+≡

```
interface
  type(c_ptr) function new_lcio_run_header (proc_id) bind(C)
  import
  integer(c_int), value :: proc_id
  end function new_lcio_run_header
end interface
```

<LCIO interface: interfaces>+≡

```
interface
  subroutine run_header_set_simstring &
    (runhdr_obj, simstring) bind(C)
  import
  type(c_ptr), value :: runhdr_obj
  character(c_char), dimension(*), intent(in) :: simstring
  end subroutine run_header_set_simstring
end interface
```

<LCIO interface: public>+≡

```
public :: lcio_run_header_init
```

<LCIO interface: procedures>+≡

```
subroutine lcio_run_header_init (runhdr, proc_id, run_id)
  type(lcio_run_header_t), intent(out) :: runhdr
  integer, intent(in), optional :: proc_id, run_id
  integer(c_int) :: rid
  rid = 0; if (present (run_id)) rid = run_id
  runhdr%obj = new_lcio_run_header (rid)
  call run_header_set_simstring (runhdr%obj, &
    "WHIZARD version:" // "{Version}")
end subroutine lcio_run_header_init
```

<LCIO interface: interfaces>+≡

```
interface
  subroutine write_run_header (lcwrt_obj, runhdr_obj) bind(C)
  import
  type(c_ptr), value :: lcwrt_obj
  type(c_ptr), value :: runhdr_obj
  end subroutine write_run_header
end interface
```

<LCIO interface: public>+≡

```
public :: lcio_run_header_write
```

<LCIO interface: procedures>+≡

```
subroutine lcio_run_header_write (wrt, hdr)
  type(lcio_writer_t), intent(inout) :: wrt
  type(lcio_run_header_t), intent(inout) :: hdr
  call write_run_header (wrt%obj, hdr%obj)
end subroutine lcio_run_header_write
```

18.13.3 LCIO Event and LC Collection

The main object of LCIO is a LCEventImpl. The object is filled by MCParticle objects, which are set as LCCollection.

```
<LCIO interface: public>+≡
  public :: lccollection_t

<LCIO interface: types>+≡
  type :: lccollection_t
  private
    type(c_ptr) :: obj = c_null_ptr
  end type lccollection_t
```

Initializer.

```
<LCIO interface: interfaces>+≡
  interface
    type(c_ptr) function new_lccollection () bind(C)
    import
    end function new_lccollection
  end interface

<LCIO interface: public>+≡
  public :: lcio_event_t

<LCIO interface: types>+≡
  type, extends (event_handle_t) :: lcio_event_t
  private
    type(c_ptr) :: obj = c_null_ptr
    type(lccollection_t) :: lccoll
  end type lcio_event_t
```

Constructor. Arguments are process ID (integer) and event ID (integer).

The Fortran version has initializer form.

```
<LCIO interface: interfaces>+≡
  interface
    type(c_ptr) function new_lcio_event (proc_id, event_id, run_id) bind(C)
    import
    integer(c_int), value :: proc_id, event_id, run_id
    end function new_lcio_event
  end interface

<LCIO interface: public>+≡
  public :: lcio_event_init

<LCIO interface: procedures>+≡
  subroutine lcio_event_init (evt, proc_id, event_id, run_id)
    type(lcio_event_t), intent(out) :: evt
    integer, intent(in), optional :: proc_id, event_id, run_id
    integer(c_int) :: pid, eid, rid
    pid = 0; if (present (proc_id)) pid = proc_id
    eid = 0; if (present (event_id)) eid = event_id
    rid = 0; if (present (run_id)) rid = run_id
    evt%obj = new_lcio_event (pid, eid, rid)
    evt%lccoll%obj = new_lccollection ()
  end subroutine lcio_event_init
```

Destructor.

```
<LCIO interface: interfaces>+≡  
interface  
  subroutine lcio_event_delete (evt_obj) bind(C)  
    import  
    type(c_ptr), value :: evt_obj  
  end subroutine lcio_event_delete  
end interface
```

Show event on screen.

```
<LCIO interface: interfaces>+≡  
interface  
  subroutine dump_lcio_event (evt_obj) bind(C)  
    import  
    type(c_ptr), value :: evt_obj  
  end subroutine dump_lcio_event  
end interface
```

```
<LCIO interface: public>+≡  
public :: show_lcio_event
```

```
<LCIO interface: procedures>+≡  
subroutine show_lcio_event (evt)  
  type(lcio_event_t), intent(in) :: evt  
  if (c_associated (evt%obj)) then  
    call dump_lcio_event (evt%obj)  
  else  
    call msg_error ("LCIO event is not allocated.")  
  end if  
end subroutine show_lcio_event
```

Put a single event to file.

```
<LCIO interface: interfaces>+≡  
interface  
  subroutine lcio_event_to_file (evt_obj, filename) bind(C)  
    import  
    type(c_ptr), value :: evt_obj  
    character(c_char), dimension(*), intent(in) :: filename  
  end subroutine lcio_event_to_file  
end interface
```

```
<LCIO interface: public>+≡  
public :: write_lcio_event
```

```
<LCIO interface: procedures>+≡  
subroutine write_lcio_event (evt, filename)  
  type(lcio_event_t), intent(in) :: evt  
  type(string_t), intent(in) :: filename  
  call lcio_event_to_file (evt%obj, char (filename) // c_null_char)  
end subroutine write_lcio_event
```

Finalize: use the LCIO destructor. Also nullify the pointer explicitly, to be on the safe side.

```
<LCIO interface: public>+≡  
public :: lcio_event_final
```

```

<LCIO interface: procedures>+≡
subroutine lcio_event_final (evt, delete)
  type(lcio_event_t), intent(inout) :: evt
  logical, intent(in) :: delete
  if (c_associated (evt%obj)) then
    if (delete) call lcio_event_delete (evt%obj)
    evt%obj = c_null_ptr
    evt%lccoll%obj = c_null_ptr
  end if
end subroutine lcio_event_final

```

Nullify: do not call the destructor, just nullify the C pointer. There should be another pointer associated with the object.

```

<LCIO interface: public>+≡
public :: lcio_event_nullify

<LCIO interface: procedures>+≡
subroutine lcio_event_nullify (evt)
  type(lcio_event_t), intent(inout) :: evt
  evt%obj = c_null_ptr
  evt%lccoll%obj = c_null_ptr
end subroutine lcio_event_nullify

```

Return the actual object as a C pointer. For use in the native C++ interface only.

```

<LCIO interface: public>+≡
public :: lcio_event_get_c_ptr

<LCIO interface: procedures>+≡
function lcio_event_get_c_ptr (evt) result (p)
  type(lcio_event_t), intent(in) :: evt
  type(c_ptr) :: p
  p = evt%obj
end function lcio_event_get_c_ptr

```

```

<LCIO interface: interfaces>+≡
interface
  subroutine lcio_set_weight (evt_obj, weight) bind(C)
    import
    type(c_ptr), value :: evt_obj
    real(c_double), value :: weight
  end subroutine lcio_set_weight
end interface
interface
  subroutine lcio_set_alpha_qcd (evt_obj, alphas) bind(C)
    import
    type(c_ptr), value :: evt_obj
    real(c_double), value :: alphas
  end subroutine lcio_set_alpha_qcd
end interface
interface
  subroutine lcio_set_scale (evt_obj, scale) bind(C)
    import

```

```

        type(c_ptr), value :: evt_obj
        real(c_double), value :: scale
    end subroutine lcio_set_scale
end interface
interface
    subroutine lcio_set_sqrts (evt_obj, sqrts) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: sqrts
    end subroutine lcio_set_sqrts
end interface
interface
    subroutine lcio_set_xsec (evt_obj, xsec, xsec_err) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: xsec, xsec_err
    end subroutine lcio_set_xsec
end interface
interface
    subroutine lcio_set_beam (evt_obj, pdg, beam) bind(C)
        import
        type(c_ptr), value :: evt_obj
        integer(c_int), value :: pdg, beam
    end subroutine lcio_set_beam
end interface
interface
    subroutine lcio_set_pol (evt_obj, pol1, pol2) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: pol1, pol2
    end subroutine lcio_set_pol
end interface
interface
    subroutine lcio_set_beam_file (evt_obj, file) bind(C)
        import
        type(c_ptr), value :: evt_obj
        character(len=1, kind=c_char), dimension(*), intent(in) :: file
    end subroutine lcio_set_beam_file
end interface
interface
    subroutine lcio_set_process_name (evt_obj, name) bind(C)
        import
        type(c_ptr), value :: evt_obj
        character(len=1, kind=c_char), dimension(*), intent(in) :: name
    end subroutine lcio_set_process_name
end interface
interface
    subroutine lcio_set_sqme (evt_obj, sqme) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: sqme
    end subroutine lcio_set_sqme
end interface
interface

```

```

        subroutine lcio_set_alt_sqme (evt_obj, sqme, index) bind(C)
            import
            type(c_ptr), value :: evt_obj
            real(c_double), value :: sqme
            integer(c_int), value :: index
        end subroutine lcio_set_alt_sqme
    end interface
interface
    subroutine lcio_set_alt_weight (evt_obj, weight, index) bind(C)
        import
        type(c_ptr), value :: evt_obj
        real(c_double), value :: weight
        integer(c_int), value :: index
    end subroutine lcio_set_alt_weight
end interface

<LCIO interface: public>+=
    public :: lcio_event_set_weight

<LCIO interface: procedures>+=
    subroutine lcio_event_set_weight (evt, weight)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: weight
        call lcio_set_weight (evt%obj, real (weight, c_double))
    end subroutine lcio_event_set_weight

<LCIO interface: public>+=
    public :: lcio_event_set_alpha_qcd

<LCIO interface: procedures>+=
    subroutine lcio_event_set_alpha_qcd (evt, alphas)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: alphas
        call lcio_set_alpha_qcd (evt%obj, real (alphas, c_double))
    end subroutine lcio_event_set_alpha_qcd

<LCIO interface: public>+=
    public :: lcio_event_set_scale

<LCIO interface: procedures>+=
    subroutine lcio_event_set_scale (evt, scale)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: scale
        call lcio_set_scale (evt%obj, real (scale, c_double))
    end subroutine lcio_event_set_scale

<LCIO interface: public>+=
    public :: lcio_event_set_sqrts

<LCIO interface: procedures>+=
    subroutine lcio_event_set_sqrts (evt, sqrts)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqrts
        call lcio_set_sqrts (evt%obj, real (sqrts, c_double))
    end subroutine lcio_event_set_sqrts

```

```

<LCIO interface: public>+≡
    public :: lcio_event_set_xsec

<LCIO interface: procedures>+≡
    subroutine lcio_event_set_xsec (evt, xsec, xsec_err)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: xsec, xsec_err
        call lcio_set_xsec (evt%obj, &
            real (xsec, c_double), real (xsec_err, c_double))
    end subroutine lcio_event_set_xsec

<LCIO interface: public>+≡
    public :: lcio_event_set_beam

<LCIO interface: procedures>+≡
    subroutine lcio_event_set_beam (evt, pdg, beam)
        type(lcio_event_t), intent(inout) :: evt
        integer, intent(in) :: pdg, beam
        call lcio_set_beam (evt%obj, &
            int (pdg, c_int), int (beam, c_int))
    end subroutine lcio_event_set_beam

<LCIO interface: public>+≡
    public :: lcio_event_set_polarization

<LCIO interface: procedures>+≡
    subroutine lcio_event_set_polarization (evt, pol)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in), dimension(2) :: pol
        call lcio_set_pol (evt%obj, &
            real (pol(1), c_double), real (pol(2), c_double))
    end subroutine lcio_event_set_polarization

<LCIO interface: public>+≡
    public :: lcio_event_set_beam_file

<LCIO interface: procedures>+≡
    subroutine lcio_event_set_beam_file (evt, file)
        type(lcio_event_t), intent(inout) :: evt
        type(string_t), intent(in) :: file
        call lcio_set_beam_file (evt%obj, &
            char (file) // c_null_char)
    end subroutine lcio_event_set_beam_file

<LCIO interface: public>+≡
    public :: lcio_event_set_process_name

<LCIO interface: procedures>+≡
    subroutine lcio_event_set_process_name (evt, name)
        type(lcio_event_t), intent(inout) :: evt
        type(string_t), intent(in) :: name
        call lcio_set_process_name (evt%obj, &
            char (name) // c_null_char)
    end subroutine lcio_event_set_process_name

```



```

<LCIO interface: public>+≡
    public :: lcio_event_set_alt_sqme

<LCIO interface: procedures>+≡
    subroutine lcio_event_set_alt_sqme (evt, sqme, index)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqme
        integer, intent(in) :: index
        call lcio_set_alt_sqme (evt%obj, real (sqme, c_double), &
            int (index, c_int))
    end subroutine lcio_event_set_alt_sqme

<LCIO interface: public>+≡
    public :: lcio_event_set_sqme

<LCIO interface: procedures>+≡
    subroutine lcio_event_set_sqme (evt, sqme)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: sqme
        call lcio_set_sqme (evt%obj, real (sqme, c_double))
    end subroutine lcio_event_set_sqme

<LCIO interface: public>+≡
    public :: lcio_event_set_alt_weight

<LCIO interface: procedures>+≡
    subroutine lcio_event_set_alt_weight (evt, weight, index)
        type(lcio_event_t), intent(inout) :: evt
        real(default), intent(in) :: weight
        integer, intent(in) :: index
        call lcio_set_alt_weight (evt%obj, real (weight, c_double), &
            int (index, c_int))
    end subroutine lcio_event_set_alt_weight

<LCIO interface: interfaces>+≡
    interface
        subroutine lcio_event_add_collection &
            (evt_obj, lccoll_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj, lccoll_obj
    end subroutine lcio_event_add_collection
    end interface

<LCIO interface: public>+≡
    public :: lcio_event_add_coll

<LCIO interface: procedures>+≡
    subroutine lcio_event_add_coll (evt)
        type(lcio_event_t), intent(inout) :: evt
        call lcio_event_add_collection (evt%obj, &
            evt%lccoll%obj)
    end subroutine lcio_event_add_coll

```

18.13.4 LCIO Particle

Particle objects have the obvious meaning.

```
<LCIO interface: public>+≡  
    public :: lcio_particle_t  
  
<LCIO interface: types>+≡  
    type :: lcio_particle_t  
    private  
        type(c_ptr) :: obj  
    end type lcio_particle_t
```

Constructor.

```
<LCIO interface: interfaces>+≡  
    interface  
        type(c_ptr) function new_lcio_particle &  
            (px, py, pz, pdg_id, mass, charge, status) bind(C)  
        import  
            integer(c_int), value :: pdg_id, status  
            real(c_double), value :: px, py, pz, mass, charge  
        end function new_lcio_particle  
    end interface  
  
<LCIO interface: interfaces>+≡  
    interface  
        subroutine add_particle_to_collection &  
            (prt_obj, lccoll_obj) bind(C)  
        import  
            type(c_ptr), value :: prt_obj, lccoll_obj  
        end subroutine add_particle_to_collection  
    end interface  
  
<LCIO interface: public>+≡  
    public :: lcio_particle_add_to_evt_coll  
  
<LCIO interface: procedures>+≡  
    subroutine lcio_particle_add_to_evt_coll &  
        (lprt, evt)  
        type(lcio_particle_t), intent(in) :: lprt  
        type(lcio_event_t), intent(inout) :: evt  
        call add_particle_to_collection (lprt%obj, evt%lccoll%obj)  
    end subroutine lcio_particle_add_to_evt_coll  
  
  
<LCIO interface: public>+≡  
    public :: lcio_particle_init  
  
<LCIO interface: procedures>+≡  
    subroutine lcio_particle_init (prt, p, pdg, charge, status)  
        type(lcio_particle_t), intent(out) :: prt  
        type(vector4_t), intent(in) :: p  
        real(default), intent(in) :: charge  
        real(default) :: mass  
        real(default) :: px, py, pz  
        integer, intent(in) :: pdg, status  
        px = vector4_get_component (p, 1)
```

```

py = vector4_get_component (p, 2)
pz = vector4_get_component (p, 3)
mass = p**1
prt%obj = new_lcio_particle (real (px, c_double), real (py, c_double), &
    real (pz, c_double), int (pdg, c_int), &
    real (mass, c_double), real (charge, c_double), int (status, c_int))
end subroutine lcio_particle_init

```

Set the particle color flow.

(LCIO interface: interfaces)+≡

```

interface
    subroutine lcio_set_color_flow (prt_obj, col1, col2) bind(C)
        import
        type(c_ptr), value :: prt_obj
        integer(c_int), value :: col1, col2
    end subroutine lcio_set_color_flow
end interface

```

Set the particle color. Either from a `color_t` object or directly from a pair of integers.

(LCIO interface: interfaces)+≡

```

interface lcio_particle_set_color
    module procedure lcio_particle_set_color_col
    module procedure lcio_particle_set_color_int
end interface lcio_particle_set_color

```

(LCIO interface: public)+≡

```

public :: lcio_particle_set_color

```

(LCIO interface: procedures)+≡

```

subroutine lcio_particle_set_color_col (prt, col)
    type(lcio_particle_t), intent(inout) :: prt
    type(color_t), intent(in) :: col
    integer(c_int), dimension(2) :: c
    c(1) = col%get_col ()
    c(2) = col%get_acl ()
    if (c(1) /= 0 .or. c(2) /= 0) then
        call lcio_set_color_flow (prt%obj, c(1), c(2))
    end if
end subroutine lcio_particle_set_color_col

subroutine lcio_particle_set_color_int (prt, col)
    type(lcio_particle_t), intent(inout) :: prt
    integer, dimension(2), intent(in) :: col
    integer(c_int), dimension(2) :: c
    c = col
    if (c(1) /= 0 .or. c(2) /= 0) then
        call lcio_set_color_flow (prt%obj, c(1), c(2))
    end if
end subroutine lcio_particle_set_color_int

```

Return the particle color as a two-dimensional array (color, anticolor).

(LCIO interface: interfaces)+≡

```

interface

```

```

        integer(c_int) function lcio_particle_flow (prt_obj, col_index) bind(C)
            use iso_c_binding !NODEP!
            type(c_ptr), value :: prt_obj
            integer(c_int), value :: col_index
        end function lcio_particle_flow
    end interface

    <LCIO interface: public>+≡
        public :: lcio_particle_get_flow

    <LCIO interface: procedures>+≡
        function lcio_particle_get_flow (prt) result (col)
            integer, dimension(2) :: col
            type(lcio_particle_t), intent(in) :: prt
            col(1) = lcio_particle_flow (prt%obj, 0_c_int)
            col(2) = - lcio_particle_flow (prt%obj, 1_c_int)
        end function lcio_particle_get_flow

```

Return the four-momentum of a LCIO particle.

```

    <LCIO interface: interfaces>+≡
        interface
            real(c_double) function lcio_three_momentum (prt_obj, p_index) bind(C)
                use iso_c_binding !NODEP!
                type(c_ptr), value :: prt_obj
                integer(c_int), value :: p_index
            end function lcio_three_momentum
        end interface

    <LCIO interface: interfaces>+≡
        interface
            real(c_double) function lcio_energy (prt_obj) bind(C)
                import
                type(c_ptr), intent(in), value :: prt_obj
            end function lcio_energy
        end interface

    <LCIO interface: public>+≡
        public :: lcio_particle_get_momentum

    <LCIO interface: procedures>+≡
        function lcio_particle_get_momentum (prt) result (p)
            type(vector4_t) :: p
            type(lcio_particle_t), intent(in) :: prt
            real(default) :: E, px, py, pz
            E = lcio_energy (prt%obj)
            px = lcio_three_momentum (prt%obj, 0_c_int)
            py = lcio_three_momentum (prt%obj, 1_c_int)
            pz = lcio_three_momentum (prt%obj, 2_c_int)
            p = vector4_moving ( E, vector3_moving ([ px, py, pz ]))
        end function lcio_particle_get_momentum

```

Return the invariant mass squared of the particle object. LCIO stores the signed invariant mass (no squaring).

```

    <LCIO interface: interfaces>+≡
        interface

```

```

        function lcio_mass (prt_obj) result (mass) bind(C)
            import
            real(c_double) :: mass
            type(c_ptr), value :: prt_obj
        end function lcio_mass
    end interface

    <LCIO interface: public>+≡
        public :: lcio_particle_get_mass_squared

    <LCIO interface: procedures>+≡
        function lcio_particle_get_mass_squared (prt) result (m2)
            real(default) :: m2
            type(lcio_particle_t), intent(in) :: prt
            real(default) :: m
            m = lcio_mass (prt%obj)
            m2 = sign (m**2, m)
        end function lcio_particle_get_mass_squared

```

Return vertex and production time of a LCIO particle.

```

    <LCIO interface: interfaces>+≡
        interface
            real(c_double) function lcio_vtx_x (prt) bind(C)
                import
                type(c_ptr), value :: prt
            end function lcio_vtx_x
        end interface
        interface
            real(c_double) function lcio_vtx_y (prt) bind(C)
                import
                type(c_ptr), value :: prt
            end function lcio_vtx_y
        end interface
        interface
            real(c_double) function lcio_vtx_z (prt) bind(C)
                import
                type(c_ptr), value :: prt
            end function lcio_vtx_z
        end interface
        interface
            real(c_float) function lcio_prt_time (prt) bind(C)
                import
                type(c_ptr), value :: prt
            end function lcio_prt_time
        end interface

```

(Decay) times in LCIO are in nanoseconds, so they need to get converted to mm for the internal format.

```

    <LCIO interface: public>+≡
        public :: lcio_particle_get_vertex
        public :: lcio_particle_get_time

    <LCIO interface: procedures>+≡
        function lcio_particle_get_vertex (prt) result (vtx)
            type(vector3_t) :: vtx

```

```

    type(lcio_particle_t), intent(in) :: prt
    real(default) :: vx, vy, vz
    vx = lcio_vtx_x (prt%obj)
    vy = lcio_vtx_y (prt%obj)
    vz = lcio_vtx_z (prt%obj)
    vtx = vector3_moving ([vx, vy, vz])
end function lcio_particle_get_vertex

function lcio_particle_get_time (prt) result (time)
    real(default) :: time
    type(lcio_particle_t), intent(in) :: prt
    time = lcio_prt_time (prt%obj)
    time = time / ns_per_mm
end function lcio_particle_get_time

```

18.13.5 Polarization

For polarization there is a three-component float entry foreseen in the LCIO format. Completely generic density matrices can in principle be attached to events as float vectors added to LCCollection of the LCEvent. This is not yet implemented currently. Here, we restrict ourselves to the same implementation as in HepMC format: we use two entries as the polarization angles, while the first entry gives the degree of polarization (something not specified in the HepMC format). *For massive vector bosons, we arbitrarily choose the convention that the longitudinal (zero) helicity state is mapped to the theta angle $\pi/2$. This works under the condition that helicity is projected onto one of the basis states.*

<LCIO interface: interfaces>+≡

```

interface
    subroutine lcio_particle_set_spin (prt_obj, s1, s2, s3) bind(C)
        import
        type(c_ptr), value :: prt_obj
        real(c_double), value :: s1, s2, s3
    end subroutine lcio_particle_set_spin
end interface

```

<LCIO interface: public>+≡

```

public :: lcio_polarization_init

```

<LCIO interface: interfaces>+≡

```

interface lcio_polarization_init
    module procedure lcio_polarization_init_pol
    module procedure lcio_polarization_init_hel
    module procedure lcio_polarization_init_int
end interface

```

<LCIO interface: procedures>+≡

```

subroutine lcio_polarization_init_pol (prt, pol)
    type(lcio_particle_t), intent(inout) :: prt
    type(polarization_t), intent(in) :: pol
    real(default) :: r, theta, phi
    if (pol%is_polarized ()) then
        call pol%to_angles (r, theta, phi)
        call lcio_particle_set_spin (prt%obj, &

```

```

        real(r, c_double), real (theta, c_double), real (phi, c_double))
    end if
end subroutine lcio_polarization_init_pol

subroutine lcio_polarization_init_hel (prt, hel)
    type(lcio_particle_t), intent(inout) :: prt
    type(helicity_t), intent(in) :: hel
    integer, dimension(2) :: h
    if (hel%is_defined ()) then
        h = hel%to_pair ()
        select case (h(1))
        case (1:)
            call lcio_particle_set_spin (prt%obj, 1._c_double, &
                0._c_double, 0._c_double)
        case (:-1)
            call lcio_particle_set_spin (prt%obj, 1._c_double, &
                real (pi, c_double), 0._c_double)
        case (0)
            call lcio_particle_set_spin (prt%obj, 1._c_double, &
                real (pi/2, c_double), 0._c_double)
        end select
    end if
end subroutine lcio_polarization_init_hel

subroutine lcio_polarization_init_int (prt, hel)
    type(lcio_particle_t), intent(inout) :: prt
    integer, intent(in) :: hel
    call lcio_particle_set_spin (prt%obj, 0._c_double, &
        0._c_double, real (hel, c_double))
end subroutine lcio_polarization_init_int

```

Recover polarization from LCIO particle (with the abovementioned deficiencies).

(LCIO interface: interfaces)+≡

```

interface
    function lcio_polarization_degree (prt_obj) result (degree) bind(C)
        import
        real(c_double) :: degree
        type(c_ptr), value :: prt_obj
    end function lcio_polarization_degree
end interface

interface
    function lcio_polarization_theta (prt_obj) result (theta) bind(C)
        import
        real(c_double) :: theta
        type(c_ptr), value :: prt_obj
    end function lcio_polarization_theta
end interface

interface
    function lcio_polarization_phi (prt_obj) result (phi) bind(C)
        import
        real(c_double) :: phi
        type(c_ptr), value :: prt_obj
    end function lcio_polarization_phi
end interface

```

```

end interface
<LCIO interface: public>+≡
public :: lcio_particle_to_pol
<LCIO interface: procedures>+≡
subroutine lcio_particle_to_pol (prt, flv, pol)
  type(lcio_particle_t), intent(in) :: prt
  type(flavor_t), intent(in) :: flv
  type(polarization_t), intent(out) :: pol
  real(default) :: degree, theta, phi
  degree = lcio_polarization_degree (prt%obj)
  theta = lcio_polarization_theta (prt%obj)
  phi = lcio_polarization_phi (prt%obj)
  call pol%init_angles (flv, degree, theta, phi)
end subroutine lcio_particle_to_pol

```

Recover helicity. Here, ϕ and `degree` is ignored and only the sign of $\cos\theta$ is relevant, mapped to positive/negative helicity.

```

<LCIO interface: public>+≡
public :: lcio_particle_to_hel
<LCIO interface: procedures>+≡
subroutine lcio_particle_to_hel (prt, flv, hel)
  type(lcio_particle_t), intent(in) :: prt
  type(flavor_t), intent(in) :: flv
  type(helicity_t), intent(out) :: hel
  real(default) :: theta
  integer :: hmax
  theta = lcio_polarization_theta (prt%obj)
  hmax = flv%get_spin_type () / 2
  call hel%init (sign (hmax, nint (cos (theta))))
end subroutine lcio_particle_to_hel

```

Set the vertex of a particle.

```

<LCIO interface: interfaces>+≡
interface
  subroutine lcio_particle_set_vertex (prt_obj, vx, vy, vz) bind(C)
    import
    type(c_ptr), value :: prt_obj
    real(c_double), value :: vx, vy, vz
  end subroutine lcio_particle_set_vertex
end interface
interface
  subroutine lcio_particle_set_time (prt_obj, t) bind(C)
    import
    type(c_ptr), value :: prt_obj
    real(c_float), value :: t
  end subroutine lcio_particle_set_time
end interface

<LCIO interface: public>+≡
public :: lcio_particle_set_vtx

```



```

<LCIO interface: procedures>+≡
  subroutine lcio_particle_set_vtx (prt, vtx)
    type(lcio_particle_t), intent(inout) :: prt
    type(vector3_t), intent(in) :: vtx
    call lcio_particle_set_vertex (prt%obj, real(vtx%p(1), c_double), &
      real(vtx%p(2), c_double), real(vtx%p(3), c_double))
  end subroutine lcio_particle_set_vtx

```

Times in LCIO are in nanoseconds, not in mm, so need to be converted.

```

<LCIO interface: public>+≡
  public :: lcio_particle_set_t

<LCIO interface: procedures>+≡
  subroutine lcio_particle_set_t (prt, t)
    type(lcio_particle_t), intent(inout) :: prt
    real(default), intent(in) :: t
    real(default) :: ns_from_t_mm
    ns_from_t_mm = ns_per_mm * t
    call lcio_particle_set_time (prt%obj, real(ns_from_t_mm, c_float))
  end subroutine lcio_particle_set_t

```

```

<LCIO interface: interfaces>+≡
  interface
    subroutine lcio_particle_add_parent (prt_obj1, prt_obj2) bind(C)
      import
      type(c_ptr), value :: prt_obj1, prt_obj2
    end subroutine lcio_particle_add_parent
  end interface

```

```

<LCIO interface: public>+≡
  public :: lcio_particle_set_parent

```

```

<LCIO interface: procedures>+≡
  subroutine lcio_particle_set_parent (daughter, parent)
    type(lcio_particle_t), intent(inout) :: daughter, parent
    call lcio_particle_add_parent (daughter%obj, parent%obj)
  end subroutine lcio_particle_set_parent

```

```

<LCIO interface: interfaces>+≡
  interface
    integer(c_int) function lcio_particle_get_generator_status &
      (prt_obj) bind(C)
    import
    type(c_ptr), value :: prt_obj
    end function lcio_particle_get_generator_status
  end interface

```

```

<LCIO interface: public>+≡
  public :: lcio_particle_get_status

```

```

<LCIO interface: procedures>+≡
  function lcio_particle_get_status (lptr) result (status)
    integer :: status
    type(lcio_particle_t), intent(in) :: lptr
    status = lcio_particle_get_generator_status (lptr%obj)
  end function

```

```
end function lcio_particle_get_status
```

Getting the PDG code.

```
<LCIO interface: interfaces>+≡
interface
  integer(c_int) function lcio_particle_get_pdg_code (prt_obj) bind(C)
  import
  type(c_ptr), value :: prt_obj
  end function lcio_particle_get_pdg_code
end interface

<LCIO interface: public>+≡
public :: lcio_particle_get_pdg

<LCIO interface: procedures>+≡
function lcio_particle_get_pdg (lptr) result (pdg)
  integer :: pdg
  type(lcio_particle_t), intent(in) :: lptr
  pdg = lcio_particle_get_pdg_code (lptr%obj)
end function lcio_particle_get_pdg
```

Obtaining the number of parents and daughters of an LCIO particle.

```
<LCIO interface: interfaces>+≡
interface
  integer(c_int) function lcio_n_parents (prt_obj) bind(C)
  import
  type(c_ptr), value :: prt_obj
  end function lcio_n_parents
end interface

<LCIO interface: interfaces>+≡
interface
  integer(c_int) function lcio_n_daughters (prt_obj) bind(C)
  import
  type(c_ptr), value :: prt_obj
  end function lcio_n_daughters
end interface

<LCIO interface: public>+≡
public :: lcio_particle_get_n_parents

<LCIO interface: procedures>+≡
function lcio_particle_get_n_parents (lptr) result (n_parents)
  integer :: n_parents
  type(lcio_particle_t), intent(in) :: lptr
  n_parents = lcio_n_parents (lptr%obj)
end function lcio_particle_get_n_parents

<LCIO interface: public>+≡
public :: lcio_particle_get_n_children
```

```

<LCIO interface: procedures>+≡
function lcio_particle_get_n_children (lptr) result (n_children)
integer :: n_children
type(lcio_particle_t), intent(in) :: lptr
n_children = lcio_n_daughters (lptr%obj)
end function lcio_particle_get_n_children

```

This provides access from the LCIO event `lcio_event_t` to the array entries of the parent and daughter arrays of the LCIO particles.

```

<LCIO interface: interfaces>+≡
interface
integer(c_int) function lcio_event_parent_k &
    (evt_obj, num_part, k_parent) bind (C)
use iso_c_binding !NODEP!
type(c_ptr), value :: evt_obj
integer(c_int), value :: num_part, k_parent
end function lcio_event_parent_k
end interface

```

```

<LCIO interface: interfaces>+≡
interface
integer(c_int) function lcio_event_daughter_k &
    (evt_obj, num_part, k_daughter) bind (C)
use iso_c_binding !NODEP!
type(c_ptr), value :: evt_obj
integer(c_int), value :: num_part, k_daughter
end function lcio_event_daughter_k
end interface

```

```

<LCIO interface: public>+≡
public :: lcio_get_n_parents

```

```

<LCIO interface: procedures>+≡
function lcio_get_n_parents (evt, num_part, k_parent) result (index_parent)
type(lcio_event_t), intent(in) :: evt
integer, intent(in) :: num_part, k_parent
integer :: index_parent
index_parent = lcio_event_parent_k (evt%obj, int (num_part, c_int), &
    int (k_parent, c_int))
end function lcio_get_n_parents

```

```

<LCIO interface: public>+≡
public :: lcio_get_n_children

```

```

<LCIO interface: procedures>+≡
function lcio_get_n_children (evt, num_part, k_daughter) result (index_daughter)
type(lcio_event_t), intent(in) :: evt
integer, intent(in) :: num_part, k_daughter
integer :: index_daughter
index_daughter = lcio_event_daughter_k (evt%obj, int (num_part, c_int), &
    int (k_daughter, c_int))
end function lcio_get_n_children

```

18.13.6 LCIO Writer type

There is a specific LCIO Writer type for handling the output of LCEventImpl objects (i.e., Monte Carlo event samples) to file. Opening the file is done by the constructor, closing by the destructor.

```
<LCIO interface: public>+≡
    public :: lcio_writer_t

<LCIO interface: types>+≡
    type :: lcio_writer_t
    private
        type(c_ptr) :: obj
    end type lcio_writer_t
```

Constructor for an output associated to a file.

```
<LCIO interface: interfaces>+≡
    interface
        type(c_ptr) function open_lcio_writer_new (filename, complevel) bind(C)
        import
            character(c_char), dimension(*), intent(in) :: filename
            integer(c_int), intent(in) :: complevel
        end function open_lcio_writer_new
    end interface

<LCIO interface: public>+≡
    public :: lcio_writer_open_out

<LCIO interface: procedures>+≡
    subroutine lcio_writer_open_out (lcio_writer, filename)
        type(lcio_writer_t), intent(out) :: lcio_writer
        type(string_t), intent(in) :: filename
        lcio_writer%obj = open_lcio_writer_new (char (filename) // &
            c_null_char, 9_c_int)
    end subroutine lcio_writer_open_out
```

Destructor:

```
<LCIO interface: interfaces>+≡
    interface
        subroutine lcio_writer_delete (io_obj) bind(C)
        import
            type(c_ptr), value :: io_obj
        end subroutine lcio_writer_delete
    end interface

<LCIO interface: public>+≡
    public :: lcio_writer_close

<LCIO interface: procedures>+≡
    subroutine lcio_writer_close (lcio_writer)
        type(lcio_writer_t), intent(inout) :: lcio_writer
        call lcio_writer_delete (lcio_writer%obj)
    end subroutine lcio_writer_close
```

Write a single event to the LCIO writer.

```

<LCIO interface: interfaces>+≡
  interface
    subroutine lcio_write_event (io_obj, evt_obj) bind(C)
      import
        type(c_ptr), value :: io_obj, evt_obj
    end subroutine lcio_write_event
  end interface

<LCIO interface: public>+≡
  public :: lcio_event_write

<LCIO interface: procedures>+≡
  subroutine lcio_event_write (wrt, evt)
    type(lcio_writer_t), intent(inout) :: wrt
    type(lcio_event_t), intent(in) :: evt
    call lcio_write_event (wrt%obj, evt%obj)
  end subroutine lcio_event_write

```

18.13.7 LCIO Reader type

There is a specific LCIO Reader type for handling the input of LCEventImpl objects (i.e., Monte Carlo event samples) from file. Opening the file is done by the constructor, closing by the destructor.

```

<LCIO interface: public>+≡
  public :: lcio_reader_t

<LCIO interface: types>+≡
  type :: lcio_reader_t
  private
    type(c_ptr) :: obj
  end type lcio_reader_t

```

Constructor for an output associated to a file.

```

<LCIO interface: interfaces>+≡
  interface
    type(c_ptr) function open_lcio_reader (filename) bind(C)
      import
        character(c_char), dimension(*), intent(in) :: filename
    end function open_lcio_reader
  end interface

<LCIO interface: public>+≡
  public :: lcio_open_file

<LCIO interface: procedures>+≡
  subroutine lcio_open_file (lcio_reader, filename)
    type(lcio_reader_t), intent(out) :: lcio_reader
    type(string_t), intent(in) :: filename
    lcio_reader%obj = open_lcio_reader (char (filename) // c_null_char)
  end subroutine lcio_open_file

```

Destructor:

```
<LCIO interface: interfaces>+≡  
  interface  
    subroutine lcio_reader_delete (io_obj) bind(C)  
      import  
      type(c_ptr), value :: io_obj  
    end subroutine lcio_reader_delete  
  end interface  
  
<LCIO interface: public>+≡  
  public :: lcio_reader_close  
  
<LCIO interface: procedures>+≡  
  subroutine lcio_reader_close (lcioreader)  
    type(lcio_reader_t), intent(inout) :: lcioreader  
    call lcio_reader_delete (lcioreader%obj)  
  end subroutine lcio_reader_close
```

Read a single event from the event file. Return true if successful.

```
<LCIO interface: interfaces>+≡  
  interface  
    type(c_ptr) function read_lcio_event (io_obj) bind(C)  
      import  
      type(c_ptr), value :: io_obj  
    end function read_lcio_event  
  end interface  
  
<LCIO interface: public>+≡  
  public :: lcio_read_event  
  
<LCIO interface: procedures>+≡  
  subroutine lcio_read_event (lcrdr, evt, ok)  
    type(lcio_reader_t), intent(inout) :: lcrdr  
    type(lcio_event_t), intent(out) :: evt  
    logical, intent(out) :: ok  
    evt%obj = read_lcio_event (lcrdr%obj)  
    ok = c_associated (evt%obj)  
  end subroutine lcio_read_event
```

Get the event index.

```
<LCIO interface: interfaces>+≡  
  interface  
    integer(c_int) function lcio_event_get_event_number (evt_obj) bind(C)  
      import  
      type(c_ptr), value :: evt_obj  
    end function lcio_event_get_event_number  
  end interface  
  
<LCIO interface: public>+≡  
  public :: lcio_event_get_event_index  
  
<LCIO interface: procedures>+≡  
  function lcio_event_get_event_index (evt) result (i_evt)  
    integer :: i_evt  
    type(lcio_event_t), intent(in) :: evt
```

```

        i_evt = lcio_event_get_event_number (evt%obj)
    end function lcio_event_get_event_index

```

Extract the process ID. This is stored (at the moment abusively) in the RUN ID as well as in an additional event parameter.

```

<LCIO interface: interfaces>+≡
    interface
        integer(c_int) function lcio_event_signal_process_id (evt_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj
        end function lcio_event_signal_process_id
    end interface

<LCIO interface: public>+≡
    public :: lcio_event_get_process_id

<LCIO interface: procedures>+≡
    function lcio_event_get_process_id (evt) result (i_proc)
        integer :: i_proc
        type(lcio_event_t), intent(in) :: evt
        i_proc = lcio_event_signal_process_id (evt%obj)
    end function lcio_event_get_process_id

```

Number of particles in an LCIO event.

```

<LCIO interface: interfaces>+≡
    interface
        integer(c_int) function lcio_event_get_n_particles (evt_obj) bind(C)
        import
        type(c_ptr), value :: evt_obj
        end function lcio_event_get_n_particles
    end interface

<LCIO interface:>≡

<LCIO interface: public>+≡
    public :: lcio_event_get_n_tot

<LCIO interface: procedures>+≡
    function lcio_event_get_n_tot (evt) result (n_tot)
        integer :: n_tot
        type(lcio_event_t), intent(in) :: evt
        n_tot = lcio_event_get_n_particles (evt%obj)
    end function lcio_event_get_n_tot

```

Extracting α_s and the scale.

```

<LCIO interface: interfaces>+≡
    interface
        function lcio_event_get_alpha_qcd (evt_obj) result (as) bind(C)
        import
        real(c_double) :: as
        type(c_ptr), value :: evt_obj
        end function lcio_event_get_alpha_qcd
    end interface
    interface

```

```

        function lcio_event_get_scale (evt_obj) result (scale) bind(C)
            import
            real(c_double) :: scale
            type(c_ptr), value :: evt_obj
        end function lcio_event_get_scale
    end interface

    <LCIO interface: public>+≡
        public :: lcio_event_get_alphas

    <LCIO interface: procedures>+≡
        function lcio_event_get_alphas (evt) result (as)
            type(lcio_event_t), intent(in) :: evt
            real(default) :: as
            as = lcio_event_get_alpha_qcd (evt%obj)
        end function lcio_event_get_alphas

    <LCIO interface: public>+≡
        public :: lcio_event_get_scaleval

    <LCIO interface: procedures>+≡
        function lcio_event_get_scaleval (evt) result (scale)
            type(lcio_event_t), intent(in) :: evt
            real(default) :: scale
            scale = lcio_event_get_scale (evt%obj)
        end function lcio_event_get_scaleval

```

Extracting particles by index from an LCIO event.

```

    <LCIO interface: interfaces>+≡
        interface
            type(c_ptr) function lcio_event_particle_k (evt_obj, k) bind(C)
                import
                type(c_ptr), value :: evt_obj
                integer(c_int), value :: k
            end function lcio_event_particle_k
        end interface

    <LCIO interface: public>+≡
        public :: lcio_event_get_particle

    <LCIO interface: procedures>+≡
        function lcio_event_get_particle (evt, n) result (prt)
            type(lcio_event_t), intent(in) :: evt
            integer, intent(in) :: n
            type(lcio_particle_t) :: prt
            prt%obj = lcio_event_particle_k (evt%obj, int (n, c_int))
        end function lcio_event_get_particle

```

18.13.8 Unit tests

Test module, followed by the corresponding implementation module.

```

    <lcio_interface_ut.f90>≡
    <File header>

```



```

module lcio_interface_ut
  use unit_tests
  use lcio_interface_util

  <Standard module head>

  <LCIO interface: public test>

  contains

  <LCIO interface: test driver>

end module lcio_interface_ut
<lcio_interface_util.f90>≡
  <File header>

  module lcio_interface_util

    <Use kinds>
    <Use strings>
    use io_units
    use lorentz
    use flavors
    use colors
    use polarizations

    use lcio_interface

    <Standard module head>

    <LCIO interface: test declarations>

    contains

    <LCIO interface: tests>

  end module lcio_interface_util
API: driver for the unit tests below.
<LCIO interface: public test>≡
  public :: lcio_interface_test
<LCIO interface: test driver>≡
  subroutine lcio_interface_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <LCIO interface: execute tests>
  end subroutine lcio_interface_test

  <LCIO interface: execute tests>≡
    call test (lcio_interface_1, "lcio_interface_1", &
      "check LCIO interface", &
      u, results)

```

```

<LCIO interface: test declarations>=
  public :: lcio_interface_1

<LCIO interface: tests>=
  subroutine lcio_interface_1 (u)
    use physics_defs, only: VECTOR
    use model_data, only: field_data_t
    integer, intent(in) :: u
    integer :: u_file, iostat
    type(lcio_event_t) :: evt
    type(lcio_particle_t) :: prt1, prt2, prt3, prt4, prt5, prt6, prt7, prt8
    type(flavor_t) :: flv
    type(color_t) :: col
    type(polarization_t) :: pol
    type(field_data_t), target :: photon_data
    character(220) :: buffer

    write (u, "(A)")  "* Test output: LCIO interface"
    write (u, "(A)")  "* Purpose: test LCIO interface"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    ! Initialize a photon flavor object and some polarization
    call photon_data%init (var_str ("PHOTON"), 22)
    call photon_data%set (spin_type=VECTOR)
    call photon_data%freeze ()
    call flv%init (photon_data)
    call pol%init_angles &
      (flv, 0.6_default, 1._default, 0.5_default)

    ! Event initialization
    call lcio_event_init (evt, 20, 1, 42)

    write (u, "(A)")  "* p -> q splitting"
    write (u, "(A)")

    ! $p\to q$ splittings
    call particle_init (prt1, &
      0._default, 0._default, 7000._default, 7000._default, &
      2212, 1._default, 3)
    call particle_init (prt2, &
      0._default, 0._default, -7000._default, 7000._default, &
      2212, 1._default, 3)
    call particle_init (prt3, &
      .750_default, -1.569_default, 32.191_default, 32.238_default, &
      1, -1._default/3._default, 3)
    call color_init_from_array (col, [501])
    call lcio_particle_set_color (prt3, col)
    call lcio_particle_set_parent (prt3, prt1)
    call lcio_particle_set_parent (prt3, prt2)
    call particle_init (prt4, &
      -3.047_default, -19._default, -54.629_default, 57.920_default, &
      -2, -2._default/3._default, 3)

```

```

call color_init_from_array (col, [-501])
call lcio_particle_set_color (prt4, col)
call lcio_particle_set_parent (prt4, prt1)
call lcio_particle_set_parent (prt4, prt2)

write (u, "(A)")  "* Hard interaction"
write (u, "(A)")

! Hard interaction
call particle_init (prt6, &
    -3.813_default, 0.113_default, -1.833_default, 4.233_default, &
    22, 0._default, 1)
call lcio_polarization_init (prt6, pol)
call particle_init (prt5, &
    1.517_default, -20.68_default, -20.605_default, 85.925_default, &
    -24, -1._default, 3)
call lcio_particle_set_parent (prt5, prt3)
call lcio_particle_set_parent (prt5, prt4)
call lcio_particle_set_parent (prt6, prt3)
call lcio_particle_set_parent (prt6, prt4)

! $W^-$ decay
call particle_init (prt7, &
    -2.445_default, 28.816_default, 6.082_default, 29.552_default, &
    1, -1._default/3._default, 1)
call particle_init (prt8, &
    3.962_default, -49.498_default, -26.687_default, 56.373_default, &
    -2, -2._default/3._default, 1)
call lcio_particle_set_t (prt7, 0.12_default)
call lcio_particle_set_t (prt8, 0.12_default)
call lcio_particle_set_vtx &
    (prt7, vector3_moving ([-0.3_default, 0.05_default, 0.004_default]))
call lcio_particle_set_vtx &
    (prt8, vector3_moving ([-0.3_default, 0.05_default, 0.004_default]))
call lcio_particle_set_parent (prt7, prt5)
call lcio_particle_set_parent (prt8, prt5)
call lcio_particle_add_to_evt_coll (prt1, evt)
call lcio_particle_add_to_evt_coll (prt2, evt)
call lcio_particle_add_to_evt_coll (prt3, evt)
call lcio_particle_add_to_evt_coll (prt4, evt)
call lcio_particle_add_to_evt_coll (prt5, evt)
call lcio_particle_add_to_evt_coll (prt6, evt)
call lcio_particle_add_to_evt_coll (prt7, evt)
call lcio_particle_add_to_evt_coll (prt8, evt)
call lcio_event_add_coll (evt)

! Event output
write (u, "(A)")  "Writing in ASCII form to file 'lcio_test.slcio'"
write (u, "(A)")

call write_lcio_event (evt, var_str ("lcio_test.slcio"))

write (u, "(A)")  "Writing completed"

```

```

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "lcio_test.slcio", &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (trim (buffer) == "")  cycle
  if (buffer(1:12) == " - timestamp")  buffer = "[...]"
  if (buffer(1:6) == " date:")  buffer = "[...]"
  if (iostat /= 0)  exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

! Wrapup
! call pol%final ()
call lcio_event_final (evt, .true.)

write (u, "(A)")
write (u, "(A)")  "* Test output end: lcio_interface_1"

contains

subroutine particle_init &
  (prt, px, py, pz, E, pdg, charge, status)
  type(lcio_particle_t), intent(out) :: prt
  real(default), intent(in) :: px, py, pz, E, charge
  integer, intent(in) :: pdg, status
  type(vector4_t) :: p
  p = vector4_moving (E, vector3_moving ([px, py, pz]))
  call lcio_particle_init (prt, p, pdg, charge, status)
end subroutine particle_init

end subroutine lcio_interface_1

```

18.14 HEP Common and Events

This is a separate module that manages data exchange between the common blocks and `event_t` objects. We separate this from the previous module in order to avoid a circular module dependency. It also contains the functions necessary for communication between `hepmc_event_t` and `event_t` or `lcio_event_t` and `event_t` as well as `particle_set_t` and `particle_t` objects.

`<hep_events.f90>`≡
<File header>

```

module hep_events

  <Use kinds>
  <Use strings>
  use system_dependencies, only: HEPMC2_AVAILABLE
  use system_dependencies, only: HEPMC3_AVAILABLE
  use diagnostics
  use lorentz
  use numeric_utils
  use flavors
  use colors
  use helicities
  use polarizations
  use model_data
  use subevents, only: PRT_BEAM, PRT_INCOMING, PRT_OUTGOING
  use subevents, only: PRT_UNDEFINED
  use subevents, only: PRT_VIRTUAL, PRT_RESONANT, PRT_BEAM_REMNANT
  use particles
  use hep_common
  use hepmc_interface
  use lcio_interface
  use event_base

  <Standard module head>

  <HEP events: public>

  contains

  <HEP events: procedures>

end module hep_events

```

18.14.1 Data Transfer: events

Fill the HEPEUP block, given a WHIZARD event object.

```

<HEP events: public>≡
  public :: hepeup_from_event

<HEP events: procedures>≡
  subroutine hepeup_from_event &
    (event, keep_beams, keep_remnants, process_index)
    class(generic_event_t), intent(in), target :: event
    logical, intent(in), optional :: keep_beams
    logical, intent(in), optional :: keep_remnants
    integer, intent(in), optional :: process_index
    type(particle_set_t), pointer :: particle_set
    real(default) :: scale, alpha_qcd
    if (event%has_valid_particle_set ()) then
      particle_set => event%get_particle_set_ptr ()
      call hepeup_from_particle_set (particle_set, keep_beams, keep_remnants)
      if (present (process_index)) then
        call hepeup_set_event_parameters (proc_id = process_index)

```

```

end if
scale = event%get_fac_scale ()
if (.not. vanishes (scale)) then
    call hepeup_set_event_parameters (scale = scale)
end if
alpha_qcd = event%get_alpha_s ()
if (.not. vanishes (alpha_qcd)) then
    call hepeup_set_event_parameters (alpha_qcd = alpha_qcd)
end if
if (event%weight_prc_is_known ()) then
    call hepeup_set_event_parameters (weight = event%get_weight_prc ())
end if
else
    call msg_bug ("HEPEUP: event incomplete")
end if
end subroutine hepeup_from_event

```

Reverse.

Note: The current implementation sets the particle set of the hard process and is therefore not useful if the event on file is dressed. This should be reconsidered.

Note: setting of scale or alpha is not yet supported by the `event_t` object. Ticket #628.

```

<HEP events: public>+≡
    public :: hepeup_to_event
<HEP events: procedures>+≡
    subroutine hepeup_to_event &
        (event, fallback_model, process_index, recover_beams, &
         use_alpha_s, use_scale)
        class(generic_event_t), intent(inout), target :: event
        class(model_data_t), intent(in), target :: fallback_model
        integer, intent(out), optional :: process_index
        logical, intent(in), optional :: recover_beams
        logical, intent(in), optional :: use_alpha_s
        logical, intent(in), optional :: use_scale
        class(model_data_t), pointer :: model
        real(default) :: weight, scale, alpha_qcd
        type(particle_set_t) :: particle_set
        model => event%get_model_ptr ()
        call hepeup_to_particle_set &
            (particle_set, recover_beams, model, fallback_model)
        call event%set_hard_particle_set (particle_set)
        call particle_set%final ()
        if (present (process_index)) then
            call hepeup_get_event_parameters (proc_id = process_index)
        end if
        call hepeup_get_event_parameters (weight = weight, &
            scale = scale, alpha_qcd = alpha_qcd)
        call event%set_weight_ref (weight)
        if (present (use_alpha_s)) then
            if (use_alpha_s .and. alpha_qcd > 0) &
                call event%set_alpha_qcd_forced (alpha_qcd)
        end if
    end if

```

```

    if (present (use_scale)) then
      if (use_scale .and. scale > 0) &
        call event%set_scale_forced (scale)
    end if
  end subroutine hepevt_to_event

```

Fill the HEPEVT (event) common block.

The `i_evt` argument overrides the index stored in the `event` object.

```

<HEP events: public>+≡
  public :: hepevt_from_event

<HEP events: procedures>+≡
  subroutine hepevt_from_event  &
    (event, process_index, i_evt, keep_beams, keep_remnants, &
     ensure_order, fill_hepev4)
    class(generic_event_t), intent(in), target :: event
    integer, intent(in), optional :: i_evt, process_index
    logical, intent(in), optional :: keep_beams
    logical, intent(in), optional :: keep_remnants
    logical, intent(in), optional :: ensure_order
    logical, intent(in), optional :: fill_hepev4
    type(particle_set_t), pointer :: particle_set
    real(default) :: alpha_qcd, scale
    if (event%has_valid_particle_set ()) then
      particle_set => event%get_particle_set_ptr ()
      call hepevt_from_particle_set (particle_set, keep_beams, &
        keep_remnants, ensure_order, fill_hepev4)
    if (present (process_index)) then
      call hepevt_set_event_parameters (proc_id = process_index)
    end if
    if (event%weight_prc_is_known ()) then
      call hepevt_set_event_parameters (weight = event%get_weight_prc ())
    end if
    if (event%sqme_prc_is_known ()) then
      call hepevt_set_event_parameters &
        (function_value = event%get_sqme_prc ())
    end if
    scale = event%get_fac_scale ()
    if (.not. vanishes (scale)) then
      call hepevt_set_event_parameters (scale = scale)
    end if
    alpha_qcd = event%get_alpha_s ()
    if (.not. vanishes (alpha_qcd)) then
      call hepevt_set_event_parameters (alpha_qcd = alpha_qcd)
    end if
    if (present (i_evt)) then
      call hepevt_set_event_parameters (i_evt = i_evt)
    else if (event%has_index ()) then
      call hepevt_set_event_parameters (i_evt = event%get_index ())
    else
      call hepevt_set_event_parameters (i_evt = 0)
    end if
  else
    call msg_bug ("HEPEVT: event incomplete")
  end

```

```

end if
end subroutine hepevt_from_event

```

HepMC format

The master output function fills a HepMC GenEvent object that is already initialized, but has no vertices in it.

We first set up the vertex lists and enter the vertices into the HepMC event. Then, we assign first all incoming particles and then all outgoing particles to their associated vertices. Particles which have neither parent nor children entries (this should not happen) are dropped.

Finally, we insert the beam particles. If there are none, use the incoming particles instead. Transform a particle into a `hepmc_particle` object, including color and polarization. The HepMC status is equivalent to the HEPEVT status, in particular: 0 = null entry, 1 = physical particle, 2 = decayed/fragmented SM hadron, tau or muon, 3 = other unphysical particle entry, 4 = incoming particles, 11 = intermediate resonance such as squarks. The use of 11 for intermediate resonances is as done by HERWIG, see <http://herwig.hepforge.org/trac/wiki/FaQs>.

(HEP events: procedures) +≡

```

subroutine particle_to_hepmc (prt, hpert)
  type(particle_t), intent(in) :: prt
  type(hepmc_particle_t), intent(out) :: hpert
  integer :: hepmc_status
  select case (prt%get_status ())
  case (PRT_UNDEFINED)
    hepmc_status = 0
  case (PRT_OUTGOING)
    hepmc_status = 1
  case (PRT_BEAM)
    hepmc_status = 4
  case (PRT_RESONANT)
    hepmc_status = 2
  case (PRT_BEAM_REMNANT)
    if (prt%get_n_children () == 0) then
      hepmc_status = 1
    else
      hepmc_status = 3
    end if
  case default
    hepmc_status = 3
  end select
  call hepmc_particle_init (hpert, &
    prt%get_momentum (), prt%get_pdg (), &
    hepmc_status)
  if (HEPMC2_AVAILABLE) then
    call hepmc_particle_set_color (hpert, prt%get_color ())
    select case (prt%get_polarization_status ())
    case (PRT_DEFINITE_HELICITY)
      call hepmc_particle_set_polarization (hpert, &
        prt%get_helicity ())
    case (PRT_GENERIC_POLARIZATION)

```



```

        call hepmc_particle_set_polarization (hprrt, &
            prt%get_polarization ())
    end select
end if
end subroutine particle_to_hepmc

```

For HepMC3, a HepMC particle needs first to be attached to a vertex and an event before non-intrinsic particle properties (color flow and helicity) could be set.

```

<HEP events: public>+≡
    public :: hepmc_event_from_particle_set

<HEP events: procedures>+≡
    subroutine hepmc_event_from_particle_set &
        (evt, particle_set, cross_section, error)
        type(hepmc_event_t), intent(inout) :: evt
        type(particle_set_t), intent(in) :: particle_set
        real(default), intent(in), optional :: cross_section, error
        type(hepmc_vertex_t), dimension(:), allocatable :: v
        type(hepmc_particle_t), dimension(:), allocatable :: hprrt
        type(hepmc_particle_t), dimension(2) :: hbeam
        type(vector4_t), dimension(:), allocatable :: vtx
        logical, dimension(:), allocatable :: is_beam
        integer, dimension(:), allocatable :: v_from, v_to
        integer :: n_vertices, n_tot, i
        n_tot = particle_set%get_n_tot ()
        allocate (v_from (n_tot), v_to (n_tot))
        call particle_set%assign_vertices (v_from, v_to, n_vertices)
        allocate (hprrt (n_tot))
        allocate (vtx (n_vertices))
        vtx = vector4_null
        do i = 1, n_tot
            if (v_to(i) /= 0 .or. v_from(i) /= 0) then
                call particle_to_hepmc (particle_set%prt(i), hprrt(i))
                if (v_from(i) /= 0) then
                    vtx(v_from(i)) = particle_set%prt(i)%get_vertex ()
                end if
            end if
        end do
        if (present (cross_section) .and. present(error)) &
            call hepmc_event_set_cross_section (evt, cross_section, error)
        allocate (v (n_vertices))
        do i = 1, n_vertices
            call hepmc_vertex_init (v(i), vtx(i))
            call hepmc_event_add_vertex (evt, v(i))
        end do
        allocate (is_beam (n_tot))
        is_beam = particle_set%prt(1:n_tot)%get_status () == PRT_BEAM
        if (.not. any (is_beam)) then
            is_beam = particle_set%prt(1:n_tot)%get_status () == PRT_INCOMING
        end if
        if (count (is_beam) == 2) then
            hbeam = pack (hprrt, is_beam)
            call hepmc_event_set_beam_particles (evt, hbeam(1), hbeam(2))
        end if
    end subroutine

```

```

end if
do i = 1, n_tot
  if (v_to(i) /= 0) then
    call hepvc_vertex_add_particle_in (v(v_to(i)), hpvt(i))
  end if
end do
do i = 1, n_tot
  if (v_from(i) /= 0) then
    call hepvc_vertex_add_particle_out (v(v_from(i)), hpvt(i))
  end if
end do
FIND_SIGNAL_PROCESS: do i = 1, n_tot
  if (particle_set%prt(i)%get_status () == PRT_INCOMING) then
    call hepvc_event_set_signal_process_vertex (evt, v(v_to(i)))
    exit FIND_SIGNAL_PROCESS
  end if
end do FIND_SIGNAL_PROCESS
if (HEPMC3_AVAILABLE) then
  do i = 1, n_tot
    call hepvc_particle_set_color (hpvt(i), &
      particle_set%prt(i)%get_color ())
    select case (particle_set%prt(i)%get_polarization_status ())
    case (PRT_DEFINITE_HELICITY)
      call hepvc_particle_set_polarization (hpvt(i), &
        particle_set%prt(i)%get_helicity ())
    case (PRT_GENERIC_POLARIZATION)
      call hepvc_particle_set_polarization (hpvt(i), &
        particle_set%prt(i)%get_polarization ())
    end select
  end do
end if
end subroutine hepvc_event_from_particle_set

```

Initialize a particle from a HepMC particle object. The model is necessary for making a fully qualified flavor component. We have the additional flag `polarized` which tells whether the polarization information should be interpreted or ignored, and the lookup array of barcodes. Note that the lookup array is searched linearly, a possible bottleneck for large particle arrays. If necessary, the barcode array could be replaced by a hash table.

(HEP events: procedures)+≡

```

subroutine particle_from_hepmc_particle &
  (prt, hpvt, model, fallback_model, polarization, barcode)
  type(particle_t), intent(out) :: prt
  type(hepmc_particle_t), intent(in) :: hpvt
  type(model_data_t), intent(in), target :: model
  type(model_data_t), intent(in), target :: fallback_model
  type(hepmc_vertex_t) :: vtx
  integer, intent(in) :: polarization
  integer, dimension(:), intent(in) :: barcode
  type(hepmc_polarization_t) :: hpol
  type(flavor_t) :: flv
  type(color_t) :: col
  type(helicity_t) :: hel

```

```

type(polarization_t) :: pol
type(vector4_t) :: vertex
integer :: n_parents, n_children
integer, dimension(:), allocatable :: &
    parent_barcode, child_barcode, parent, child
integer :: i
select case (hepmc_particle_get_status (hprt))
case (1); call prt%set_status (PRT_OUTGOING)
case (2); call prt%set_status (PRT_RESONANT)
case (3); call prt%set_status (PRT_VIRTUAL)
end select
if (hepmc_particle_is_beam (hprt)) call prt%set_status (PRT_BEAM)
call flv%init (hepmc_particle_get_pdg (hprt), model, fallback_model)
call col%init (hepmc_particle_get_color (hprt))
call prt%set_flavor (flv)
call prt%set_color (col)
call prt%set_polarization (polarization)
select case (polarization)
case (PRT_DEFINITE_HELICITY)
    hpol = hepmc_particle_get_polarization (hprt)
    call hepmc_polarization_to_hel (hpol, prt%get_flv (), hel)
    call prt%set_helicity (hel)
    call hepmc_polarization_final (hpol)
case (PRT_GENERIC_POLARIZATION)
    hpol = hepmc_particle_get_polarization (hprt)
    call hepmc_polarization_to_pol (hpol, prt%get_flv (), pol)
    call prt%set_pol (pol)
    call hepmc_polarization_final (hpol)
end select
call prt%set_momentum (hepmc_particle_get_momentum (hprt), &
    hepmc_particle_get_mass_squared (hprt))
n_parents = hepmc_particle_get_n_parents (hprt)
n_children = hepmc_particle_get_n_children (hprt)
if (HEPMC2_AVAILABLE) then
    allocate (parent_barcode (n_parents), parent (n_parents))
    allocate (child_barcode (n_children), child (n_children))
    parent_barcode = hepmc_particle_get_parent_barcodes (hprt)
    child_barcode = hepmc_particle_get_child_barcodes (hprt)
    do i = 1, size (barcode)
        where (parent_barcode == barcode(i)) parent = i
        where (child_barcode == barcode(i)) child = i
    end do
    call prt%set_parents (parent)
    call prt%set_children (child)
else if (HEPMC3_AVAILABLE) then
    allocate (parent_barcode (n_parents), parent (n_parents))
    allocate (child_barcode (n_children), child (n_children))
    parent_barcode = hepmc_particle_get_parent_barcodes (hprt)
    child_barcode = hepmc_particle_get_child_barcodes (hprt)
    do i = 1, size (barcode)
        where (parent_barcode == barcode(i)) parent = i
        where (child_barcode == barcode(i)) child = i
    end do
    call prt%set_parents (parent)

```

```

        call prt%set_children (child)
    end if
    if (prt%get_status () == PRT_VIRTUAL .and. n_parents == 0) &
        call prt%set_status (PRT_INCOMING)
    if (HEPMC2_AVAILABLE) then
        vtx = hePMC_particle_get_decay_vertex (hprt)
        if (hePMC_vertex_is_valid (vtx)) then
            vertex = hePMC_vertex_to_vertex (vtx)
            if (vertex /= vector4_null) call prt%set_vertex (vertex)
        end if
    end if
end if
end subroutine particle_from_hePMC_particle

```

If a particle set is initialized from a HepMC event record, we have to specify the treatment of polarization (unpolarized or density matrix) which is common to all particles. Correlated polarization information is not available.

There is some complication in reconstructing incoming particles and beam remnants. First of all, they all will be tagged as virtual. We then define an incoming particle as

```

<HEP events: public>+≡
    public :: hePMC_event_to_particle_set

<HEP events: procedures>+≡
    subroutine hePMC_event_to_particle_set &
        (particle_set, evt, model, fallback_model, polarization)
    type(particle_set_t), intent(inout), target :: particle_set
    type(hePMC_event_t), intent(in) :: evt
    class(model_data_t), intent(in), target :: model, fallback_model
    integer, intent(in) :: polarization
    type(hePMC_event_particle_iterator_t) :: it
    type(hePMC_vertex_t) :: v
    type(hePMC_vertex_particle_in_iterator_t) :: v_it
    type(hePMC_particle_t) :: prt
    integer, dimension(:), allocatable :: barcode, n_parents
    integer :: n_tot, n_beam, i, bc
    n_tot = hePMC_event_get_n_particles(evt)
    allocate (barcode (n_tot))
    if (HEPMC2_AVAILABLE) then
        call hePMC_event_particle_iterator_init (it, evt)
        do i = 1, n_tot
            barcode(i) = hePMC_particle_get_barcode &
                (hePMC_event_particle_iterator_get (it))
            call hePMC_event_particle_iterator_advance (it)
        end do
        allocate (particle_set%prt (n_tot))
        call hePMC_event_particle_iterator_reset (it)
        do i = 1, n_tot
            prt = hePMC_event_particle_iterator_get (it)
            call particle_from_hePMC_particle (particle_set%prt(i), &
                prt, model, fallback_model, polarization, barcode)
            call hePMC_event_particle_iterator_advance (it)
        end do
        call hePMC_event_particle_iterator_final (it)
        v = hePMC_event_get_signal_process_vertex (evt)
    end if
end subroutine

```

```

    if (hepmc_vertex_is_valid (v)) then
        call hepmc_vertex_particle_in_iterator_init (v_it, v)
        do while (hepmc_vertex_particle_in_iterator_is_valid (v_it))
            prt = hepmc_vertex_particle_in_iterator_get (v_it)
            bc = hepmc_particle_get_barcode &
                (hepmc_vertex_particle_in_iterator_get (v_it))
            do i = 1, size(barcode)
                if (bc == barcode(i)) &
                    call particle_set%prt(i)%set_status (PRT_INCOMING)
            end do
            call hepmc_vertex_particle_in_iterator_advance (v_it)
        end do
        call hepmc_vertex_particle_in_iterator_final (v_it)
    end if
else if (HEPMC3_AVAILABLE) then
    allocate (particle_set%prt (n_tot))
    do i = 1, n_tot
        barcode(i) = hepmc_particle_get_barcode &
            (hepmc_event_get_nth_particle (evt, i))
    end do
    do i = 1, n_tot
        prt = hepmc_event_get_nth_particle (evt, i)
        call particle_from_hepmc_particle (particle_set%prt(i), &
            prt, model, fallback_model, polarization, barcode)
    end do
end if
do i = 1, n_tot
    if (particle_set%prt(i)%get_status () == PRT_VIRTUAL &
        .and. particle_set%prt(i)%get_n_children () == 0) &
        call particle_set%prt(i)%set_status (PRT_OUTGOING)
end do
if (HEPMC3_AVAILABLE) then
    n_beam = hepmc_event_get_n_beams (evt)
    do i = 1, n_beam
        bc = hepmc_event_get_nth_beam (evt, i)
        if (.not. particle_set%prt(bc)%get_status () == PRT_INCOMING) &
            call particle_set%prt(bc)%set_status (PRT_BEAM)
    end do
    do i = 1, n_tot
        if (particle_set%prt(i)%get_status () == PRT_VIRTUAL) then
            n_parents = particle_set%prt(i)%get_parents ()
            if (all &
                (particle_set%prt(n_parents)%get_status () == PRT_BEAM)) then
                call particle_set%prt(i)%set_status (PRT_INCOMING)
            end if
        end if
    end do
end if
particle_set%n_tot = n_tot
particle_set%n_beam = &
    count (particle_set%prt%get_status () == PRT_BEAM)
particle_set%n_in = &
    count (particle_set%prt%get_status () == PRT_INCOMING)
particle_set%n_out = &

```

```

        count (particle_set%prt%get_status () == PRT_OUTGOING)
particle_set%n_vir = &
        particle_set%n_tot - particle_set%n_in - particle_set%n_out
end subroutine hepmc_event_to_particle_set

```

Fill a WHIZARD event from a HepMC event record. In HepMC the weights are in a weight container. If the size of this container is larger than one, it is ambiguous to assign the event a specific weight. For now we only allow to read in unweighted events.

```

<HEP events: public>+=
    public :: hepmc_to_event

<HEP events: procedures>+=
    subroutine hepmc_to_event &
        (event, hepmc_event, fallback_model, process_index, &
         recover_beams, use_alpha_s, use_scale)
    class(generic_event_t), intent(inout), target :: event
    type(hepmc_event_t), intent(inout) :: hepmc_event
    class(model_data_t), intent(in), target :: fallback_model
    integer, intent(out), optional :: process_index
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alpha_s
    logical, intent(in), optional :: use_scale
    class(model_data_t), pointer :: model
    real(default) :: scale, alpha_qcd
    type(particle_set_t) :: particle_set
    model => event%get_model_ptr ()
    call event%set_index (hepmc_event_get_event_index (hepmc_event))
    call hepmc_event_to_particle_set (particle_set, &
        hepmc_event, model, fallback_model, PRT_DEFINITE_HELICITY)
    call event%set_hard_particle_set (particle_set)
    call particle_set%final ()
    call event%set_weight_ref (1._default)
    alpha_qcd = hepmc_event_get_alpha_qcd (hepmc_event)
    scale = hepmc_event_get_scale (hepmc_event)
    if (present (use_alpha_s)) then
        if (use_alpha_s .and. alpha_qcd > 0) &
            call event%set_alpha_qcd_forced (alpha_qcd)
    end if
    if (present (use_scale)) then
        if (use_scale .and. scale > 0) &
            call event%set_scale_forced (scale)
    end if
end subroutine hepmc_to_event

```

LCIO event format

The master output function fills a LCIO event object that is already initialized, but has no particles in it.

In contrast to HepMC in LCIO there are no vertices (except for tracker and other detector specifications). So we assign first all incoming particles and then all outgoing particles to LCIO particle types. Particles which have neither

parent nor children entries (this should not happen) are dropped. Finally, we insert the beam particles. If there are none, use the incoming particles instead.

Transform a particle into a `lcio_particle` object, including color and polarization. The LCIO status is equivalent to the HepMC status, in particular: 0 = null entry, 1 = physical particle, 2 = decayed/fragmented SM hadron, tau or muon, 3 = other unphysical particle entry, 4 = incoming particles, 11 = intermediate resonance such as squarks. The use of 11 for intermediate resonances is as done by HERWIG, see <http://herwig.hepforge.org/trac/wiki/FaQs>.

A beam-remnant particle (e.g., ISR photon) that has no children is tagged as outgoing, otherwise unphysical.

```

<HEP events: public>+=
    public :: particle_to_lcio

<HEP events: procedures>+=
    subroutine particle_to_lcio (prt, lprt)
        type(particle_t), intent(in) :: prt
        type(lcio_particle_t), intent(out) :: lprt
        integer :: lcio_status
        type(vector4_t) :: vtx
        select case (prt%get_status ())
        case (PRT_UNDEFINED)
            lcio_status = 0
        case (PRT_OUTGOING)
            lcio_status = 1
        case (PRT_BEAM_REMNANT)
            if (prt%get_n_children () == 0) then
                lcio_status = 1
            else
                lcio_status = 3
            end if
        case (PRT_BEAM)
            lcio_status = 4
        case (PRT_RESONANT)
            lcio_status = 2
        case default
            lcio_status = 3
        end select
        call lcio_particle_init (lprt, &
            prt%get_momentum (), &
            prt%get_pdg (), &
            prt%flv%get_charge (), &
            lcio_status)
        call lcio_particle_set_color (lprt, prt%get_color ())
        vtx = prt%get_vertex ()
        call lcio_particle_set_vtx (lprt, space_part (vtx))
        call lcio_particle_set_t (lprt, vtx%p(0))
        select case (prt%get_polarization_status ())
        case (PRT_DEFINITE_HELICITY)
            call lcio_polarization_init (lprt, prt%get_helicity ())
        case (PRT_GENERIC_POLARIZATION)
            call lcio_polarization_init (lprt, prt%get_polarization ())
        end select
    end subroutine particle_to_lcio

```

Initialize a particle from a LCIO particle object. The model is necessary for making a fully qualified flavor component.

(HEP events: public)+≡

public :: particle_from_lcio_particle

(HEP events: procedures)+≡

```
subroutine particle_from_lcio_particle &
  (prt, lpert, model, fallback_model, daughters, parents, polarization)
  type(particle_t), intent(out) :: prt
  type(lcio_particle_t), intent(in) :: lpert
  type(model_data_t), intent(in), target :: model
  type(model_data_t), intent(in), target :: fallback_model
  integer, dimension(:), intent(in) :: daughters, parents
  type(vector4_t) :: vtx4
  type(flavor_t) :: flv
  type(color_t) :: col
  type(helicity_t) :: hel
  type(polarization_t) :: pol
  integer, intent(in) :: polarization
  select case (lcio_particle_get_status (lpert))
  case (1); call prt%set_status (PRT_OUTGOING)
  case (2); call prt%set_status (PRT_RESONANT)
  case (3)
    select case (size (parents))
    case (0)
      call prt%set_status (PRT_INCOMING)
    case default
      call prt%set_status (PRT_VIRTUAL)
    end select
  case (4); call prt%set_status (PRT_BEAM)
  end select
  call flv%init (lcio_particle_get_pdg (lpert), model, fallback_model)
  call col%init (lcio_particle_get_flow (lpert))
  if (flv%is_beam_remnant ()) call prt%set_status (PRT_BEAM_REMNANT)
  call prt%set_flavor (flv)
  call prt%set_color (col)
  call prt%set_polarization (polarization)
  select case (polarization)
  case (PRT_DEFINITE_HELICITY)
    call lcio_particle_to_hel (lpert, prt%get_flv (), hel)
    call prt%set_helicity (hel)
  case (PRT_GENERIC_POLARIZATION)
    call lcio_particle_to_pol (lpert, prt%get_flv (), pol)
    call prt%set_pol (pol)
  end select
  call prt%set_momentum (lcio_particle_get_momentum (lpert), &
    lcio_particle_get_mass_squared (lpert))
  call prt%set_parents (parents)
  call prt%set_children (daughters)
  vtx4 = vector4_moving (lcio_particle_get_time (lpert), &
    lcio_particle_get_vertex (lpert))
  if (vtx4 /= vector4_null) call prt%set_vertex (vtx4)
end subroutine particle_from_lcio_particle
```



```

<HEP events: public>+≡
  public :: lcio_event_from_particle_set

<HEP events: procedures>+≡
  subroutine lcio_event_from_particle_set (evt, particle_set)
    type(lcio_event_t), intent(inout) :: evt
    type(particle_set_t), intent(in) :: particle_set
    type(lcio_particle_t), dimension(:), allocatable :: lpvt
    type(particle_set_t), target :: pset_filtered
    integer, dimension(:), allocatable :: parent
    integer :: n_tot, i, j, n_beam, n_parents, type, beam_count

    call particle_set%filter_particles ( pset_filtered, real_parents = .true. , &
      keep_beams = .true. , keep_virtuals = .false.)
    n_tot = pset_filtered%n_tot
    n_beam = count (pset_filtered%prt%get_status () == PRT_BEAM)
    if (n_beam == 0) then
      type = PRT_INCOMING
    else
      type = PRT_BEAM
    end if
    beam_count = 0
    allocate (lpvt (n_tot))
    do i = 1, n_tot
      call particle_to_lcio (pset_filtered%prt(i), lpvt(i))
      n_parents = pset_filtered%prt(i)%get_n_parents ()
      if (n_parents /= 0) then
        allocate (parent (n_parents))
        parent = pset_filtered%prt(i)%get_parents ()
        do j = 1, n_parents
          call lcio_particle_set_parent (lpvt(i), lpvt(parent(j)))
        end do
        deallocate (parent)
      end if
      if (pset_filtered%prt(i)%get_status () == type) then
        beam_count = beam_count + 1
        call lcio_event_set_beam &
          (evt, pset_filtered%prt(i)%get_pdg (), beam_count)
      end if
      call lcio_particle_add_to_evt_coll (lpvt(i), evt)
    end do
    call lcio_event_add_coll (evt)
  end subroutine lcio_event_from_particle_set

```

If a particle set is initialized from a LCIO event record, we have to specify the treatment of polarization (unpolarized or density matrix) which is common to all particles. Correlated polarization information is not available.

```

<HEP events: public>+≡
  public :: lcio_event_to_particle_set

<HEP events: procedures>+≡
  subroutine lcio_event_to_particle_set &
    (particle_set, evt, model, fallback_model, polarization)
    type(particle_set_t), intent(inout), target :: particle_set

```

```

type(lcio_event_t), intent(in) :: evt
class(model_data_t), intent(in), target :: model, fallback_model
integer, intent(in) :: polarization
type(lcio_particle_t) :: prt
integer, dimension(:), allocatable :: parents, daughters
integer :: n_tot, i, j, n_parents, n_children
n_tot = lcio_event_get_n_tot (evt)
allocate (particle_set%prt (n_tot))
do i = 1, n_tot
    prt = lcio_event_get_particle (evt, i-1)
    n_parents = lcio_particle_get_n_parents (prt)
    n_children = lcio_particle_get_n_children (prt)
    allocate (daughters (n_children))
    allocate (parents (n_parents))
    if (n_children > 0) then
        do j = 1, n_children
            daughters(j) = lcio_get_n_children (evt,i,j)
        end do
    end if
    if (n_parents > 0) then
        do j = 1, n_parents
            parents(j) = lcio_get_n_parents (evt,i,j)
        end do
    end if
    call particle_from_lcio_particle (particle_set%prt(i), &
        prt, model, fallback_model, &
        daughters, parents, polarization)
    deallocate (daughters, parents)
end do
do i = 1, n_tot
    if (particle_set%prt(i)%get_status () == PRT_VIRTUAL) then
        CHECK_BEAM: do j = 1, particle_set%prt(i)%get_n_parents ()
            if (particle_set%prt(j)%get_status () == PRT_BEAM) &
                call particle_set%prt(i)%set_status (PRT_INCOMING)
            exit CHECK_BEAM
        end do CHECK_BEAM
    end if
end do
particle_set%n_tot = n_tot
particle_set%n_beam = &
    count (particle_set%prt%get_status () == PRT_BEAM)
particle_set%n_in = &
    count (particle_set%prt%get_status () == PRT_INCOMING)
particle_set%n_out = &
    count (particle_set%prt%get_status () == PRT_OUTGOING)
particle_set%n_vir = &
    particle_set%n_tot - particle_set%n_in - particle_set%n_out
end subroutine lcio_event_to_particle_set

```

<HEP events: public>+≡
 public :: lcio_to_event

<HEP events: procedures>+≡
 subroutine lcio_to_event &

```

        (event, lcio_event, fallback_model, process_index, recover_beams, &
         use_alpha_s, use_scale)
class(generic_event_t), intent(inout), target :: event
type(lcio_event_t), intent(inout) :: lcio_event
class(model_data_t), intent(in), target :: fallback_model
integer, intent(out), optional :: process_index
logical, intent(in), optional :: recover_beams
logical, intent(in), optional :: use_alpha_s
logical, intent(in), optional :: use_scale
class(model_data_t), pointer :: model
real(default) :: scale, alpha_qcd
type(particle_set_t) :: particle_set
model => event%get_model_ptr ()
call lcio_event_to_particle_set (particle_set, &
                                lcio_event, fallback_model, PRT_DEFINITE_HELICITY)
call event%set_hard_particle_set (particle_set)
call particle_set%final ()
call event%set_weight_ref (1._default)
alpha_qcd = lcio_event_get_alphas (lcio_event)
scale = lcio_event_get_scaleval (lcio_event)
if (present (use_alpha_s)) then
    if (use_alpha_s .and. alpha_qcd > 0) &
        call event%set_alpha_qcd_forced (alpha_qcd)
end if
if (present (use_scale)) then
    if (use_scale .and. scale > 0) &
        call event%set_scale_forced (scale)
end if
end subroutine lcio_to_event

```

18.14.2 Unit tests

Test module, followed by the corresponding implementation module.

(*hep_events_ut.f90*)≡
⟨File header⟩

```

module hep_events_ut
  use unit_tests
  use hepmc_interface, only: HEPMC_IS_AVAILABLE
  use system_dependencies, only: HEPMC2_AVAILABLE
  use hep_events_util

```

⟨Standard module head⟩

⟨HEP events: public test⟩

contains

⟨HEP events: test driver⟩

```

end module hep_events_ut

```

```

⟨hep_events_util.f90⟩≡
  ⟨File header⟩

  module hep_events_util

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use lorentz
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use state_matrices, only: FM_SELECT_HELICITY, FM_FACTOR_HELICITY
    use interactions
    use evaluators
    use model_data
    use particles
    use subevents
    use hepmc_interface

    use hep_events

    ⟨Standard module head⟩

    ⟨HEP events: test declarations⟩

    contains

    ⟨HEP events: tests⟩

  end module hep_events_util
API: driver for the unit tests below.
⟨HEP events: public test⟩≡
  public :: hep_events_test
⟨HEP events: test driver⟩≡
  subroutine hep_events_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    ⟨HEP events: execute tests⟩
  end subroutine hep_events_test

```

If HepMC is available, check the routines via HepMC.

Set up a chain of production and decay and factorize the result into particles.
The process is $d\bar{d} \rightarrow Z \rightarrow q\bar{q}$.

```

⟨HEP events: execute tests⟩≡
  if (hepmc_is_available ()) then
    call test (hep_events_1, "hep_events_1", &
      "check HepMC event routines", &
      u, results)
  end if
⟨HEP events: test declarations⟩≡
  public :: hep_events_1

```

```

<HEP events: tests>≡
subroutine hep_events_1 (u)
  use os_interface
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t), dimension(3) :: flv
  type(color_t), dimension(3) :: col
  type(helicity_t), dimension(3) :: hel
  type(quantum_numbers_t), dimension(3) :: qn
  type(vector4_t), dimension(3) :: p
  type(interaction_t), target :: int1, int2
  type(quantum_numbers_mask_t) :: qn_mask_conn
  type(evaluator_t), target :: eval
  type(interaction_t), pointer :: int
  type(particle_set_t) :: particle_set1, particle_set2
  type(hepmc_event_t) :: hepmc_event
  type(hepmc_iostream_t) :: iostream
  real(default) :: cross_section, error, weight
  logical :: ok

  write (u, "(A)")  "* Test output: HEP events"
  write (u, "(A)")  "* Purpose: test HepMC event routines"
  write (u, "(A)")

  write (u, "(A)")  "* Reading model file"

  call model%init_sm_test ()

  write (u, "(A)")
  write (u, "(A)")  "* Initializing production process"

  call int1%basic_init (2, 0, 1, set_relations=.true.)
  call flv%init ([1, -1, 23], model)
  call col%init_col_acl ([0, 0, 0], [0, 0, 0])
  call hel(3)%init ( 1, 1)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0.25_default, 0._default))
  call hel(3)%init ( 1,-1)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0._default, 0.25_default))
  call hel(3)%init (-1, 1)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0._default,-0.25_default))
  call hel(3)%init (-1,-1)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0.25_default, 0._default))
  call hel(3)%init ( 0, 0)
  call qn%init (flv, col, hel)
  call int1%add_state (qn, value=(0.5_default, 0._default))
  call int1%freeze ()
  p(1) = vector4_moving (45._default, 45._default, 3)
  p(2) = vector4_moving (45._default,-45._default, 3)
  p(3) = p(1) + p(2)
  call int1%set_momenta (p)

```

```

write (u, "(A)")
write (u, "(A)")  "* Setup decay process"

call int2%basic_init (1, 0, 2, set_relations=.true.)
call flv%init ([23, 1, -1], model)
call col%init_col_acl ([0, 501, 0], [0, 0, 501])
call hel%init ([1, 1, 1], [1, 1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(1._default, 0._default))
call hel%init ([1, 1, 1], [-1,-1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0._default, 0.1_default))
call hel%init ([-1,-1,-1], [1, 1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0._default,-0.1_default))
call hel%init ([-1,-1,-1], [-1,-1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(1._default, 0._default))
call hel%init ([0, 1,-1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(4._default, 0._default))
call hel%init ([0,-1, 1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(2._default, 0._default))
call hel%init ([0, 1,-1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(2._default, 0._default))
call hel%init ([0,-1, 1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(4._default, 0._default))
call flv%init ([23, 2, -2], model)
call hel%init ([0, 1,-1], [0, 1,-1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0.5_default, 0._default))
call hel%init ([0,-1, 1], [0,-1, 1])
call qn%init (flv, col, hel)
call int2%add_state (qn, value=(0.5_default, 0._default))
call int2%freeze ()
p(2) = vector4_moving (45._default, 45._default, 2)
p(3) = vector4_moving (45._default,-45._default, 2)
call int2%set_momenta (p)
call int2%set_source_link (1, int1, 3)
call int1%basic_write (u)
call int2%basic_write (u)

write (u, "(A)")
write (u, "(A)")  "* Concatenate production and decay"

call eval%init_product (int1, int2, qn_mask_conn, &
    connections_are_resonant=.true.)
call eval%receive_momenta ()
call eval%evaluate ()
call eval%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (complete, polarized)"
write (u, "(A)")

int => eval%interaction_t
call particle_set1%init &
      (ok, int, int, FM_FACTOR_HELICITY, &
       [0.2_default, 0.2_default], .false., .true.)
call particle_set1%write (u)

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (in/out only, selected helicity)"
write (u, "(A)")

int => eval%interaction_t
call particle_set2%init &
      (ok, int, int, FM_SELECT_HELICITY, &
       [0.9_default, 0.9_default], .false., .false.)
call particle_set2%write (u)
call particle_set2%final ()

write (u, "(A)")
write (u, "(A)")  "* Factorize as subevent (complete, selected helicity)"
write (u, "(A)")

int => eval%interaction_t
call particle_set2%init &
      (ok, int, int, FM_SELECT_HELICITY, &
       [0.7_default, 0.7_default], .false., .true.)
call particle_set2%write (u)

write (u, "(A)")
write (u, "(A)")  "* Transfer particle_set to HepMC, print, and output to"
write (u, "(A)")  "          hep_events.hepmc.dat"
write (u, "(A)")

cross_section = 42.0_default
error = 17.0_default
weight = 1.0_default
call hepmc_event_init (hepmc_event, 11, 127)
call hepmc_event_from_particle_set (hepmc_event, particle_set2, &
      cross_section, error)
call hepmc_event_add_weight (hepmc_event, weight, .true.)
call hepmc_event_print (hepmc_event)
call hepmc_iostream_open_out &
      (iostream, var_str ("hep_events.hepmc.dat"), 2)
call hepmc_iostream_write_event (iostream, hepmc_event)
call hepmc_iostream_close (iostream)

write (u, "(A)")
write (u, "(A)")  "* Recover from HepMC file"
write (u, "(A)")

```

```

call particle_set2%final ()
call hepmc_event_final (hepmc_event)
call hepmc_event_init (hepmc_event)
call hepmc_iostream_open_in &
    (iostream , var_str ("hep_events.hepmc.dat"), HEPMC3_MODE_HEPMC3)
call hepmc_iostream_read_event (iostream, hepmc_event, ok=ok)
call hepmc_iostream_close (iostream)
call hepmc_event_to_particle_set (particle_set2, &
    hepmc_event, model, model, PRT_DEFINITE_HELICITY)
call particle_set2%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call particle_set1%final ()
call particle_set2%final ()
call eval%final ()
call int1%final ()
call int2%final ()
call hepmc_event_final (hepmc_event)
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: hep_events_1"

end subroutine hep_events_1

```

18.15 LHEF Input/Output

The LHEF event record is standardized. It is an ASCII format. We try our best at using it for both input and output.

`<eio_lhef.f90>`≡
<File header>

```

module eio_lhef

  <Use kinds>
  <Use strings>
  use io_units
  use string_utils
  use numeric_utils
  use diagnostics
  use os_interface
  use xml
  use event_base
  use event_handles, only: event_handle_t
  use eio_data
  use eio_base
  use hep_common
  use hep_events

```


⟨Standard module head⟩

⟨EIO LHEF: public⟩

⟨EIO LHEF: types⟩

contains

⟨EIO LHEF: procedures⟩

end module eio_lhef

18.15.1 Type

With sufficient confidence that it will always be three characters, we can store the version string with a default value.

⟨EIO LHEF: public⟩≡

public :: eio_lhef_t

⟨EIO LHEF: types⟩≡

```
type, extends (eio_t) :: eio_lhef_t
  logical :: writing = .false.
  logical :: reading = .false.
  integer :: unit = 0
  type(event_sample_data_t) :: data
  type(cstream_t) :: cstream
  character(3) :: version = "1.0"
  logical :: keep_beams = .false.
  logical :: keep_remnants = .true.
  logical :: keep_virtuals = .false.
  logical :: recover_beams = .true.
  logical :: unweighted = .true.
  logical :: write_sqme_ref = .false.
  logical :: write_sqme_prc = .false.
  logical :: write_sqme_alt = .false.
  logical :: use_alphas_from_file = .false.
  logical :: use_scale_from_file = .false.
  integer :: n_alt = 0
  integer, dimension(:), allocatable :: proc_num_id
  integer :: i_weight_sqme = 0
  type(xml_tag_t) :: tag_lhef, tag_head, tag_init, tag_event
  type(xml_tag_t), allocatable :: tag_gen_n, tag_gen_v
  type(xml_tag_t), allocatable :: tag_generator, tag_xsecinfo
  type(xml_tag_t), allocatable :: tag_sqme_ref, tag_sqme_prc
  type(xml_tag_t), dimension(:), allocatable :: tag_sqme_alt, tag_wgts_alt
  type(xml_tag_t), allocatable :: tag_weight, tag_weightinfo, tag_weights
contains
  ⟨EIO LHEF: eio_lhef: TBP⟩
end type eio_lhef_t
```

18.15.2 Specific Methods

Set parameters that are specifically used with LHEF.

```

<EIO LHEF: eio lhef: TBP>≡
  procedure :: set_parameters => eio_lhef_set_parameters

<EIO LHEF: procedures>≡
  subroutine eio_lhef_set_parameters (eio, &
    keep_beams, keep_remnants, recover_beams, &
    use_alphas_from_file, use_scale_from_file, &
    version, extension, write_sqme_ref, write_sqme_prc, write_sqme_alt)
    class(eio_lhef_t), intent(inout) :: eio
    logical, intent(in), optional :: keep_beams
    logical, intent(in), optional :: keep_remnants
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alphas_from_file
    logical, intent(in), optional :: use_scale_from_file
    character(*), intent(in), optional :: version
    type(string_t), intent(in), optional :: extension
    logical, intent(in), optional :: write_sqme_ref
    logical, intent(in), optional :: write_sqme_prc
    logical, intent(in), optional :: write_sqme_alt
    if (present (keep_beams)) eio%keep_beams = keep_beams
    if (present (keep_remnants)) eio%keep_remnants = keep_remnants
    if (present (recover_beams)) eio%recover_beams = recover_beams
    if (present (use_alphas_from_file)) &
      eio%use_alphas_from_file = use_alphas_from_file
    if (present (use_scale_from_file)) &
      eio%use_scale_from_file = use_scale_from_file
    if (present (version)) then
      select case (version)
      case ("1.0", "2.0", "3.0")
        eio%version = version
      case default
        call msg_error ("LHEF version " // version &
          // " is not supported. Inserting 2.0")
        eio%version = "2.0"
      end select
    end if
    if (present (extension)) then
      eio%extension = extension
    else
      eio%extension = "lhe"
    end if
    if (present (write_sqme_ref)) eio%write_sqme_ref = write_sqme_ref
    if (present (write_sqme_prc)) eio%write_sqme_prc = write_sqme_prc
    if (present (write_sqme_alt)) eio%write_sqme_alt = write_sqme_alt
  end subroutine eio_lhef_set_parameters

```

18.15.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO LHEF: eio lhef: TBP>+≡
  procedure :: write => eio_lhef_write

```

```

<EIO LHEF: procedures>+≡
subroutine eio_lhef_write (object, unit)
  class(eio_lhef_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A)") "LHEF event stream:"
  if (object%writing) then
    write (u, "(3x,A,A)") "Writing to file   = ", char (object%filename)
  else if (object%reading) then
    write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
  else
    write (u, "(3x,A)") "[closed]"
  end if
  write (u, "(3x,A,L1)") "Keep beams      = ", object%keep_beams
  write (u, "(3x,A,L1)") "Keep remnants  = ", object%keep_remnants
  write (u, "(3x,A,L1)") "Recover beams   = ", object%recover_beams
  write (u, "(3x,A,L1)") "Alpha_s from file = ", &
    object%use_alphas_from_file
  write (u, "(3x,A,L1)") "Scale from file  = ", &
    object%use_scale_from_file
  write (u, "(3x,A,A)") "Version          = ", object%version
  write (u, "(3x,A,A,A)") "File extension   = '", &
    char (object%extension), "'"
  if (allocated (object%proc_num_id)) then
    write (u, "(3x,A)") "Numerical process IDs:"
    do i = 1, size (object%proc_num_id)
      write (u, "(5x,I0,': ',I0)") i, object%proc_num_id(i)
    end do
  end if
end subroutine eio_lhef_write

```

Finalizer: close any open file.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: final => eio_lhef_final

<EIO LHEF: procedures>+≡
subroutine eio_lhef_final (object)
  class(eio_lhef_t), intent(inout) :: object
  if (allocated (object%proc_num_id)) deallocate (object%proc_num_id)
  if (object%writing) then
    write (msg_buffer, "(A,A,A)") "Events: closing LHEF file '", &
      char (object%filename), "'"
    call msg_message ()
    call object%write_footer ()
    close (object%unit)
    object%writing = .false.
  else if (object%reading) then
    write (msg_buffer, "(A,A,A)") "Events: closing LHEF file '", &
      char (object%filename), "'"
    call msg_message ()
    call object%cstream%final ()
    close (object%unit)
    object%reading = .false.
  end if
end subroutine eio_lhef_final

```

```

        end if
    end subroutine eio_lhef_final

```

Common initialization for input and output.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: common_init => eio_lhef_common_init

<EIO LHEF: procedures>+≡
    subroutine eio_lhef_common_init (eio, sample, data, extension)
        class(eio_lhef_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        if (.not. present (data)) &
            call msg_bug ("LHEF initialization: missing data")
        eio%data = data
        if (data%n_beam /= 2) &
            call msg_fatal ("LHEF: defined for scattering processes only")
        eio%unweighted = data%unweighted
        if (eio%unweighted) then
            select case (data%norm_mode)
            case (NORM_UNIT)
            case default; call msg_fatal &
                ("LHEF: normalization for unweighted events must be '1'")
            end select
        else
            select case (data%norm_mode)
            case (NORM_SIGMA)
            case default; call msg_fatal &
                ("LHEF: normalization for weighted events must be 'sigma'")
            end select
        end if
        eio%n_alt = data%n_alt
        eio%sample = sample
        if (present (extension)) then
            eio%extension = extension
        end if
        call eio%set_filename ()
        eio%unit = free_unit ()
        call eio%init_tags (data)
        allocate (eio%proc_num_id (data%n_proc), source = data%proc_num_id)
    end subroutine eio_lhef_common_init

```

Initialize the tag objects. Some tags depend on the LHEF version. In particular, the tags that in LHEF 2.0 identify individual weights by name in each event block, in LHEF 3.0 are replaced by info tags in the init block and a single **weights** tag in the event block. The name attributes of those tags are specific for WHIZARD.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: init_tags => eio_lhef_init_tags

<EIO LHEF: procedures>+≡
    subroutine eio_lhef_init_tags (eio, data)

```

```

class(eio_lhef_t), intent(inout) :: eio
type(event_sample_data_t), intent(in) :: data
real(default), parameter :: pb_per_fb = 1.e-3_default
integer :: i
call eio%tag_lhef%init ( &
    var_str ("LesHouchesEvents"), &
    [xml_attribute (var_str ("version"), var_str (eio%version))], &
    .true.)
call eio%tag_head%init ( &
    var_str ("header"), &
    .true.)
call eio%tag_init%init ( &
    var_str ("init"), &
    .true.)
call eio%tag_event%init (var_str ("event"), &
    .true.)
select case (eio%version)
case ("1.0")
    allocate (eio%tag_gen_n)
    call eio%tag_gen_n%init ( &
        var_str ("generator_name"), &
        .true.)
    allocate (eio%tag_gen_v)
    call eio%tag_gen_v%init ( &
        var_str ("generator_version"), &
        .true.)
end select
select case (eio%version)
case ("2.0", "3.0")
    allocate (eio%tag_generator)
    call eio%tag_generator%init ( &
        var_str ("generator"), &
        [xml_attribute (var_str ("version"), var_str ("<Version>"))], &
        .true.)
    allocate (eio%tag_xsecinfo)
    call eio%tag_xsecinfo%init ( &
        var_str ("xsecinfo"), &
        [xml_attribute (var_str ("neve"), str (data%n_evt)), &
        xml_attribute (var_str ("totxsec"), &
            str (data%total_cross_section * pb_per_fb))])
end select
select case (eio%version)
case ("2.0")
    allocate (eio%tag_weight)
    call eio%tag_weight%init (var_str ("weight"), &
        [xml_attribute (var_str ("name"))])
    if (eio%write_sqme_ref) then
        allocate (eio%tag_sqme_ref)
        call eio%tag_sqme_ref%init (var_str ("weight"), &
            [xml_attribute (var_str ("name"), var_str ("sqme_ref"))], &
            .true.)
    end if
    if (eio%write_sqme_prc) then
        allocate (eio%tag_sqme_prc)
    end if
end select

```

```

        call eio%tag_sqme_prc%init (var_str ("weight"), &
            [xml_attribute (var_str ("name"), var_str ("sqme_prc"))], &
            .true.)
    end if
    if (eio%n_alt > 0) then
        if (eio%write_sqme_alt) then
            allocate (eio%tag_sqme_alt (1))
            call eio%tag_sqme_alt(1)%init (var_str ("weight"), &
                [xml_attribute (var_str ("name"), var_str ("sqme_alt"))], &
                .true.)
        end if
        allocate (eio%tag_wgts_alt (1))
        call eio%tag_wgts_alt(1)%init (var_str ("weight"), &
            [xml_attribute (var_str ("name"), var_str ("wgts_alt"))], &
            .true.)
    end if
    case ("3.0")
        if (eio%write_sqme_ref) then
            allocate (eio%tag_sqme_ref)
            call eio%tag_sqme_ref%init (var_str ("weightinfo"), &
                [xml_attribute (var_str ("name"), var_str ("sqme_ref"))])
        end if
        if (eio%write_sqme_prc) then
            allocate (eio%tag_sqme_prc)
            call eio%tag_sqme_prc%init (var_str ("weightinfo"), &
                [xml_attribute (var_str ("name"), var_str ("sqme_prc"))])
        end if
        if (eio%n_alt > 0) then
            if (eio%write_sqme_alt) then
                allocate (eio%tag_sqme_alt (eio%n_alt))
                do i = 1, eio%n_alt
                    call eio%tag_sqme_alt(i)%init (var_str ("weightinfo"), &
                        [xml_attribute (var_str ("name"), &
                            var_str ("sqme_alt") // str (i))])
                end do
            end if
            allocate (eio%tag_wgts_alt (eio%n_alt))
            do i = 1, eio%n_alt
                call eio%tag_wgts_alt(i)%init (var_str ("weightinfo"), &
                    [xml_attribute (var_str ("name"), &
                        var_str ("wgts_alt") // str (i))])
            end do
        end if
        allocate (eio%tag_weightinfo)
        call eio%tag_weightinfo%init (var_str ("weightinfo"), &
            [xml_attribute (var_str ("name"))])
        allocate (eio%tag_weights)
        call eio%tag_weights%init (var_str ("weights"), .true.)
    end select
end subroutine eio_lhef_init_tags

```

Initialize event writing.

$\langle EIO\ LHEF: eio\ lhef: TBP \rangle + \equiv$

```

    procedure :: init_out => eio_lhef_init_out
<EIO LHEF: procedures>+≡
    subroutine eio_lhef_init_out (eio, sample, data, success, extension)
        class(eio_lhef_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(in), optional :: data
        logical, intent(out), optional :: success
        integer :: u, i
        call eio%set_splitting (data)
        call eio%common_init (sample, data, extension)
        write (msg_buffer, "(A,A,A)") "Events: writing to LHEF file '", &
            char (eio%filename), "'"
        call msg_message ()
        eio%writing = .true.
        u = eio%unit
        open (u, file = char (eio%filename), &
            action = "write", status = "replace")
        call eio%write_header ()
        call heprup_init &
            (data%pdg_beam, &
            data%energy_beam, &
            n_processes = data%n_proc, &
            unweighted = data%unweighted, &
            negative_weights = data%negative_weights)
        do i = 1, data%n_proc
            call heprup_set_process_parameters (i = i, &
                process_id = data%proc_num_id(i), &
                cross_section = data%cross_section(i), &
                error = data%error(i))
        end do
        call eio%tag_init%write (u); write (u, *)
        call heprup_write_lhef (u)
        select case (eio%version)
        case ("2.0"); call eio%write_init_20 (data)
        case ("3.0"); call eio%write_init_30 (data)
        end select
        call eio%tag_init%close (u); write (u, *)
        if (present (success)) success = .true.
    end subroutine eio_lhef_init_out

```

Initialize event reading. First read the LHEF tag and version, then read the header and skip over its contents, then read the init block. (We require the opening and closing tags of the init block to be placed on separate lines without extra stuff.)

For input, we do not (yet?) support split event files.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: init_in => eio_lhef_init_in
<EIO LHEF: procedures>+≡
    subroutine eio_lhef_init_in (eio, sample, data, success, extension)
        class(eio_lhef_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample

```

```

type(string_t), intent(in), optional :: extension
type(event_sample_data_t), intent(inout), optional :: data
logical, intent(out), optional :: success
logical :: exist, ok, closing
type(event_sample_data_t) :: data_file
type(string_t) :: string
integer :: u
eio%split = .false.
call eio%common_init (sample, data, extension)
write (msg_buffer, "(A,A,A)") "Events: reading from LHEF file '", &
    char (eio%filename), "'"
call msg_message ()
inquire (file = char (eio%filename), exist = exist)
if (.not. exist) call msg_fatal ("Events: LHEF file not found.")
eio%reading = .true.
u = eio%unit
open (u, file = char (eio%filename), &
    action = "read", status = "old")
call eio%cstream%init (u)
call eio%read_header ()
call eio%tag_init%read (eio%cstream, ok)
if (.not. ok) call err_init
select case (eio%version)
case ("1.0"); call eio%read_init_10 (data_file)
    call eio%tag_init%read_content (eio%cstream, string, closing)
    if (string /= "" .or. .not. closing) call err_init
case ("2.0"); call eio%read_init_20 (data_file)
case ("3.0"); call eio%read_init_30 (data_file)
end select
call eio%merge_data (data, data_file)
if (present (success)) success = .true.

contains

subroutine err_init
    call msg_fatal ("LHEF: syntax error in init tag")
end subroutine err_init

end subroutine eio_lhef_init_in

```

Merge event sample data: we can check the data in the file against our assumptions and set or reset parameters.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: merge_data => eio_merge_data

<EIO LHEF: procedures>+≡
subroutine eio_merge_data (eio, data, data_file)
    class(eio_lhef_t), intent(inout) :: eio
    type(event_sample_data_t), intent(inout) :: data
    type(event_sample_data_t), intent(in) :: data_file
    real, parameter :: tolerance = 1000 * epsilon (1._default)
    if (data%unweighted .neqv. data_file%unweighted) call err_weights
    if (data%negative_weights .neqv. data_file%negative_weights) &
        call err_weights

```



```

if (data%norm_mode /= data_file%norm_mode) call err_norm
if (data%n_beam /= data_file%n_beam) call err_beams
if (any (data%pdg_beam /= data_file%pdg_beam)) call err_beams
if (any (abs ((data%energy_beam - data_file%energy_beam)) &
    > (data%energy_beam + data_file%energy_beam) * tolerance)) &
    call err_beams
if (data%n_proc /= data_file%n_proc) call err_proc
if (any (data%proc_num_id /= data_file%proc_num_id)) call err_proc
where (data%cross_section == 0)
    data%cross_section = data_file%cross_section
    data%error = data_file%error
end where
data%total_cross_section = sum (data%cross_section)
if (data_file%n_evt > 0) then
    if (data%n_evt > 0 .and. data_file%n_evt /= data%n_evt) call err_n_evt
    data%n_evt = data_file%n_evt
end if
contains
subroutine err_weights
    call msg_fatal ("LHEF: mismatch in event weight properties")
end subroutine err_weights
subroutine err_norm
    call msg_fatal ("LHEF: mismatch in event normalization")
end subroutine err_norm
subroutine err_beams
    call msg_fatal ("LHEF: mismatch in beam properties")
end subroutine err_beams
subroutine err_proc
    call msg_fatal ("LHEF: mismatch in process definitions")
end subroutine err_proc
subroutine err_n_evt
    call msg_error ("LHEF: mismatch in specified number of events (ignored)")
end subroutine err_n_evt
end subroutine eio_merge_data

```

Switch from input to output: reopen the file for reading.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: switch_inout => eio_lhef_switch_inout

```

```

<EIO LHEF: procedures>+≡
    subroutine eio_lhef_switch_inout (eio, success)
        class(eio_lhef_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("LHEF: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_lhef_switch_inout

```

Split event file: increment the counter, close the current file, open a new one. If the file needs a header, repeat it for the new file. (We assume that the common block contents are still intact.)

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: split_out => eio_lhef_split_out

```

```

<EIO LHEF: procedures>+≡
subroutine eio_lhef_split_out (eio)
  class(eio_lhef_t), intent(inout) :: eio
  integer :: u
  if (eio%split) then
    eio%split_index = eio%split_index + 1
    call eio%set_filename ()
    write (msg_buffer, "(A,A,A)") "Events: writing to LHEF file '", &
      char (eio%filename), "'"
    call msg_message ()
    call eio%write_footer ()
    u = eio%unit
    close (u)
    open (u, file = char (eio%filename), &
      action = "write", status = "replace")
    call eio%write_header ()
    call eio%tag_init%write (u); write (u, *)
    call heprup_write_lhef (u)
    select case (eio%version)
    case ("2.0"); call eio%write_init_20 (eio%data)
    case ("3.0"); call eio%write_init_30 (eio%data)
    end select
    call eio%tag_init%close (u); write (u, *)
  end if
end subroutine eio_lhef_split_out

```

Output an event. Write first the event indices, then weight and squared matrix element, then the particle set.

```

<EIO LHEF: eio_lhef: TBP>+≡
procedure :: output => eio_lhef_output

<EIO LHEF: procedures>+≡
subroutine eio_lhef_output &
  (eio, event, i_prc, reading, passed, pacify, event_handle)
  class(eio_lhef_t), intent(inout) :: eio
  class(generic_event_t), intent(in), target :: event
  integer, intent(in) :: i_prc
  logical, intent(in), optional :: reading, passed, pacify
  class(event_handle_t), intent(inout), optional :: event_handle
  integer :: u
  u = given_output_unit (eio%unit); if (u < 0) return
  if (present (passed)) then
    if (.not. passed) return
  end if
  if (eio%writing) then
    call hepeup_from_event (event, &
      process_index = eio%proc_num_id (i_prc), &
      keep_beams = eio%keep_beams, &
      keep_remnants = eio%keep_remnants)
    write (u, '(A)') "<event>"
    call hepeup_write_lhef (eio%unit)
    select case (eio%version)
    case ("2.0"); call eio%write_event_20 (event)
    case ("3.0"); call eio%write_event_30 (event)
    end select
  end if
end subroutine eio_lhef_output

```

```

        end select
        write (u, '(A)') "</event>"
    else
        call eio%write ()
        call msg_fatal ("LHEF file is not open for writing")
    end if
end subroutine eio_lhef_output

```

Input an event. Upon input of `i_prc`, we can just read in the whole HEPEUP common block. These data are known to come first. The `i_prc` value can be deduced from the IDPRUP value by a table lookup.

Reading the common block bypasses the `cstream` which accesses the input unit. This is consistent with the LHEF specification. After the common-block data have been swallowed, we can resume reading from stream.

We don't catch actual I/O errors. However, we return a negative value in `iostat` if we reached the terminating `</LesHouchesEvents>` tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: input_i_prc => eio_lhef_input_i_prc

<EIO LHEF: procedures>+≡
    subroutine eio_lhef_input_i_prc (eio, i_prc, iostat)
        class(eio_lhef_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        integer :: i, proc_num_id
        type(string_t) :: s
        logical :: ok
        iostat = 0
        call eio%tag_lhef%read_content (eio%cstream, s, ok)
        if (ok) then
            if (s == "") then
                iostat = -1
            else
                call err_close
            end if
            return
        else
            call eio%cstream%revert_record (s)
        end if
        call eio%tag_event%read (eio%cstream, ok)
        if (.not. ok) then
            call err_evt1
            return
        end if
        call hepeup_read_lhef (eio%unit)
        call hepeup_get_event_parameters (proc_id = proc_num_id)
        i_prc = 0
        FIND_I_PRC: do i = 1, size (eio%proc_num_id)
            if (eio%proc_num_id(i) == proc_num_id) then
                i_prc = i
                exit FIND_I_PRC
            end if
        end do FIND_I_PRC
    end subroutine eio_lhef_input_i_prc

```

```

    if (i_prc == 0) call err_index
contains
  subroutine err_close
    call msg_error ("LHEF: reading events: syntax error in closing tag")
    iostat = 1
  end subroutine
  subroutine err_evt1
    call msg_error ("LHEF: reading events: invalid event tag, &
      &aborting read")
    iostat = 2
  end subroutine err_evt1
  subroutine err_index
    call msg_error ("LHEF: reading events: undefined process ID " &
      // char (str (proc_num_id)) // ", aborting read")
    iostat = 3
  end subroutine err_index
end subroutine eio_lhef_input_i_prc

```

Since we have already read the event information from file, this input routine can transfer the common-block contents to the event record. Also, we read any further information in the event record.

Since LHEF doesn't give this information, we must assume that the MCI group, term, and channel can all be safely set to 1. This works if there is only one MCI group and term. The channel doesn't matter for the matrix element.

The event index is incremented, as if the event was generated. The LHEF format does not support event indices.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: input_event => eio_lhef_input_event

<EIO LHEF: procedures>+≡
  subroutine eio_lhef_input_event (eio, event, iostat, event_handle)
    class(eio_lhef_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    type(string_t) :: s
    logical :: closing
    iostat = 0
    call event%reset_contents ()
    call event%select (1, 1, 1)
    call hepeup_to_event (event, eio%fallback_model, &
      recover_beams = eio%recover_beams, &
      use_alpha_s = eio%use_alphas_from_file, &
      use_scale = eio%use_scale_from_file)
    select case (eio%version)
    case ("1.0")
      call eio%tag_event%read_content (eio%cstream, s, closing = closing)
      if (s /= "" .or. .not. closing) call err_evt2
    case ("2.0"); call eio%read_event_20 (event)
    case ("3.0"); call eio%read_event_30 (event)
    end select
    call event%increment_index ()
contains

```

```

subroutine err_evt2
  call msg_error ("LHEF: reading events: syntax error in event record, &
    &aborting read")
  iostat = 2
end subroutine err_evt2

end subroutine eio_lhef_input_event

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: skip => eio_lhef_skip
<EIO LHEF: procedures>+≡
  subroutine eio_lhef_skip (eio, iostat)
    class(eio_lhef_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    if (eio%reading) then
      read (eio%unit, iostat = iostat)
    else
      call eio%write ()
      call msg_fatal ("Raw event file is not open for reading")
    end if
  end subroutine eio_lhef_skip

```

18.15.4 Les Houches Event File: header/footer

These two routines write the header and footer for the Les Houches Event File format (LHEF).

The current version writes no information except for the generator name and version (v.1.0 only).

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: write_header => eio_lhef_write_header
  procedure :: write_footer => eio_lhef_write_footer
<EIO LHEF: procedures>+≡
  subroutine eio_lhef_write_header (eio)
    class(eio_lhef_t), intent(in) :: eio
    integer :: u
    u = given_output_unit (eio%unit); if (u < 0) return
    call eio%tag_lhef%write (u); write (u, *)
    call eio%tag_head%write (u); write (u, *)
    select case (eio%version)
    case ("1.0")
      write (u, "(2x)", advance = "no")
      call eio%tag_gen_n%write (var_str ("WHIZARD"), u)
      write (u, *)
      write (u, "(2x)", advance = "no")
      call eio%tag_gen_v%write (var_str ("Version"), u)
      write (u, *)
    end select
    call eio%tag_head%close (u); write (u, *)
  end subroutine eio_lhef_write_header

```

```

subroutine eio_lhef_write_footer (eio)
  class(eio_lhef_t), intent(in) :: eio
  integer :: u
  u = given_output_unit (eio%unit); if (u < 0) return
  call eio%tag_lhef%close (u)
end subroutine eio_lhef_write_footer

```

Reading the header just means finding the tags and ignoring any contents. When done, we should stand just after the header tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: read_header => eio_lhef_read_header

<EIO LHEF: procedures>+≡
  subroutine eio_lhef_read_header (eio)
    class(eio_lhef_t), intent(inout) :: eio
    logical :: success, closing
    type(string_t) :: content
    call eio%tag_lhef%read (eio%cstream, success)
    if (.not. success .or. .not. eio%tag_lhef%has_content) call err_lhef
    if (eio%tag_lhef%get_attribute (1) /= eio%version) call err_version
    call eio%tag_head%read (eio%cstream, success)
    if (.not. success) call err_header
    if (eio%tag_head%has_content) then
      SKIP_HEADER_CONTENT: do
        call eio%tag_head%read_content (eio%cstream, content, closing)
        if (closing) exit SKIP_HEADER_CONTENT
      end do SKIP_HEADER_CONTENT
    end if
  contains
    subroutine err_lhef
      call msg_fatal ("LHEF: LesHouchesEvents tag absent or corrupted")
    end subroutine err_lhef
    subroutine err_header
      call msg_fatal ("LHEF: header tag absent or corrupted")
    end subroutine err_header
    subroutine err_version
      call msg_error ("LHEF: version mismatch: expected " &
        // eio%version // ", found " &
        // char (eio%tag_lhef%get_attribute (1)))
    end subroutine err_version
  end subroutine eio_lhef_read_header

```

18.15.5 Version-Specific Code: 1.0

In version 1.0, the init tag contains just HEPUP data. While a `cstream` is connected to the input unit, we bypass it temporarily for the purpose of reading the HEPUP contents. This is consistent with the LHEF standard.

This routine does not read the closing tag of the init block.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: read_init_10 => eio_lhef_read_init_10

```

```

<EIO LHEF: procedures>+≡
subroutine eio_lhef_read_init_10 (eio, data)
  class(eio_lhef_t), intent(in) :: eio
  type(event_sample_data_t), intent(out) :: data
  integer :: n_proc, i
  call heprup_read_lhef (eio%unit)
  call heprup_get_run_parameters (n_processes = n_proc)
  call data%init (n_proc)
  data%n_beam = 2
  call heprup_get_run_parameters ( &
    unweighted = data%unweighted, &
    negative_weights = data%negative_weights, &
    beam_pdg = data%pdg_beam, &
    beam_energy = data%energy_beam)
  if (data%unweighted) then
    data%norm_mode = NORM_UNIT
  else
    data%norm_mode = NORM_SIGMA
  end if
  do i = 1, n_proc
    call heprup_get_process_parameters (i, &
      process_id = data%proc_num_id(i), &
      cross_section = data%cross_section(i), &
      error = data%error(i))
  end do
end subroutine eio_lhef_read_init_10

```

18.15.6 Version-Specific Code: 2.0

This is the init information for the 2.0 format, after the HEPRUP data. We have the following tags:

- **generator** Generator name and version.
- **xsecinfo** Cross section and weights data. We have the total cross section and number of events (assuming that the event file is intact), but information on minimum and maximum weights is not available before the file is complete. We just write the mandatory tags. (Note that the default values of the other tags describe a uniform unit weight, but we can determine most values only after the sample is complete.)
- **cutsinfo** This optional tag is too specific to represent the possibilities of WHIZARD, so we skip it.
- **procinfo** This optional tag is useful for giving details of NLO calculations. Skipped.
- **mergetype** Optional, also not applicable.

```

<EIO LHEF: eio_lhef: TBP>+≡
procedure :: write_init_20 => eio_lhef_write_init_20

```

```

<EIO LHEF: procedures>+≡
subroutine eio_lhef_write_init_20 (eio, data)
  class(eio_lhef_t), intent(in) :: eio
  type(event_sample_data_t), intent(in) :: data
  integer :: u
  u = eio%unit
  call eio%tag_generator%write (u)
  write (u, "(A)", advance="no") "WHIZARD"
  call eio%tag_generator%close (u); write (u, *)
  call eio%tag_xsecinfo%write (u); write (u, *)
end subroutine eio_lhef_write_init_20

```

When reading the init block, we first call the 1.0 routine that fills HEPRUP. Then we consider the possible tags. Only the `generator` and `xsecinfo` tags are of interest. We skip everything else except for the closing tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: read_init_20 => eio_lhef_read_init_20

<EIO LHEF: procedures>+≡
subroutine eio_lhef_read_init_20 (eio, data)
  class(eio_lhef_t), intent(inout) :: eio
  type(event_sample_data_t), intent(out) :: data
  real(default), parameter :: pb_per_fb = 1.e-3_default
  type(string_t) :: content
  logical :: found, closing
  call eio_lhef_read_init_10 (eio, data)
  SCAN_INIT_TAGS: do
    call eio%tag_generator%read (eio%cstream, found)
    if (found) then
      if (.not. eio%tag_generator%has_content) call err_generator
      call eio%tag_generator%read_content (eio%cstream, content, closing)
      call msg_message ("LHEF: Event file has been generated by " &
        // char (content) // " " &
        // char (eio%tag_generator%get_attribute (1)))
      cycle SCAN_INIT_TAGS
    end if
    call eio%tag_xsecinfo%read (eio%cstream, found)
    if (found) then
      if (eio%tag_xsecinfo%has_content) call err_xsecinfo
      cycle SCAN_INIT_TAGS
    end if
    call eio%tag_init%read_content (eio%cstream, content, closing)
    if (closing) then
      if (content /= "") call err_init
      exit SCAN_INIT_TAGS
    end if
  end do SCAN_INIT_TAGS
  data%n_evt = &
    read_ival (eio%tag_xsecinfo%get_attribute (1))
  data%total_cross_section = &
    read_rval (eio%tag_xsecinfo%get_attribute (2)) / pb_per_fb
contains
subroutine err_generator
  call msg_fatal ("LHEF: invalid generator tag")

```



```

end subroutine err_generator
subroutine err_xsecinfo
  call msg_fatal ("LHEF: invalid xsecinfo tag")
end subroutine err_xsecinfo
subroutine err_init
  call msg_fatal ("LHEF: syntax error after init tag")
end subroutine err_init
end subroutine eio_lhef_read_init_20

```

This is additional event-specific information for the 2.0 format, after the HEP-EUP data. We can specify weights, starting from the master weight and adding alternative weights. The alternative weights are collected in a common tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: write_event_20 => eio_lhef_write_event_20
<EIO LHEF: procedures>+≡
  subroutine eio_lhef_write_event_20 (eio, event)
    class(eio_lhef_t), intent(in) :: eio
    class(generic_event_t), intent(in) :: event
    type(string_t) :: s
    integer :: i, u
    u = eio%unit
    if (eio%write_sqme_ref) then
      s = str (event%get_sqme_ref ())
      call eio%tag_sqme_ref%write (s, u); write (u, *)
    end if
    if (eio%write_sqme_prc) then
      s = str (event%get_sqme_prc ())
      call eio%tag_sqme_prc%write (s, u); write (u, *)
    end if
    if (eio%n_alt > 0) then
      if (eio%write_sqme_alt) then
        s = str (event%get_sqme_alt(1))
        do i = 2, eio%n_alt
          s = s // " " // str (event%get_sqme_alt(i)); write (u, *)
        end do
        call eio%tag_sqme_alt(1)%write (s, u)
      end if
      s = str (event%get_weight_alt(1))
      do i = 2, eio%n_alt
        s = s // " " // str (event%get_weight_alt(i)); write (u, *)
      end do
      call eio%tag_wgts_alt(1)%write (s, u)
    end if
  end subroutine eio_lhef_write_event_20

```

Read extra event data. If there is a weight entry labeled `sqme_prc`, we take this as the squared matrix-element value (the new *reference* value `sqme_ref`). Other tags, including tags written by the above writer, are skipped.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: read_event_20 => eio_lhef_read_event_20
<EIO LHEF: procedures>+≡

```

```

subroutine eio_lhef_read_event_20 (eio, event)
  class(eio_lhef_t), intent(inout) :: eio
  class(generic_event_t), intent(inout) :: event
  type(string_t) :: content
  logical :: found, closing
  SCAN_EVENT_TAGS: do
    call eio%tag_weight%read (eio%cstream, found)
    if (found) then
      if (.not. eio%tag_weight%has_content) call err_weight
      call eio%tag_weight%read_content (eio%cstream, content, closing)
      if (.not. closing) call err_weight
      if (eio%tag_weight%get_attribute (1) == "sqme_prc") then
        call event%set_sqme_ref (read_rval (content))
      end if
      cycle SCAN_EVENT_TAGS
    end if
    call eio%tag_event%read_content (eio%cstream, content, closing)
    if (closing) then
      if (content /= "") call err_event
      exit SCAN_EVENT_TAGS
    end if
  end do SCAN_EVENT_TAGS
contains
  subroutine err_weight
    call msg_fatal ("LHEF: invalid weight tag in event record")
  end subroutine err_weight
  subroutine err_event
    call msg_fatal ("LHEF: syntax error after event tag")
  end subroutine err_event
end subroutine eio_lhef_read_event_20

```

18.15.7 Version-Specific Code: 3.0

This is the init information for the 3.0 format, after the HEPRUP data. We have the following tags:

- **generator** Generator name and version.
- **xsecinfo** Cross section and weights data. We have the total cross section and number of events (assuming that the event file is intact), but information on minimum and maximum weights is not available before the file is complete. We just write the mandatory tags. (Note that the default values of the other tags describe a uniform unit weight, but we can determine most values only after the sample is complete.)
- **cutsinfo** This optional tag is too specific to represent the possibilities of WHIZARD, so we skip it.
- **procinfo** This optional tag is useful for giving details of NLO calculations. Skipped.
- **weightinfo** Determine the meaning of optional weights, whose values are given in the event record.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: write_init_30 => eio_lhef_write_init_30

<EIO LHEF: procedures>+≡
  subroutine eio_lhef_write_init_30 (eio, data)
    class(eio_lhef_t), intent(in) :: eio
    type(event_sample_data_t), intent(in) :: data
    integer :: u, i
    u = given_output_unit (eio%unit)
    call eio%tag_generator%write (u)
    write (u, "(A)", advance="no") "WHIZARD"
    call eio%tag_generator%close (u); write (u, *)
    call eio%tag_xsecinfo%write (u); write (u, *)
    if (eio%write_sqme_ref) then
      call eio%tag_sqme_ref%write (u); write (u, *)
    end if
    if (eio%write_sqme_prc) then
      call eio%tag_sqme_prc%write (u); write (u, *)
    end if
    if (eio%write_sqme_alt) then
      do i = 1, eio%n_alt
        call eio%tag_sqme_alt(i)%write (u); write (u, *)
      end do
    end if
    do i = 1, eio%n_alt
      call eio%tag_wgts_alt(i)%write (u); write (u, *)
    end do
  end subroutine eio_lhef_write_init_30

```

When reading the init block, we first call the 1.0 routine that fills HEPUP. Then we consider the possible tags. Only the **generator** and **xsecinfo** tags are of interest. We skip everything else except for the closing tag.

```

<EIO LHEF: eio_lhef: TBP>+≡
  procedure :: read_init_30 => eio_lhef_read_init_30

<EIO LHEF: procedures>+≡
  subroutine eio_lhef_read_init_30 (eio, data)
    class(eio_lhef_t), intent(inout) :: eio
    type(event_sample_data_t), intent(out) :: data
    real(default), parameter :: pb_per_fb = 1.e-3_default
    type(string_t) :: content
    logical :: found, closing
    integer :: n_weightinfo
    call eio_lhef_read_init_10 (eio, data)
    n_weightinfo = 0
    eio%i_weight_sqme = 0
    SCAN_INIT_TAGS: do
      call eio%tag_generator%read (eio%cstream, found)
      if (found) then
        if (.not. eio%tag_generator%has_content) call err_generator
        call eio%tag_generator%read_content (eio%cstream, content, closing)
        call msg_message ("LHEF: Event file has been generated by " &
          // char (content) // " " &
          // char (eio%tag_generator%get_attribute (1)))
      end if
    end do
  end subroutine eio_lhef_read_init_30

```

```

        cycle SCAN_INIT_TAGS
    end if
    call eio%tag_xsecinfo%read (eio%cstream, found)
    if (found) then
        if (eio%tag_xsecinfo%has_content) call err_xsecinfo
        cycle SCAN_INIT_TAGS
    end if
    call eio%tag_weightinfo%read (eio%cstream, found)
    if (found) then
        if (eio%tag_weightinfo%has_content) call err_xsecinfo
        n_weightinfo = n_weightinfo + 1
        if (eio%tag_weightinfo%get_attribute (1) == "sqme_prc") then
            eio%i_weight_sqme = n_weightinfo
        end if
        cycle SCAN_INIT_TAGS
    end if
    call eio%tag_init%read_content (eio%cstream, content, closing)
    if (closing) then
        if (content /= "") call err_init
        exit SCAN_INIT_TAGS
    end if
end do SCAN_INIT_TAGS
data%n_evt = &
    read_ival (eio%tag_xsecinfo%get_attribute (1))
data%total_cross_section = &
    read_rval (eio%tag_xsecinfo%get_attribute (2)) / pb_per_fb
contains
    subroutine err_generator
        call msg_fatal ("LHEF: invalid generator tag")
    end subroutine err_generator
    subroutine err_xsecinfo
        call msg_fatal ("LHEF: invalid xsecinfo tag")
    end subroutine err_xsecinfo
    subroutine err_init
        call msg_fatal ("LHEF: syntax error after init tag")
    end subroutine err_init
end subroutine eio_lhef_read_init_30

```

This is additional event-specific information for the 3.0 format, after the HEP-EUP data. We can specify weights, starting from the master weight and adding alternative weights. The weight tags are already allocated, so we just have to transfer the weight values to strings, assemble them and write them to file. All weights are collected in a single tag.

Note: If efficiency turns out to be an issue, we may revert to traditional character buffer writing. However, we need to know the maximum length.

```

<EIO LHEF: eio_lhef: TBP>+≡
    procedure :: write_event_30 => eio_lhef_write_event_30

<EIO LHEF: procedures>+≡
    subroutine eio_lhef_write_event_30 (eio, event)
        class(eio_lhef_t), intent(in) :: eio
        class(generic_event_t), intent(in) :: event
        type(string_t) :: s
    end subroutine

```

```

integer :: u, i
u = eio%unit
s = ""
if (eio%write_sqme_ref) then
  s = s // str (event%get_sqme_ref ()) // " "
end if
if (eio%write_sqme_prc) then
  s = s // str (event%get_sqme_prc ()) // " "
end if
if (eio%n_alt > 0) then
  if (eio%write_sqme_alt) then
    s = s // str (event%get_sqme_alt(1)) // " "
    do i = 2, eio%n_alt
      s = s // str (event%get_sqme_alt(i)) // " "
    end do
  end if
  s = s // str (event%get_weight_alt(1)) // " "
  do i = 2, eio%n_alt
    s = s // str (event%get_weight_alt(i)) // " "
  end do
end if
if (len_trim (s) > 0) then
  call eio%tag_weights%write (trim (s), u); write (u, *)
end if
end subroutine eio_lhef_write_event_30

```

Read extra event data. If there is a `weights` tag and if there was a `weightinfo` entry labeled `sqme_prc`, we extract the corresponding entry from the `weights` string and store this as the event's squared matrix-element value. Other tags, including tags written by the above writer, are skipped.

(EIO LHEF: eio_lhef: TBP)+≡

```

procedure :: read_event_30 => eio_lhef_read_event_30

```

(EIO LHEF: procedures)+≡

```

subroutine eio_lhef_read_event_30 (eio, event)
  class(eio_lhef_t), intent(inout) :: eio
  class(generic_event_t), intent(inout) :: event
  type(string_t) :: content, string
  logical :: found, closing
  integer :: i
  SCAN_EVENT_TAGS: do
    call eio%tag_weights%read (eio%cstream, found)
    if (found) then
      if (.not. eio%tag_weights%has_content) call err_weights
      call eio%tag_weights%read_content (eio%cstream, content, closing)
      if (.not. closing) call err_weights
      if (eio%i_weight_sqme > 0) then
        SCAN_WEIGHTS: do i = 1, eio%i_weight_sqme
          call split (content, string, " ")
          content = adjustl (content)
          if (i == eio%i_weight_sqme) then
            call event%set_sqme_ref (read_rval (string))
            exit SCAN_WEIGHTS
          end if
        end do
      end if
    end if
  end do

```

```

        end do SCAN_WEIGHTS
    end if
    cycle SCAN_EVENT_TAGS
end if
call eio%tag_event%read_content (eio%cstream, content, closing)
if (closing) then
    if (content /= "") call err_event
    exit SCAN_EVENT_TAGS
end if
end do SCAN_EVENT_TAGS
contains
subroutine err_weights
    call msg_fatal ("LHEF: invalid weights tag in event record")
end subroutine err_weights
subroutine err_event
    call msg_fatal ("LHEF: syntax error after event tag")
end subroutine err_event
end subroutine eio_lhef_read_event_30

```

18.15.8 Unit tests

Test module, followed by the corresponding implementation module.

`<eio_lhef.ut.f90>`≡

<File header>

```

module eio_lhef_ut
    use unit_tests
    use eio_lhef_uti

```

<Standard module head>

<EIO LHEF: public test>

contains

<EIO LHEF: test driver>

```

end module eio_lhef_ut

```

`<eio_lhef.uti.f90>`≡

<File header>

```

module eio_lhef_uti

```

<Use kinds>

<Use strings>

```

    use io_units
    use model_data
    use event_base
    use eio_data
    use eio_base

```

```

    use eio_lhef

```

```

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test
    use eio_base_ut, only: eio_prepare_fallback_model, eio_cleanup_fallback_model

    <Standard module head>

    <EIO LHEF: test declarations>

contains

    <EIO LHEF: tests>

end module eio_lhef_ut

API: driver for the unit tests below.
<EIO LHEF: public test>≡
    public :: eio_lhef_test

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

```

Version 1.0 Output

We test the implementation of all I/O methods. We start with output according to version 1.0.

```

<EIO LHEF: execute tests>≡
    call test (eio_lhef_1, "eio_lhef_1", &
        "write version 1.0", &
        u, results)

<EIO LHEF: test declarations>≡
    public :: eio_lhef_1

<EIO LHEF: tests>≡
    subroutine eio_lhef_1 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_lhef_1"
        write (u, "(A)")  "* Purpose: generate an event and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

```

```

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_lhef_1"

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
    call eio%set_parameters ()
end select

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // "." // eio%extension), &
      action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (buffer(1:21) == " <generator_version>") buffer = "[...]"
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_lhef_t :: eio)
select type (eio)

```



```

type is (eio_lhef_t)
  call eio%set_parameters ()
end select

select type (eio)
type is (eio_lhef_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_1"

end subroutine eio_lhef_1

```

Version 2.0 Output

Version 2.0 has added a lot of options to the LHEF format. We implement some of them.

```

<EIO LHEF: execute tests>+≡
  call test (eio_lhef_2, "eio_lhef_2", &
    "write version 2.0", &
    u, results)

<EIO LHEF: test declarations>+≡
  public :: eio_lhef_2

<EIO LHEF: tests>+≡
  subroutine eio_lhef_2 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat
    character(80) :: buffer

    write (u, "(A)")  "* Test output: eio_lhef_2"
    write (u, "(A)")  "* Purpose: generate an event and write weight to file"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    call eio_prepare_test (event, unweighted = .false.)

    call data%init (1)
    data%unweighted = .false.
    data%norm_mode = NORM_SIGMA

```

```

data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_lhef_2"

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
  call eio%set_parameters (version = "2.0", write_sqme_prc = .true.)
end select

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // "." // eio%extension), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:10) == "<generator") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_2"

end subroutine eio_lhef_2

```

Version 3.0 Output

Version 3.0 is an update which removes some tags (which we didn't use anyway) and suggests a new treatment of weights.

```
(EIO LHEF: execute tests)+≡
    call test (eio_lhef_3, "eio_lhef_3", &
        "write version 3.0", &
        u, results)

(EIO LHEF: test declarations)+≡
    public :: eio_lhef_3

(EIO LHEF: tests)+≡
    subroutine eio_lhef_3 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(80) :: buffer

        write (u, "(A)")  "* Test output: eio_lhef_3"
        write (u, "(A)")  "* Purpose: generate an event and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted = .false.)

        call data%init (1)
        data%unweighted = .false.
        data%norm_mode = NORM_SIGMA
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

        sample = "eio_lhef_3"

        allocate (eio_lhef_t :: eio)
        select type (eio)
        type is (eio_lhef_t)
            call eio%set_parameters (version = "3.0", write_sqme_prc = .true.)
        end select

        call eio%init_out (sample, data)
```

```

call event%generate (1, [0._default, 0._default])

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents:"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".lhe"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (buffer(1:10) == "<generator") buffer = "[...]"
  if (iostat /= 0) exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_3"

end subroutine eio_lhef_3

```

Version 1.0 Input

Check input of a version-1.0 conforming LHEF file.

```

<EIO LHEF: execute tests>+≡
  call test (eio_lhef_4, "eio_lhef_4", &
    "read version 1.0", &
    u, results)

<EIO LHEF: test declarations>+≡
  public :: eio_lhef_4

<EIO LHEF: tests>+≡
  subroutine eio_lhef_4 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: fallback_model
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat, i_prc

    write (u, "(A)")  "* Test output: eio_lhef_4"

```

```

write (u, "(A)")  "*" Purpose: read a LHEF 1.0 file"
write (u, "(A)")

write (u, "(A)")  "*" Write a LHEF data file"
write (u, "(A)")

u_file = free_unit ()
sample = "eio_lhef_4"
open (u_file, file = char (sample // ".lhe"), &
      status = "replace", action = "readwrite")

write (u_file, "(A)")  '<LesHouchesEvents version="1.0">'
write (u_file, "(A)")  '<header>'
write (u_file, "(A)")  '  <arbitrary_tag opt="foo">content</arbitrary_tag>'
write (u_file, "(A)")  '  Text'
write (u_file, "(A)")  '  <another_tag />'
write (u_file, "(A)")  '</header>'
write (u_file, "(A)")  '<init>'
write (u_file, "(A)")  '  25 25  5.0000000000E+02  5.0000000000E+02 &
& -1 -1 -1 -1 3 1'
write (u_file, "(A)")  '  1.0000000000E-01  1.0000000000E-03 &
& 1.0000000000E+00 42'
write (u_file, "(A)")  '</init>'
write (u_file, "(A)")  '<event>'
write (u_file, "(A)")  '  4 42  3.0574068604E+08  1.0000000000E+03 &
& -1.0000000000E+00 -1.0000000000E+00'
write (u_file, "(A)")  '  25 -1 0 0 0 0  0.0000000000E+00  0.0000000000E+00 &
& 4.8412291828E+02  5.0000000000E+02  1.2500000000E+02 &
& 0.0000000000E+00  9.0000000000E+00'
write (u_file, "(A)")  '  25 -1 0 0 0 0  0.0000000000E+00  0.0000000000E+00 &
& -4.8412291828E+02  5.0000000000E+02  1.2500000000E+02 &
& 0.0000000000E+00  9.0000000000E+00'
write (u_file, "(A)")  '  25 1 1 2 0 0 -1.4960220911E+02 -4.6042825611E+02 &
& 0.0000000000E+00  5.0000000000E+02  1.2500000000E+02 &
& 0.0000000000E+00  9.0000000000E+00'
write (u_file, "(A)")  '  25 1 1 2 0 0  1.4960220911E+02  4.6042825611E+02 &
& 0.0000000000E+00  5.0000000000E+02  1.2500000000E+02 &
& 0.0000000000E+00  9.0000000000E+00'
write (u_file, "(A)")  '</event>'
write (u_file, "(A)")  '</LesHouchesEvents>'
close (u_file)

write (u, "(A)")  "*" Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
  call eio%set_parameters (recover_beams = .false.)

```

```

end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize and read header"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, *)

select type (eio)
type is (eio_lhef_t)
    call eio%tag_lhef%write (u); write (u, *)
end select

write (u, *)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_lhef_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_4"

end subroutine eio_lhef_4

```

Version 2.0 Input

Check input of a version-2.0 conforming LHEF file.

```

<EIO LHEF: execute tests>+≡
call test (eio_lhef_5, "eio_lhef_5", &
  "read version 2.0", &
  u, results)

<EIO LHEF: test declarations>+≡
public :: eio_lhef_5

<EIO LHEF: tests>+≡
subroutine eio_lhef_5 (u)
  integer, intent(in) :: u
  class(model_data_t), pointer :: fallback_model
  class(generic_event_t), pointer :: event
  type(event_sample_data_t) :: data
  class(eio_t), allocatable :: eio
  type(string_t) :: sample
  integer :: u_file, iostat, i_prc

  write (u, "(A)")  "* Test output: eio_lhef_5"
  write (u, "(A)")  "* Purpose: read a LHEF 2.0 file"
  write (u, "(A)")

  write (u, "(A)")  "* Write a LHEF data file"
  write (u, "(A)")

  u_file = free_unit ()
  sample = "eio_lhef_5"
  open (u_file, file = char (sample // ".lhe"), &
    status = "replace", action = "readwrite")

  write (u_file, "(A)")  '<LesHouchesEvents version="2.0">'
  write (u_file, "(A)")  '<header>'
  write (u_file, "(A)")  '</header>'
  write (u_file, "(A)")  '<init>'
  write (u_file, "(A)")  ' 25 25 5.0000000000E+02 5.0000000000E+02 &
    &-1 -1 -1 -1 4 1'
  write (u_file, "(A)")  ' 1.0000000000E-01 1.0000000000E-03 &
    & 0.0000000000E+00 42'
  write (u_file, "(A)")  '<generator version="2.2.3">WHIZARD&

```

```

        &</generator>'
write (u_file, "(A)") '<xsecinfo neve="1" totxsec="1.0000000000E-01" />'
write (u_file, "(A)") '</init>'
write (u_file, "(A)") '<event>'
write (u_file, "(A)") ' 4 42 3.0574068604E+08 1.0000000000E+03 &
&-1.0000000000E+00 -1.0000000000E+00'
write (u_file, "(A)") ' 25 -1 0 0 0 0 0.0000000000E+00 &
& 0.0000000000E+00 4.8412291828E+02 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") ' 25 -1 0 0 0 0 0.0000000000E+00 &
& 0.0000000000E+00 -4.8412291828E+02 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") ' 25 1 1 2 0 0 -1.4960220911E+02 &
&-4.6042825611E+02 0.0000000000E+00 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") ' 25 1 1 2 0 0 1.4960220911E+02 &
& 4.6042825611E+02 0.0000000000E+00 5.0000000000E+02 &
& 1.2500000000E+02 0.0000000000E+00 9.0000000000E+00'
write (u_file, "(A)") '<weight name="sqme_prc">1.0000000000E+00</weight>'
write (u_file, "(A)") '</event>'
write (u_file, "(A)") '</LesHouchesEvents>'
close (u_file)

write (u, "(A)") "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
    call eio%set_parameters (version = "2.0", recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%unweighted = .false.
data%norm_mode = NORM_SIGMA
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)") "* Initialize and read header"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, *)

```



```

select type (eio)
type is (eio_lhef_t)
    call eio%tag_lhef%write (u); write (u, *)
end select

write (u, *)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_lhef_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_5"

end subroutine eio_lhef_5

```

Version 3.0 Input

Check input of a version-3.0 conforming LHEF file.

```

<EIO LHEF: execute tests>+≡
    call test (eio_lhef_6, "eio_lhef_6", &
        "read version 3.0", &
        u, results)

```

```

<EIO LHEF: test declarations>+≡
    public :: eio_lhef_6

<EIO LHEF: tests>+≡
    subroutine eio_lhef_6 (u)
        integer, intent(in) :: u
        class(model_data_t), pointer :: fallback_model
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat, i_prc

        write (u, "(A)")  "* Test output: eio_lhef_6"
        write (u, "(A)")  "* Purpose: read a LHEF 3.0 file"
        write (u, "(A)")

        write (u, "(A)")  "* Write a LHEF data file"
        write (u, "(A)")

        u_file = free_unit ()
        sample = "eio_lhef_6"
        open (u_file, file = char (sample // ".lhe"), &
            status = "replace", action = "readwrite")

        write (u_file, "(A)")  '<LesHouchesEvents version="3.0">'
        write (u_file, "(A)")  '<header>'
        write (u_file, "(A)")  '</header>'
        write (u_file, "(A)")  '<init>'
        write (u_file, "(A)")  ' 25 25  5.0000000000E+02  5.0000000000E+02 &
            &-1 -1 -1 -1 4 1'
        write (u_file, "(A)")  '  1.0000000000E-01  1.0000000000E-03 &
            & 0.0000000000E+00 42'
        write (u_file, "(A)")  '<generator version="2.2.3">WHIZARD&
            &</generator>'
        write (u_file, "(A)")  '<xsecinfo neve="1" totxsec="1.0000000000E-01" />'
        write (u_file, "(A)")  '<weightinfo name="sqme_prc" />'
        write (u_file, "(A)")  '</init>'
        write (u_file, "(A)")  '<event>'
        write (u_file, "(A)")  ' 4 42  3.0574068604E+08  1.0000000000E+03 &
            &-1.0000000000E+00 -1.0000000000E+00'
        write (u_file, "(A)")  ' 25 -1 0 0 0 0  0.0000000000E+00 &
            & 0.0000000000E+00 4.8412291828E+02  5.0000000000E+02 &
            & 1.2500000000E+02  0.0000000000E+00  9.0000000000E+00'
        write (u_file, "(A)")  ' 25 -1 0 0 0 0  0.0000000000E+00 &
            & 0.0000000000E+00 -4.8412291828E+02  5.0000000000E+02 &
            & 1.2500000000E+02  0.0000000000E+00  9.0000000000E+00'
        write (u_file, "(A)")  ' 25 1 1 2 0 0 -1.4960220911E+02 &
            &-4.6042825611E+02  0.0000000000E+00  5.0000000000E+02 &
            & 1.2500000000E+02  0.0000000000E+00  9.0000000000E+00'
        write (u_file, "(A)")  ' 25 1 1 2 0 0  1.4960220911E+02 &
            & 4.6042825611E+02  0.0000000000E+00  5.0000000000E+02 &
            & 1.2500000000E+02  0.0000000000E+00  9.0000000000E+00'
        write (u_file, "(A)")  '<weights>1.0000000000E+00</weights>'
        write (u_file, "(A)")  '</event>'

```

```

write (u_file, "(A)") '</LesHouchesEvents>'
close (u_file)

write (u, "(A)")  "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_lhef_t :: eio)
select type (eio)
type is (eio_lhef_t)
    call eio%set_parameters (version = "3.0", recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%unweighted = .false.
data%norm_mode = NORM_SIGMA
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize and read header"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, *)

select type (eio)
type is (eio_lhef_t)
    call eio%tag_lhef%write (u); write (u, *)
end select

write (u, *)
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_lhef_t)
    write (u, "(A,I0,A,I0)") "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

```

```

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,IO)")  "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lhef_6"

end subroutine eio_lhef_6

```

18.16 STDHEP File Formats

Here, we implement the two existing STDHEP file formats, one based on the HEPRUP/HEPEUP common blocks, the other based on the HEPEVT common block. The second one is actually the standard STDHEP format.

```

<eio_stdhep.f90>≡
  <File header>

  module eio_stdhep

    use kinds, only: i32, i64
    <Use strings>
    use io_units
    use string_utils
    use diagnostics
    use event_base
    use event_handles, only: event_handle_t
    use hep_common
    use hep_events
    use eio_data
    use eio_base

    <Standard module head>

    <EIO stdhep: public>

```

```

    <EIO stdhep: types>

    <EIO stdhep: variables>

    contains

    <EIO stdhep: procedures>

    end module eio_stdhep

```

18.16.1 Type

```

<EIO stdhep: public>≡
    public :: eio_stdhep_t

<EIO stdhep: types>≡
    type, abstract, extends (eio_t) :: eio_stdhep_t
        logical :: writing = .false.
        logical :: reading = .false.
        integer :: unit = 0
        logical :: keep_beams = .false.
        logical :: keep_remnants = .true.
        logical :: ensure_order = .false.
        logical :: recover_beams = .false.
        logical :: use_alphas_from_file = .false.
        logical :: use_scale_from_file = .false.
        integer, dimension(:), allocatable :: proc_num_id
        integer(i64) :: n_events_expected = 0
    contains
        <EIO stdhep: eio stdhep: TBP>
    end type eio_stdhep_t

<EIO stdhep: public>+≡
    public :: eio_stdhep_hepevt_t

<EIO stdhep: types>+≡
    type, extends (eio_stdhep_t) :: eio_stdhep_hepevt_t
    end type eio_stdhep_hepevt_t

<EIO stdhep: public>+≡
    public :: eio_stdhep_hepeup_t

<EIO stdhep: types>+≡
    type, extends (eio_stdhep_t) :: eio_stdhep_hepeup_t
    end type eio_stdhep_hepeup_t

<EIO stdhep: public>+≡
    public :: eio_stdhep_hepev4_t

<EIO stdhep: types>+≡
    type, extends (eio_stdhep_t) :: eio_stdhep_hepev4_t
    end type eio_stdhep_hepev4_t

```

18.16.2 Specific Methods

Set parameters that are specifically used with STDHEP file formats.

(EIO stdhep: eio stdhep: TBP)≡

```
procedure :: set_parameters => eio_stdhep_set_parameters
```

(EIO stdhep: procedures)≡

```
subroutine eio_stdhep_set_parameters (eio, &
    keep_beams, keep_remnants, ensure_order, recover_beams, &
    use_alphas_from_file, use_scale_from_file, extension)
class(eio_stdhep_t), intent(inout) :: eio
logical, intent(in), optional :: keep_beams
logical, intent(in), optional :: keep_remnants
logical, intent(in), optional :: ensure_order
logical, intent(in), optional :: recover_beams
logical, intent(in), optional :: use_alphas_from_file
logical, intent(in), optional :: use_scale_from_file
type(string_t), intent(in), optional :: extension
if (present (keep_beams)) eio%keep_beams = keep_beams
if (present (keep_remnants)) eio%keep_remnants = keep_remnants
if (present (ensure_order)) eio%ensure_order = ensure_order
if (present (recover_beams)) eio%recover_beams = recover_beams
if (present (use_alphas_from_file)) &
    eio%use_alphas_from_file = use_alphas_from_file
if (present (use_scale_from_file)) &
    eio%use_scale_from_file = use_scale_from_file
if (present (extension)) then
    eio%extension = extension
else
    select type (eio)
    type is (eio_stdhep_hepevt_t)
        eio%extension = "hep"
    type is (eio_stdhep_hepev4_t)
        eio%extension = "ev4.hep"
    type is (eio_stdhep_hepeup_t)
        eio%extension = "up.hep"
    end select
end if
end subroutine eio_stdhep_set_parameters
```

18.16.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

(EIO stdhep: eio stdhep: TBP)+≡

```
procedure :: write => eio_stdhep_write
```

(EIO stdhep: procedures)+≡

```
subroutine eio_stdhep_write (object, unit)
class(eio_stdhep_t), intent(in) :: object
integer, intent(in), optional :: unit
integer :: u, i
u = given_output_unit (unit)
```

```

write (u, "(1x,A)") "STDHEP event stream:"
if (object%writing) then
  write (u, "(3x,A,A)") "Writing to file  = ", char (object%filename)
else if (object%reading) then
  write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
else
  write (u, "(3x,A)") "[closed]"
end if
write (u, "(3x,A,L1)") "Keep beams      = ", object%keep_beams
write (u, "(3x,A,L1)") "Keep remnants  = ", object%keep_remnants
write (u, "(3x,A,L1)") "Recover beams   = ", object%recover_beams
write (u, "(3x,A,L1)") "Alpha_s from file = ", &
  object%use_alphas_from_file
write (u, "(3x,A,L1)") "Scale from file  = ", &
  object%use_scale_from_file
if (allocated (object%proc_num_id)) then
  write (u, "(3x,A)") "Numerical process IDs:"
  do i = 1, size (object%proc_num_id)
    write (u, "(5x,I0,' ':',I0)") i, object%proc_num_id(i)
  end do
end if
end subroutine eio_stdhep_write

```

Finalizer: close any open file.

<EIO stdhep: eio stdhep: TBP>+≡

```
procedure :: final => eio_stdhep_final
```

<EIO stdhep: procedures>+≡

```

subroutine eio_stdhep_final (object)
  class(eio_stdhep_t), intent(inout) :: object
  if (allocated (object%proc_num_id)) deallocate (object%proc_num_id)
  if (object%writing) then
    write (msg_buffer, "(A,A,A)") "Events: closing STDHEP file '", &
      char (object%filename), "'"
    call msg_message ()
    call stdhep_write (200)
    call stdhep_end ()
    object%writing = .false.
  else if (object%reading) then
    write (msg_buffer, "(A,A,A)") "Events: closing STDHEP file '", &
      char (object%filename), "'"
    call msg_message ()
    object%reading = .false.
  end if
end subroutine eio_stdhep_final

```

Common initialization for input and output.

<EIO stdhep: eio stdhep: TBP>+≡

```
procedure :: common_init => eio_stdhep_common_init
```

<EIO stdhep: procedures>+≡

```

subroutine eio_stdhep_common_init (eio, sample, data, extension)
  class(eio_stdhep_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample

```

```

type(string_t), intent(in), optional :: extension
type(event_sample_data_t), intent(in), optional :: data
if (.not. present (data)) &
    call msg_bug ("STDHEP initialization: missing data")
if (data%n_beam /= 2) &
    call msg_fatal ("STDHEP: defined for scattering processes only")
if (present (extension)) then
    eio%extension = extension
end if
eio%sample = sample
call eio%set_filename ()
eio%unit = free_unit ()
allocate (eio%proc_num_id (data%n_proc), source = data%proc_num_id)
end subroutine eio_stdhep_common_init

```

Split event file: increment the counter, close the current file, open a new one. If the file needs a header, repeat it for the new file. (We assume that the common block contents are still intact.)

```

<EIO stdhep: eio stdhep: TBP>+≡
    procedure :: split_out => eio_stdhep_split_out

<EIO stdhep: procedures>+≡
    subroutine eio_stdhep_split_out (eio)
        class(eio_stdhep_t), intent(inout) :: eio
        if (eio%split) then
            eio%split_index = eio%split_index + 1
            call eio%set_filename ()
            write (msg_buffer, "(A,A,A)") "Events: writing to STDHEP file '", &
                char (eio%filename), "'"
            call msg_message ()
            call stdhep_write (200)
            call stdhep_end ()
            select type (eio)
            type is (eio_stdhep_hepeup_t)
                call stdhep_init_out (char (eio%filename), &
                    "WHIZARD <Version>", eio%n_events_expected)
                call stdhep_write (100)
                call stdhep_write (STDHEP_HEPRUP)
            type is (eio_stdhep_hepevt_t)
                call stdhep_init_out (char (eio%filename), &
                    "WHIZARD <Version>", eio%n_events_expected)
                call stdhep_write (100)
            type is (eio_stdhep_hepev4_t)
                call stdhep_init_out (char (eio%filename), &
                    "WHIZARD <Version>", eio%n_events_expected)
                call stdhep_write (100)
            end select
        end if
    end subroutine eio_stdhep_split_out

```

Initialize event writing.

```

<EIO stdhep: eio stdhep: TBP>+≡
    procedure :: init_out => eio_stdhep_init_out

```


<EIO stdhep: procedures>+≡

```

subroutine eio_stdhep_init_out (eio, sample, data, success, extension)
  class(eio_stdhep_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(in), optional :: data
  logical, intent(out), optional :: success
  integer :: i
  if (.not. present (data)) &
    call msg_bug ("STDHEP initialization: missing data")
  call eio%set_splitting (data)
  call eio%common_init (sample, data, extension)
  eio%n_events_expected = data%n_evt
  write (msg_buffer, "(A,A,A)") "Events: writing to STDHEP file '", &
    char (eio%filename), "'"
  call msg_message ()
  eio%writing = .true.
  select type (eio)
  type is (eio_stdhep_hepeup_t)
    call heprup_init &
      (data%pdg_beam, &
       data%energy_beam, &
       n_processes = data%n_proc, &
       unweighted = data%unweighted, &
       negative_weights = data%negative_weights)
    do i = 1, data%n_proc
      call heprup_set_process_parameters (i = i, &
        process_id = data%proc_num_id(i), &
        cross_section = data%cross_section(i), &
        error = data%error(i))
    end do
    call stdhep_init_out (char (eio%filename), &
      "WHIZARD <Version>", eio%n_events_expected)
    call stdhep_write (100)
    call stdhep_write (STDHEP_HEPRUP)
  type is (eio_stdhep_hepevt_t)
    call stdhep_init_out (char (eio%filename), &
      "WHIZARD <Version>", eio%n_events_expected)
    call stdhep_write (100)
  type is (eio_stdhep_hepev4_t)
    call stdhep_init_out (char (eio%filename), &
      "WHIZARD <Version>", eio%n_events_expected)
    call stdhep_write (100)
  end select
  if (present (success)) success = .true.
end subroutine eio_stdhep_init_out

```

Initialize event reading.

<EIO stdhep: eio stdhep: TBP>+≡

```

procedure :: init_in => eio_stdhep_init_in

```

<EIO stdhep: procedures>+≡

```

subroutine eio_stdhep_init_in (eio, sample, data, success, extension)
  class(eio_stdhep_t), intent(inout) :: eio

```

```

type(string_t), intent(in) :: sample
type(string_t), intent(in), optional :: extension
type(event_sample_data_t), intent(inout), optional :: data
logical, intent(out), optional :: success
integer :: ilbl, lok
logical :: exist
call eio%common_init (sample, data, extension)
write (msg_buffer, "(A,A,A)") "Events: reading from STDHEP file '", &
    char (eio%filename), "'"
call msg_message ()
inquire (file = char (eio%filename), exist = exist)
if (.not. exist) call msg_fatal ("Events: STDHEP file not found.")
eio%reading = .true.
call stdhep_init_in (char (eio%filename), eio%n_events_expected)
call stdhep_read (ilbl, lok)
if (lok /= 0) then
    call stdhep_end ()
    write (msg_buffer, "(A)") "Events: STDHEP file appears to" // &
        " be empty."
    call msg_message ()
end if
if (ilbl == 100) then
    write (msg_buffer, "(A)") "Events: reading in STDHEP events"
    call msg_message ()
end if
if (present (success)) success = .false.
end subroutine eio_stdhep_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO stdhep: eio stdhep: TBP>+≡
    procedure :: switch_inout => eio_stdhep_switch_inout

<EIO stdhep: procedures>+≡
    subroutine eio_stdhep_switch_inout (eio, success)
        class(eio_stdhep_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("STDHEP: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_stdhep_switch_inout

```

Output an event. Write first the event indices, then weight and squared matrix element, then the particle set.

```

<EIO stdhep: eio stdhep: TBP>+≡
    procedure :: output => eio_stdhep_output

<EIO stdhep: procedures>+≡
    subroutine eio_stdhep_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_stdhep_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        if (present (passed)) then

```

```

        if (.not. passed) return
    end if
    if (eio%writing) then
        select type (eio)
            type is (eio_stdhep_hepeup_t)
                call hepeup_from_event (event, &
                    process_index = eio%proc_num_id (i_prc), &
                    keep_beams = eio%keep_beams, &
                    keep_remnants = eio%keep_remnants)
                call stdhep_write (STDHEP_HEPEUP)
            type is (eio_stdhep_hepevt_t)
                call hepevt_from_event (event, &
                    keep_beams = eio%keep_beams, &
                    keep_remnants = eio%keep_remnants, &
                    ensure_order = eio%ensure_order)
                call stdhep_write (STDHEP_HEPEVT)
            type is (eio_stdhep_hepev4_t)
                call hepevt_from_event (event, &
                    process_index = eio%proc_num_id (i_prc), &
                    keep_beams = eio%keep_beams, &
                    keep_remnants = eio%keep_remnants, &
                    ensure_order = eio%ensure_order, &
                    fill_hepev4 = .true.)
                call stdhep_write (STDHEP_HEPEV4)
        end select
    else
        call eio%write ()
        call msg_fatal ("STDHEP file is not open for writing")
    end if
end subroutine eio_stdhep_output

```

Input an event. We do not allow to read in STDHEP files written via the HEPEVT common block as there is no control on the process ID. This implies that the event index cannot be read; it is simply incremented to count the current event sample.

(EIO stdhep: eio stdhep: TBP)+≡

```

    procedure :: input_i_prc => eio_stdhep_input_i_prc
    procedure :: input_event => eio_stdhep_input_event

```

(EIO stdhep: procedures)+≡

```

    subroutine eio_stdhep_input_i_prc (eio, i_prc, iostat)
        class(eio_stdhep_t), intent(inout) :: eio
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        integer :: i, ilbl, proc_num_id
        iostat = 0
        select type (eio)
            type is (eio_stdhep_hepevt_t)
                if (size (eio%proc_num_id) > 1) then
                    call msg_fatal ("Events: only single processes allowed " // &
                        "with the STDHEP HEPEVT format.")
                else
                    proc_num_id = eio%proc_num_id (1)
                    call stdhep_read (ilbl, lok)
                end if
            type is (eio_stdhep_hepeup_t)
                call hepeup_read (ilbl, lok)
            type is (eio_stdhep_hepev4_t)
                call hepev4_read (ilbl, lok)
        end select
    end subroutine eio_stdhep_input_i_prc

```

```

        end if
type is (eio_stdhep_hepev4_t)
    call stdhep_read (ilbl, lok)
    proc_num_id = idruplh
type is (eio_stdhep_hepeup_t)
    call stdhep_read (ilbl, lok)
    if (lok /= 0) call msg_error ("Events: STDHEP appears to be " // &
        "empty or corrupted.")
    if (ilbl == 12) then
        call stdhep_read (ilbl, lok)
    end if
    if (ilbl == 11) then
        proc_num_id = IDPRUP
    end if
end select
FIND_I_PRC: do i = 1, size (eio%proc_num_id)
    if (eio%proc_num_id(i) == proc_num_id) then
        i_prc = i
        exit FIND_I_PRC
    end if
end do FIND_I_PRC
if (i_prc == 0) call err_index
contains
subroutine err_index
    call msg_error ("STDHEP: reading events: undefined process ID " &
        // char (str (proc_num_id)) // ", aborting read")
    iostat = 1
end subroutine err_index
end subroutine eio_stdhep_input_i_prc

subroutine eio_stdhep_input_event (eio, event, iostat, event_handle)
    class(eio_stdhep_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    iostat = 0
    call event%reset_contents ()
    call event%select (1, 1, 1)
    call hepeup_to_event (event, eio%fallback_model, &
        recover_beams = eio%recover_beams, &
        use_alpha_s = eio%use_alphas_from_file, &
        use_scale = eio%use_scale_from_file)
    call event%increment_index ()
end subroutine eio_stdhep_input_event

<EIO stdhep: eio stdhep: TBP>+≡
    procedure :: skip => eio_stdhep_skip

<EIO stdhep: procedures>+≡
    subroutine eio_stdhep_skip (eio, iostat)
        class(eio_stdhep_t), intent(inout) :: eio
        integer, intent(out) :: iostat
        if (eio%reading) then
            read (eio%unit, iostat = iostat)

```

```

    else
        call eio%write ()
        call msg_fatal ("Raw event file is not open for reading")
    end if
end subroutine eio_stdhep_skip

```

STDHEP specific routines.

```

<EIO stdhep: public>+≡
public :: stdhep_init_out
public :: stdhep_init_in
public :: stdhep_write
public :: stdhep_end

<EIO stdhep: procedures>+≡
subroutine stdhep_init_out (file, title, nevt)
    character(len=*), intent(in) :: file, title
    integer(i64), intent(in) :: nevt
    integer(i32) :: nevt32
    nevt32 = min (nevt, int (huge (1_i32), i64))
    call stdxwinit (file, title, nevt32, istr, lok)
end subroutine stdhep_init_out

subroutine stdhep_init_in (file, nevt)
    character(len=*), intent(in) :: file
    integer(i64), intent(out) :: nevt
    integer(i32) :: nevt32
    call stdxrinit (file, nevt32, istr, lok)
    if (lok /= 0) call msg_fatal ("STDHEP: error in reading file '" // &
        file // "'.")
    nevt = int (nevt32, i64)
end subroutine stdhep_init_in

subroutine stdhep_write (ilbl)
    integer, intent(in) :: ilbl
    call stdxwrt (ilbl, istr, lok)
end subroutine stdhep_write

subroutine stdhep_read (ilbl, lok)
    integer, intent(out) :: ilbl, lok
    call stdxrd (ilbl, istr, lok)
    if (lok /= 0) return
end subroutine stdhep_read

subroutine stdhep_end
    call stdxend (istr)
end subroutine stdhep_end

```

18.16.4 Variables

```

<EIO stdhep: variables>≡
integer, save :: istr, lok

```

```

integer, parameter :: &
    STDHEP_HEPEVT = 1, STDHEP_HEPEV4 = 4, &
    STDHEP_HEPEUP = 11, STDHEP_HEPRUP = 12

```

18.16.5 Unit tests

Test module, followed by the corresponding implementation module.

```

(eio_stdhep_ut.f90)≡
  <File header>

```

```

module eio_stdhep_ut
  use unit_tests
  use eio_stdhep_util

```

```

  <Standard module head>

```

```

  <EIO stdhep: public test>

```

```

contains

```

```

  <EIO stdhep: test driver>

```

```

end module eio_stdhep_ut

```

```

(eio_stdhep_util.f90)≡
  <File header>

```

```

module eio_stdhep_util

```

```

  <Use kinds>

```

```

  <Use strings>

```

```

    use io_units
    use model_data
    use event_base
    use eio_data
    use eio_base
    use xdr_wo_stdhep

```

```

    use eio_stdhep

```

```

    use eio_base_util, only: eio_prepare_test, eio_cleanup_test

```

```

    use eio_base_util, only: eio_prepare_fallback_model, eio_cleanup_fallback_model

```

```

  <Standard module head>

```

```

  <EIO stdhep: test declarations>

```

```

contains

```

```

  <EIO stdhep: tests>

```

```

end module eio_stdhep_util

```

API: driver for the unit tests below.

```

<EIO stdhep: public test>≡
    public :: eio_stdhep_test

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

```

Test I/O methods

We test the implementation of the STDHEP HEPEVT I/O method:

```

<EIO stdhep: execute tests>≡
    call test (eio_stdhep_1, "eio_stdhep_1", &
        "read and write event contents, format [stdhep]", &
        u, results)

<EIO stdhep: test declarations>≡
    public :: eio_stdhep_1

<EIO stdhep: tests>≡
    subroutine eio_stdhep_1 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(215) :: buffer

        write (u, "(A)")  "* Test output: eio_stdhep_1"
        write (u, "(A)")  "*   Purpose: generate an event in STDHEP HEPEVT format"
        write (u, "(A)")  "*           and write weight to file"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

```

```

sample = "eio_stdhep_1"

allocate (eio_stdhep_hepevt_t :: eio)
select type (eio)
type is (eio_stdhep_hepevt_t)
    call eio%set_parameters ()
end select

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (61) ! not supported by reader, actually
call event%evaluate_expressions ()
call event%pacify_particle_set ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* Write STDHEP file contents to ASCII file"
write (u, "(A)")

call write_stdhep_event &
    (sample // ".hep", var_str ("eio_stdhep_1.hep.out"), 1)

write (u, "(A)")
write (u, "(A)")  "* Read in ASCII contents of STDHEP file"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "eio_stdhep_1.hep.out", &
    action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (iostat /= 0) exit
    if (trim (buffer) == "") cycle
    if (buffer(1:18) == "    total blocks: ") &
        buffer = "    total blocks: [...]"
    if (buffer(1:25) == "    title: WHIZARD") &
        buffer = "    title: WHIZARD [version]"
    if (buffer(1:17) == "    date:") &
        buffer = "    date: [...]"
    if (buffer(1:17) == "    closing date:") &
        buffer = "    closing date: [...]"
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)

```



```

allocate (eio_stdhep_hepevt_t :: eio)

select type (eio)
type is (eio_stdhep_hepevt_t)
  call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_stdhep_1"

end subroutine eio_stdhep_1

```

We test the implementation of the STDHEP HEPEUP I/O method:

```

<EIO stdhep: execute tests>+≡
  call test (eio_stdhep_2, "eio_stdhep_2", &
    "read and write event contents, format [stdhep]", &
    u, results)

<EIO stdhep: test declarations>+≡
  public :: eio_stdhep_2

<EIO stdhep: tests>+≡
  subroutine eio_stdhep_2 (u)
    integer, intent(in) :: u
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(model_data_t), pointer :: fallback_model
    class(eio_t), allocatable :: eio
    type(string_t) :: sample
    integer :: u_file, iostat
    character(215) :: buffer

    write (u, "(A)")  "* Test output: eio_stdhep_2"
    write (u, "(A)")  "*   Purpose: generate an event in STDHEP HEPEUP format"
    write (u, "(A)")  "*           and write weight to file"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize test process"

    allocate (fallback_model)
    call eio_prepare_fallback_model (fallback_model)
    call eio_prepare_test (event, unweighted = .false.)

    call data%init (1)
    data%n_evt = 1
    data%n_beam = 2
    data%pdg_beam = 25
    data%energy_beam = 500
    data%proc_num_id = [42]

```

```

data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_stdhep_2"

allocate (eio_stdhep_hepeup_t :: eio)
select type (eio)
type is (eio_stdhep_hepeup_t)
    call eio%set_parameters ()
end select
call eio%set_fallback_model (fallback_model)

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (62) ! not supported by reader, actually
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* Write STDHEP file contents to ASCII file"
write (u, "(A)")

call write_stdhep_event &
    (sample // ".up.hep", var_str ("eio_stdhep_2.hep.out"), 2)

write (u, "(A)")
write (u, "(A)")  "* Read in ASCII contents of STDHEP file"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "eio_stdhep_2.hep.out", &
    action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (iostat /= 0) exit
    if (trim (buffer) == "") cycle
    if (buffer(1:18) == "    total blocks: ") &
        buffer = "    total blocks: [...]"
    if (buffer(1:25) == "                title: WHIZARD") &
        buffer = "                title: WHIZARD [version]"
    if (buffer(1:17) == "                date:") &
        buffer = "                date: [...]"
    if (buffer(1:17) == "    closing date:") &
        buffer = "    closing date: [...]"
    write (u, "(A)") trim (buffer)
end do

```

```

close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_stdhep_hepeup_t :: eio)

select type (eio)
type is (eio_stdhep_hepeup_t)
    call eio%set_parameters (keep_beams = .true.)
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_stdhep_2"

end subroutine eio_stdhep_2

```

Check input from a StdHep file, HEPEVT block.

```

<EIO stdhep: execute tests>+≡
    call test (eio_stdhep_3, "eio_stdhep_3", &
        "read StdHep file, HEPEVT block", &
        u, results)
<EIO stdhep: test declarations>+≡
    public :: eio_stdhep_3
<EIO stdhep: tests>+≡
    subroutine eio_stdhep_3 (u)
        integer, intent(in) :: u
        class(model_data_t), pointer :: fallback_model
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: iostat, i_prc

        write (u, "(A)")  "* Test output: eio_stdhep_3"
        write (u, "(A)")  "* Purpose: read a StdHep file, HEPEVT block"
        write (u, "(A)")

        write (u, "(A)")  "* Write a StdHep data file, HEPEVT block"
        write (u, "(A)")

        allocate (fallback_model)
        call eio_prepare_fallback_model (fallback_model)

```

```

call eio_prepare_test (event)

call data%init (1)
data%n_evt = 1
data%n_beam = 2
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_stdhep_3"

allocate (eio_stdhep_hepevt_t :: eio)
select type (eio)
type is (eio_stdhep_hepevt_t)
    call eio%set_parameters ()
end select
call eio%set_fallback_model (fallback_model)

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (63) ! not supported by reader, actually
call event%evaluate_expressions ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (eio)
deallocate (fallback_model)

write (u, "(A)")  "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_stdhep_hepevt_t :: eio)
select type (eio)
type is (eio_stdhep_hepevt_t)
    call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)

```

```

data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_stdhep_hepevt_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_stdhep_3"

end subroutine eio_stdhep_3

```

Check input from a StdHep file, HEPEVT block.

```

<EIO stdhep: execute tests>+≡
    call test (eio_stdhep_4, "eio_stdhep_4", &
        "read StdHep file, HEPRUP/HEPEUP block", &
        u, results)

<EIO stdhep: test declarations>+≡
    public :: eio_stdhep_4

<EIO stdhep: tests>+≡
    subroutine eio_stdhep_4 (u)
        integer, intent(in) :: u
        class(model_data_t), pointer :: fallback_model
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: iostat, i_prc

        write (u, "(A)")  "* Test output: eio_stdhep_3"
        write (u, "(A)")  "* Purpose: read a StdHep file, HEPRUP/HEPEUP block"
        write (u, "(A)")

        write (u, "(A)")  "* Write a StdHep data file, HEPRUP/HEPEUP block"
        write (u, "(A)")

        allocate (fallback_model)
        call eio_prepare_fallback_model (fallback_model)
        call eio_prepare_test (event)

        call data%init (1)
        data%n_evt = 1
        data%n_beam = 2
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 100
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event, HEPEUP/HEPRUP"
        write (u, "(A)")

        sample = "eio_stdhep_4"

        allocate (eio_stdhep_hepeup_t :: eio)
        select type (eio)
        type is (eio_stdhep_hepeup_t)
            call eio%set_parameters ()
        end select
        call eio%set_fallback_model (fallback_model)

        call eio%init_out (sample, data)
        call event%generate (1, [0._default, 0._default])
        call event%set_index (64)  ! not supported by reader, actually

```

```

call event%evaluate_expressions ()
call event%pacify_particle_set ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (eio)
deallocate (fallback_model)

write (u, "(A)")  "* Initialize test process"
write (u, "(A)")

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event, unweighted = .false.)

allocate (eio_stdhep_hepeup_t :: eio)
select type (eio)
type is (eio_stdhep_hepeup_t)
    call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_stdhep_hepeup_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

```

```

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,IO)") "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_stdhep_4"

end subroutine eio_stdhep_4

```

18.17 HepMC Output

The HepMC event record is standardized. It is an ASCII format. We try our best at using it for both input and output.

```

<eio_hepmc.f90>≡
  <File header>

  module eio_hepmc

    <Use kinds>
    <Use strings>
    use io_units
    use string_utils
    use diagnostics
    use particles
    use model_data
    use event_base
    use event_handles, only: event_handle_t
    use hep_events
    use eio_data
    use eio_base
    use hepmc_interface

    <Standard module head>

    <EIO HepMC: public>

```


<EIO HepMC: types>

contains

<EIO HepMC: procedures>

end module eio_hepmc

18.17.1 Type

A type `hepmc_event` is introduced as container to store HepMC event data, particularly for splitting the reading into read out of the process index and the proper event data.

Note: the `keep_beams` flag is not supported. Beams will always be written. Tools like `Rivet` can use the cross section information of a HepMC file for scaling plots. As there is no header in HepMC and this is written for every event, we make it optional with `output_cross_section`.

<EIO HepMC: public>≡

public :: eio_hepmc_t

<EIO HepMC: types>≡

```
type, extends (eio_t) :: eio_hepmc_t
  logical :: writing = .false.
  logical :: reading = .false.
  type(event_sample_data_t) :: data
  ! logical :: keep_beams = .false.
  logical :: recover_beams = .false.
  logical :: use_alphas_from_file = .false.
  logical :: use_scale_from_file = .false.
  logical :: output_cross_section = .false.
  integer :: hepmc3_mode = HEPMC3_MODE_HEPMC3
  type(hepmc_iostream_t) :: iostream
  type(hepmc_event_t) :: hepmc_event
  integer, dimension(:), allocatable :: proc_num_id
contains
  <EIO HepMC: eio hepmc: TBP>
end type eio_hepmc_t
```

18.17.2 Specific Methods

Set parameters that are specifically used with HepMC.

<EIO HepMC: eio hepmc: TBP>≡

procedure :: set_parameters => eio_hepmc_set_parameters

<EIO HepMC: procedures>≡

```
subroutine eio_hepmc_set_parameters &
  (eio, &
    recover_beams, use_alphas_from_file, use_scale_from_file, &
    extension, output_cross_section, hepmc3_mode)
class(eio_hepmc_t), intent(inout) :: eio
logical, intent(in), optional :: recover_beams
```

```

logical, intent(in), optional :: use_alphas_from_file
logical, intent(in), optional :: use_scale_from_file
logical, intent(in), optional :: output_cross_section
type(string_t), intent(in), optional :: extension
integer, intent(in), optional :: hepmc3_mode
if (present (recover_beams)) &
    eio%recover_beams = recover_beams
if (present (use_alphas_from_file)) &
    eio%use_alphas_from_file = use_alphas_from_file
if (present (use_scale_from_file)) &
    eio%use_scale_from_file = use_scale_from_file
if (present (extension)) then
    eio%extension = extension
else
    eio%extension = "hepmc"
end if
if (present (output_cross_section)) &
    eio%output_cross_section = output_cross_section
if (present (hepmc3_mode)) &
    eio%hepmc3_mode = hepmc3_mode
end subroutine eio_hepmc_set_parameters

```

18.17.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

(EIO HepMC: eio hepmc: TBP)+≡

```

procedure :: write => eio_hepmc_write

```

(EIO HepMC: procedures)+≡

```

subroutine eio_hepmc_write (object, unit)
    class(eio_hepmc_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A)") "HepMC event stream:"
    if (object%writing) then
        write (u, "(3x,A,A)") "Writing to file   = ", char (object%filename)
    else if (object%reading) then
        write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
    else
        write (u, "(3x,A)") "[closed]"
    end if
    write (u, "(3x,A,L1)") "Recover beams      = ", object%recover_beams
    write (u, "(3x,A,L1)") "Alpha_s from file = ", &
        object%use_alphas_from_file
    write (u, "(3x,A,L1)") "Scale from file   = ", &
        object%use_scale_from_file
    write (u, "(3x,A,A,A)") "File extension    = '", &
        char (object%extension), "'"
    write (u, "(3x,A,I0)") "HepMC3 mode       = ", object%hepmc3_mode
    if (allocated (object%proc_num_id)) then
        write (u, "(3x,A)") "Numerical process IDs:"
    end if
end subroutine eio_hepmc_write

```

```

        do i = 1, size (object%proc_num_id)
            write (u, "(5x,I0,' ': ',I0)") i, object%proc_num_id(i)
        end do
    end if
end subroutine eio_hepmc_write

```

Finalizer: close any open file.

```

(EIO HepMC: eio hepmc: TBP)+≡
    procedure :: final => eio_hepmc_final

(EIO HepMC: procedures)+≡
    subroutine eio_hepmc_final (object)
        class(eio_hepmc_t), intent(inout) :: object
        if (allocated (object%proc_num_id)) deallocate (object%proc_num_id)
        if (object%writing) then
            write (msg_buffer, "(A,A,A)") "Events: closing HepMC file '", &
                char (object%filename), "'"
            call msg_message ()
            call hepmc_iostream_close (object%iostream)
            object%writing = .false.
        else if (object%reading) then
            write (msg_buffer, "(A,A,A)") "Events: closing HepMC file '", &
                char (object%filename), "'"
            call msg_message ()
            call hepmc_iostream_close (object%iostream)
            object%reading = .false.
        end if
    end subroutine eio_hepmc_final

```

Split event file: increment the counter, close the current file, open a new one.
If the file needs a header, repeat it for the new file.

```

(EIO HepMC: eio hepmc: TBP)+≡
    procedure :: split_out => eio_hepmc_split_out

(EIO HepMC: procedures)+≡
    subroutine eio_hepmc_split_out (eio)
        class(eio_hepmc_t), intent(inout) :: eio
        if (eio%split) then
            eio%split_index = eio%split_index + 1
            call eio%set_filename ()
            write (msg_buffer, "(A,A,A)") "Events: writing to HepMC file '", &
                char (eio%filename), "'"
            call msg_message ()
            call hepmc_iostream_close (eio%iostream)
            call hepmc_iostream_open_out (eio%iostream, &
                eio%filename, eio%hepmc3_mode)
        end if
    end subroutine eio_hepmc_split_out

```

Common initialization for input and output.

```

(EIO HepMC: eio hepmc: TBP)+≡
    procedure :: common_init => eio_hepmc_common_init

```

```

<EIO HepMC: procedures>+≡
subroutine eio_hepmc_common_init (eio, sample, data, extension)
  class(eio_hepmc_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(in), optional :: data
  if (.not. present (data)) &
    call msg_bug ("HepMC initialization: missing data")
  eio%data = data
  if (data%n_beam /= 2) &
    call msg_fatal ("HepMC: defined for scattering processes only")
  ! We could relax this condition now with weighted hepmc events
  if (data%unweighted) then
    select case (data%norm_mode)
    case (NORM_UNIT)
    case default; call msg_fatal &
      ("HepMC: normalization for unweighted events must be '1'")
    end select
  end if
  eio%sample = sample
  if (present (extension)) then
    eio%extension = extension
  end if
  call eio%set_filename ()
  allocate (eio%proc_num_id (data%n_proc), source = data%proc_num_id)
end subroutine eio_hepmc_common_init

```

Initialize event writing.

```

<EIO HepMC: eio hepmc: TBP>+≡
  procedure :: init_out => eio_hepmc_init_out

<EIO HepMC: procedures>+≡
subroutine eio_hepmc_init_out (eio, sample, data, success, extension)
  class(eio_hepmc_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(in), optional :: data
  logical, intent(out), optional :: success
  call eio%set_splitting (data)
  call eio%common_init (sample, data, extension)
  write (msg_buffer, "(A,A,A)") "Events: writing to HepMC file '", &
    char (eio%filename), "'"
  call msg_message ()
  eio%writing = .true.
  call hepmc_iostream_open_out (eio%iostream, &
    eio%filename, eio%hepmc3_mode)
  if (present (success)) success = .true.
end subroutine eio_hepmc_init_out

```

Initialize event reading. For input, we do not (yet) support split event files.

```

<EIO HepMC: eio hepmc: TBP>+≡
  procedure :: init_in => eio_hepmc_init_in

```

```

<EIO HepMC: procedures>+≡
subroutine eio_hepmc_init_in (eio, sample, data, success, extension)
  class(eio_hepmc_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(inout), optional :: data
  logical, intent(out), optional :: success
  logical :: exist
  eio%split = .false.
  call eio%common_init (sample, data, extension)
  write (msg_buffer, "(A,A,A)") "Events: reading from HepMC file '", &
    char (eio%filename), "'"
  call msg_message ()
  inquire (file = char (eio%filename), exist = exist)
  if (.not. exist) call msg_fatal ("Events: HepMC file not found.")
  eio%reading = .true.
  call hepmc_iostream_open_in (eio%iostream, &
    eio%filename, eio%hepmc3_mode)
  if (present (success)) success = .true.
end subroutine eio_hepmc_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO HepMC: eio hepmc: TBP>+≡
  procedure :: switch_inout => eio_hepmc_switch_inout

<EIO HepMC: procedures>+≡
subroutine eio_hepmc_switch_inout (eio, success)
  class(eio_hepmc_t), intent(inout) :: eio
  logical, intent(out), optional :: success
  call msg_bug ("HepMC: in-out switch not supported")
  if (present (success)) success = .false.
end subroutine eio_hepmc_switch_inout

```

Output an event to the allocated HepMC output stream. For the moment, we set `alpha_qed` always to -1. There should be methods for the handling of α in `me.methods` in the same way as for α_s .

If an `event_handle` is in the argument list, and it is of the correct HepMC type, do not destroy the event but transfer it there (i.e., the enclosed C pointer).

```

<EIO HepMC: eio hepmc: TBP>+≡
  procedure :: output => eio_hepmc_output

<EIO HepMC: procedures>+≡
subroutine eio_hepmc_output &
  (eio, event, i_prc, reading, passed, pacify, event_handle)
  class(eio_hepmc_t), intent(inout) :: eio
  class(generic_event_t), intent(in), target :: event
  integer, intent(in) :: i_prc
  logical, intent(in), optional :: reading, passed, pacify
  class(event_handle_t), intent(inout), optional :: event_handle
  type(particle_set_t), pointer :: pset_ptr
  if (present (passed)) then
    if (.not. passed) return
  end if

```

```

if (eio%writing) then
  pset_ptr => event%get_particle_set_ptr ()
  call hepmc_event_init (eio%hepmc_event, &
    proc_id = eio%proc_num_id(i_prc), &
    event_id = event%get_index ())
  if (eio%output_cross_section) then
    call hepmc_event_from_particle_set (eio%hepmc_event, pset_ptr, &
      eio%data%cross_section(i_prc), eio%data%error(i_prc))
  else
    call hepmc_event_from_particle_set (eio%hepmc_event, pset_ptr)
  end if
  call hepmc_event_set_scale (eio%hepmc_event, event%get_fac_scale ())
  call hepmc_event_set_alpha_qcd (eio%hepmc_event, event%get_alpha_s ())
  call hepmc_event_set_alpha_qed (eio%hepmc_event, -1._default)
  if (.not. eio%data%unweighted) then
    select case (eio%data%norm_mode)
    case (NORM_UNIT, NORM_N_EVT)
      call hepmc_event_add_weight &
        (eio%hepmc_event, event%weight_prc, .false.)
    case default
      call hepmc_event_add_weight &
        (eio%hepmc_event, event%weight_prc, .true.)
    end select
  end if
  call hepmc_iostream_write_event (eio%iostream, &
    eio%hepmc_event, eio%hepmc3_mode)
  call maybe_transfer_event_to_handle (eio%hepmc_event, event_handle)
  call hepmc_event_final (eio%hepmc_event)
else
  call eio%write ()
  call msg_fatal ("HepMC file is not open for writing")
end if
end subroutine eio_hepmc_output

```

Input an event.

(EIO HepMC: eio hepmc: TBP)+≡

```

procedure :: input_i_prc => eio_hepmc_input_i_prc
procedure :: input_event => eio_hepmc_input_event

```

(EIO HepMC: procedures)+≡

```

subroutine eio_hepmc_input_i_prc (eio, i_prc, iostat)
  class(eio_hepmc_t), intent(inout) :: eio
  integer, intent(out) :: i_prc
  integer, intent(out) :: iostat
  logical :: ok
  integer :: i, proc_num_id
  iostat = 0
  call hepmc_event_init (eio%hepmc_event)
  call hepmc_iostream_read_event (eio%iostream, &
    eio%hepmc_event, ok=ok)
  proc_num_id = hepmc_event_get_process_id (eio%hepmc_event)
  if (.not. ok) then
    iostat = -1
  return

```

```

end if
i_prc = 0
FIND_I_PRC: do i = 1, size (eio%proc_num_id)
  if (eio%proc_num_id(i) == proc_num_id) then
    i_prc = i
    exit FIND_I_PRC
  end if
end do FIND_I_PRC
if (i_prc == 0) call err_index
contains
subroutine err_index
  call msg_error ("HepMC: reading events: undefined process ID " &
    // char (str (proc_num_id)) // ", aborting read")
  iostat = 1
end subroutine err_index
end subroutine eio_hepmc_input_i_prc

subroutine eio_hepmc_input_event (eio, event, iostat, event_handle)
  class(eio_hepmc_t), intent(inout) :: eio
  class(generic_event_t), intent(inout), target :: event
  integer, intent(out) :: iostat
  class(event_handle_t), intent(inout), optional :: event_handle
  iostat = 0
  call event%reset_contents ()
  call event%select (1, 1, 1)
  call hepmc_to_event (event, eio%hepmc_event, &
    eio%fallback_model, &
    recover_beams = eio%recover_beams, &
    use_alpha_s = eio%use_alphas_from_file, &
    use_scale = eio%use_scale_from_file)
  call maybe_transfer_event_to_handle (eio%hepmc_event, event_handle)
  call hepmc_event_final (eio%hepmc_event)
end subroutine eio_hepmc_input_event

```

If an `event_handle` is in the argument list, and it is of the correct HepMC type, do not destroy the event but transfer it to the handle (i.e., the enclosed C pointer). Nullify the original pointer, so the event does not get destroyed.

(EIO HepMC: procedures)+≡

```

subroutine maybe_transfer_event_to_handle (hepmc_event, event_handle)
  type(hepmc_event_t), intent(inout) :: hepmc_event
  class(event_handle_t), intent(inout), optional :: event_handle
  if (present (event_handle)) then
    select type (event_handle)
    type is (hepmc_event_t)
      call hepmc_event_final (event_handle) ! just in case
      event_handle = hepmc_event
      call hepmc_event_nullify (hepmc_event) ! avoid destructor call
    end select
  end if
end subroutine maybe_transfer_event_to_handle

```

(EIO HepMC: eio hepmc: TBP)+≡

```

procedure :: skip => eio_hepmc_skip

```

```

⟨EIO HepMC: procedures⟩+≡
  subroutine eio_hepmc_skip (eio, iostat)
    class(eio_hepmc_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    iostat = 0
  end subroutine eio_hepmc_skip

```

18.17.4 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨eio_hepmc_ut.f90⟩≡
  ⟨File header⟩

  module eio_hepmc_ut
    use unit_tests
    use system_dependencies, only: HEPMC2_AVAILABLE
    use system_dependencies, only: HEPMC3_AVAILABLE
    use eio_hepmc_util

    ⟨Standard module head⟩

    ⟨EIO HepMC: public test⟩

    contains

    ⟨EIO HepMC: test driver⟩

  end module eio_hepmc_ut

⟨eio_hepmc_util.f90⟩≡
  ⟨File header⟩

  module eio_hepmc_util

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use system_dependencies, only: HEPMC2_AVAILABLE
    use system_dependencies, only: HEPMC3_AVAILABLE
    use io_units
    use diagnostics
    use model_data
    use event_base
    use eio_data
    use eio_base

    use eio_hepmc

    use eio_base_ut, only: eio_prepare_test, eio_cleanup_test
    use eio_base_ut, only: eio_prepare_fallback_model, eio_cleanup_fallback_model

    ⟨Standard module head⟩

    ⟨EIO HepMC: test declarations⟩

```


contains

<EIO HepMC: tests>

end module eio_hepmc_util

API: driver for the unit tests below.

<EIO HepMC: public test>≡

public :: eio_hepmc_test

<EIO HepMC: test driver>≡

subroutine eio_hepmc_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<EIO HepMC: execute tests>

end subroutine eio_hepmc_test

Test I/O methods

We test the implementation of all I/O methods.

<EIO HepMC: execute tests>≡

if (HEPMC2_AVAILABLE) then

call test (eio_hepmc_1, "eio_hepmc2_1", &
"write event contents", &
u, results)

else if (HEPMC3_AVAILABLE) then

call test (eio_hepmc_1, "eio_hepmc3_1", &
"write event contents", &
u, results)

end if

<EIO HepMC: test declarations>≡

public :: eio_hepmc_1

<EIO HepMC: tests>≡

subroutine eio_hepmc_1 (u)

integer, intent(in) :: u

class(generic_event_t), pointer :: event

type(event_sample_data_t) :: data

class(eio_t), allocatable :: eio

type(string_t) :: sample

integer :: u_file, iostat

character(116) :: buffer

write (u, "(A)") "* Test output: eio_hepmc_1"

write (u, "(A)") "* Purpose: write a HepMC file"

write (u, "(A)")

write (u, "(A)") "* Initialize test process"

call eio_prepare_test (event, unweighted=.false.)

call data%init (1)

data%n_beam = 2

```

data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_hepmc_1"

allocate (eio_hepmc_t :: eio)
select type (eio)
type is (eio_hepmc_t)
  call eio%set_parameters ()
end select

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (55)

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* File contents (blanking out last two digits):"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".hepmc"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (iostat /= 0) exit
  if (trim (buffer) == "") cycle
  if (buffer(1:14) == "HepMC::Version") cycle
  if (HEPMC2_AVAILABLE) then
    if (buffer(1:10) == "P 10001 25") &
      call buffer_blanker (buffer, 32, 55, 78)
    if (buffer(1:10) == "P 10002 25") &
      call buffer_blanker (buffer, 33, 56, 79)
    if (buffer(1:10) == "P 10003 25") &
      call buffer_blanker (buffer, 29, 53, 78, 101)
    if (buffer(1:10) == "P 10004 25") &
      call buffer_blanker (buffer, 28, 51, 76, 99)
  else if (HEPMC3_AVAILABLE) then
    if (buffer(1:8) == "P 1 0 25") &
      call buffer_blanker (buffer, 26, 49, 72)
    if (buffer(1:8) == "P 2 0 25") &

```

```

        call buffer_blanker (buffer, 26, 49, 73)
    if (buffer(1:9) == "P 3 -1 25") &
        call buffer_blanker (buffer, 28, 52, 75)
    if (buffer(1:9) == "P 4 -1 25") &
        call buffer_blanker (buffer, 27, 50, 73)
    end if
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_hepmc_t :: eio)

select type (eio)
type is (eio_hepmc_t)
    call eio%set_parameters ()
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_hepmc_1"

contains

subroutine buffer_blanker (buf, pos1, pos2, pos3, pos4)
    character(len=*), intent(inout) :: buf
    integer, intent(in) :: pos1, pos2, pos3
    integer, intent(in), optional :: pos4
    type(string_t) :: line
    line = var_str (trim (buf))
    line = replace (line, pos1, "XX")
    line = replace (line, pos2, "XX")
    line = replace (line, pos3, "XX")
    if (present (pos4)) then
        line = replace (line, pos4, "XX")
    end if
    line = replace (line, "4999999999999", "5000000000000")
    buf = char (line)
end subroutine buffer_blanker

end subroutine eio_hepmc_1

```

Test also the reading of HepMC events.

(EIO HepMC: execute tests)+≡

```

if (HEPMC2_AVAILABLE) then
  call test (eio_hePMC_2, "eio_hePMC2_2", &
    "read event contents", &
    u, results)
else if (HEPMC3_AVAILABLE) then
  call test (eio_hePMC_2, "eio_hePMC3_2", &
    "read event contents", &
    u, results)
end if

<EIO HepMC: test declarations>+≡
public :: eio_hePMC_2

<EIO HepMC: tests>+≡
subroutine eio_hePMC_2 (u)
  integer, intent(in) :: u
  class(model_data_t), pointer :: fallback_model
  class(generic_event_t), pointer :: event
  type(event_sample_data_t) :: data
  class(eio_t), allocatable :: eio
  type(string_t) :: sample
  integer :: u_file, iostat, i_prc

  write (u, "(A)")  "* Test output: eio_hePMC_2"
  write (u, "(A)")  "* Purpose: read a HepMC event"
  write (u, "(A)")

  write (u, "(A)")  "* Write a HepMC data file"
  write (u, "(A)")

  u_file = free_unit ()
  sample = "eio_hePMC_2"
  open (u_file, file = char (sample // ".hePMC"), &
    status = "replace", action = "readwrite")

  if (HEPMC2_AVAILABLE) then
    write (u_file, "(A)")  "HepMC::Version 2.06.09"
    write (u_file, "(A)")  "HepMC::IO_GenEvent-START_EVENT_LISTING"
    write (u_file, "(A)")  "E 66 -1 -1.0000000000000000e+00 &
      &-1.0000000000000000e+00 &
      &-1.0000000000000000e+00 42 0 1 10001 10002 0 0"
    write (u_file, "(A)")  "U GEV MM"
    write (u_file, "(A)")  "V -1 0 0 0 0 2 2 0"
    write (u_file, "(A)")  "P 10001 25 0 0 4.8412291827592713e+02 &
      &5.0000000000000000e+02 &
      &1.2499999999999999e+02 3 0 0 -1 0"
    write (u_file, "(A)")  "P 10002 25 0 0 -4.8412291827592713e+02 &
      &5.0000000000000000e+02 &
      &1.2499999999999999e+02 3 0 0 -1 0"
    write (u_file, "(A)")  "P 10003 25 -1.4960220911365536e+02 &
      &-4.6042825611414656e+02 &
      &0 5.0000000000000000e+02 1.2500000000000000e+02 1 0 0 0 0"
    write (u_file, "(A)")  "P 10004 25 1.4960220911365536e+02 &
      &4.6042825611414656e+02 &
      &0 5.0000000000000000e+02 1.2500000000000000e+02 1 0 0 0 0"

```

```

        write (u_file, "(A)") "HepMC::IO_GenEvent-END_EVENT_LISTING"
    else if (HEPMC3_AVAILABLE) then
        write (u_file, "(A)") "HepMC::Version 3.01.01"
        write (u_file, "(A)") "HepMC::Ascii3-START_EVENT_LISTING"
        write (u_file, "(A)") "E 55 1 4"
        write (u_file, "(A)") "U GEV MM"
        write (u_file, "(A)") "A 0 alphaQCD -1"
        write (u_file, "(A)") "A 0 event_scale 1000"
        write (u_file, "(A)") "A 0 signal_process_id 42"
        write (u_file, "(A)") "P 1 0 25 0.0000000000000000e+00 &
            &0.0000000000000000e+00 4.8412291827592713e+02 &
            &5.0000000000000000e+02 1.2499999999999989e+02 3"
        write (u_file, "(A)") "P 2 0 25 0.0000000000000000e+00 &
            &0.0000000000000000e+00 -4.8412291827592713e+02 &
            &5.0000000000000000e+02 1.2499999999999989e+02 3"
        write (u_file, "(A)") "V -1 0 [1,2]"
        write (u_file, "(A)") "P 3 -1 25 -1.4960220911365536e+02 &
            &-4.6042825611414656e+02 0.0000000000000000e+00 &
            &5.0000000000000000e+02 1.2500000000000000e+02 1"
        write (u_file, "(A)") "P 4 -1 25 1.4960220911365536e+02 &
            &4.6042825611414656e+02 0.0000000000000000e+00 &
            &5.0000000000000000e+02 1.2500000000000000e+02 1"
        write (u_file, "(A)") "HepMC::Ascii3-END_EVENT_LISTING"
    else
        call msg_fatal &
            ("Trying to execute eio_hepmc unit tests without a linked HepMC")
    end if
    close (u_file)

    write (u, "(A)") "* Initialize test process"
    write (u, "(A)")

    allocate (fallback_model)
    call eio_prepare_fallback_model (fallback_model)
    call eio_prepare_test (event, unweighted=.false.)

    allocate (eio_hepmc_t :: eio)
    select type (eio)
    type is (eio_hepmc_t)
        call eio%set_parameters (recover_beams = .false.)
    end select
    call eio%set_fallback_model (fallback_model)

    call data%init (1)
    data%n_beam = 2
    data%unweighted = .true.
    data%norm_mode = NORM_UNIT
    data%pdg_beam = 25
    data%energy_beam = 500
    data%proc_num_id = [42]
    call data%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Initialize"

```

```

write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_hepmc_t)
  write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
    " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)

call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_hepmc_2"

end subroutine eio_hepmc_2

```

Test also the correct normalization of weighted HepMC events.

```

(EIO HepMC: execute tests)+≡
  if (HEPMC2_AVAILABLE) then
    call test (eio_hepmc_3, "eio_hepmc2_3", &
      "write event contents", &
      u, results)
  else if (HEPMC3_AVAILABLE) then
    call test (eio_hepmc_3, "eio_hepmc3_3", &
      "event contents weighted, '1' normalization", &
      u, results)
  end if

```

```

<EIO HepMC: test declarations>+≡
    public :: eio_hepmc_3

<EIO HepMC: tests>+≡
    subroutine eio_hepmc_3 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(string_t) :: sample
        integer :: u_file, iostat
        character(126) :: buffer

        write (u, "(A)")  "* Test output: eio_hepmc_3"
        write (u, "(A)")  "* Purpose: test correct HepMC normalization"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize test process"

        call eio_prepare_test (event, unweighted=.false., &
                               sample_norm = var_str ("1"))

        call data%init (1)
        data%n_beam = 2
        data%unweighted = .false.
        data%norm_mode = NORM_UNIT
        data%pdg_beam = 25
        data%energy_beam = 500
        data%proc_num_id = [42]
        data%cross_section(1) = 20
        data%error(1) = 1
        data%total_cross_section = sum (data%cross_section)

        write (u, "(A)")
        write (u, "(A)")  "* Generate and write an event"
        write (u, "(A)")

        sample = "eio_hepmc_3"

        allocate (eio_hepmc_t :: eio)
        select type (eio)
        type is (eio_hepmc_t)
            call eio%set_parameters ()
        end select

        call eio%init_out (sample, data)
        call event%generate (1, [0._default, 0._default])
        call event%set_index (55)

        call eio%output (event, i_prc = 1)
        call eio%write (u)
        call eio%final ()

        write (u, "(A)")
        write (u, "(A)")  "* File contents (blanking out last two digits):"

```

```

write (u, "(A)")

u_file = free_unit ()
open (u_file, file = char (sample // ".hepmc"), &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (iostat /= 0) exit
  if (trim (buffer) == "") cycle
  if (buffer(1:14) == "HepMC::Version") cycle
  if (HEPMC2_AVAILABLE) then
    if (buffer(1:4) == "E 55") then
      buffer = replace (buffer, 113, "XXXXXXXX")
    end if
    if (buffer(1:10) == "P 10001 25") &
      call buffer_blanker (buffer, 32, 55, 78)
    if (buffer(1:10) == "P 10002 25") &
      call buffer_blanker (buffer, 33, 56, 79)
    if (buffer(1:10) == "P 10003 25") &
      call buffer_blanker (buffer, 29, 53, 78, 101)
    if (buffer(1:10) == "P 10004 25") &
      call buffer_blanker (buffer, 28, 51, 76, 99)
  else if (HEPMC3_AVAILABLE) then
    if (buffer(1:4) == "W 3.") then
      buffer = replace (buffer, 11, "XXXXXXXXXXXXXXXXXX")
    end if
    if (buffer(1:8) == "P 1 0 25") &
      call buffer_blanker (buffer, 26, 49, 72, 118)
    if (buffer(1:8) == "P 2 0 25") &
      call buffer_blanker (buffer, 26, 49, 73, 119)
    if (buffer(1:9) == "P 3 -1 25") &
      call buffer_blanker (buffer, 28, 52, 75, 121)
    if (buffer(1:9) == "P 4 -1 25") &
      call buffer_blanker (buffer, 27, 50, 73, 119)
  end if
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_hepmc_t :: eio)

select type (eio)
type is (eio_hepmc_t)
  call eio%set_parameters ()
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```



```

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "** Test output end: eio_hepmc_3"

contains

subroutine buffer_blanker (buf, pos1, pos2, pos3, pos4)
  character(len=*), intent(inout) :: buf
  integer, intent(in) :: pos1, pos2, pos3
  integer, intent(in), optional :: pos4
  type(string_t) :: line
  line = var_str (trim (buf))
  line = replace (line, pos1, "XX")
  line = replace (line, pos2, "XX")
  line = replace (line, pos3, "XX")
  if (present (pos4)) then
    line = replace (line, pos4, "XX")
  end if
  line = replace (line, "4999999999999", "50000000000000")
  buf = char (line)
end subroutine buffer_blanker

end subroutine eio_hepmc_3

```

18.18 LCIO Output

The LCIO event record is standardized for the use with Linear e^+e^- colliders. It is a binary event format. We try our best at using it for both input and output.

```

⟨eio_lcio.f90⟩≡
  ⟨File header⟩

module eio_lcio

  ⟨Use kinds⟩
  ⟨Use strings⟩
  use io_units
  use string_utils
  use diagnostics
  use particles
  use event_base
  use event_handles, only: event_handle_t
  use hep_events
  use eio_data
  use eio_base
  use lcio_interface

  ⟨Standard module head⟩

```

```

    <EIO LCIO: public>

    <EIO LCIO: types>

contains

    <EIO LCIO: procedures>

end module eio_lcio

```

18.18.1 Type

A type `lcio_event` is introduced as container to store LCIO event data, particularly for splitting the reading into read out of the process index and the proper event data.

Note: the `keep_beams` flag is not supported.

```

<EIO LCIO: public>≡
    public :: eio_lcio_t

<EIO LCIO: types>≡
    type, extends (eio_t) :: eio_lcio_t
        logical :: writing = .false.
        logical :: reading = .false.
        type(event_sample_data_t) :: data
        logical :: recover_beams = .false.
        logical :: use_alphas_from_file = .false.
        logical :: use_scale_from_file = .false.
        logical :: proc_as_run_id = .true.
        integer :: n_alt = 0
        integer :: lcio_run_id = 0
        type(lcio_writer_t) :: lcio_writer
        type(lcio_reader_t) :: lcio_reader
        type(lcio_run_header_t) :: lcio_run_hdr
        type(lcio_event_t) :: lcio_event
        integer, dimension(:), allocatable :: proc_num_id
    contains
        <EIO LCIO: eio lcio: TBP>
    end type eio_lcio_t

```

18.18.2 Specific Methods

Set parameters that are specifically used with LCIO.

```

<EIO LCIO: eio lcio: TBP>≡
    procedure :: set_parameters => eio_lcio_set_parameters

<EIO LCIO: procedures>≡
    subroutine eio_lcio_set_parameters &
        (eio, recover_beams, use_alphas_from_file, use_scale_from_file, &
         extension, proc_as_run_id, lcio_run_id)
    class(eio_lcio_t), intent(inout) :: eio
    logical, intent(in), optional :: recover_beams
    logical, intent(in), optional :: use_alphas_from_file

```

```

logical, intent(in), optional :: use_scale_from_file
logical, intent(in), optional :: proc_as_run_id
integer, intent(in), optional :: lcio_run_id
type(string_t), intent(in), optional :: extension
if (present (recover_beams)) eio%recover_beams = recover_beams
if (present (use_alphas_from_file)) &
    eio%use_alphas_from_file = use_alphas_from_file
if (present (use_scale_from_file)) &
    eio%use_scale_from_file = use_scale_from_file
if (present (proc_as_run_id)) &
    eio%proc_as_run_id = proc_as_run_id
if (present (lcio_run_id)) &
    eio%lcio_run_id = lcio_run_id
if (present (extension)) then
    eio%extension = extension
else
    eio%extension = "slcio"
end if
end subroutine eio_lcio_set_parameters

```

18.18.3 Common Methods

Output. This is not the actual event format, but a readable account of the current object status.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: write => eio_lcio_write

<EIO LCIO: procedures>+≡
    subroutine eio_lcio_write (object, unit)
        class(eio_lcio_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1x,A)") "LCIO event stream:"
        if (object%writing) then
            write (u, "(3x,A,A)") "Writing to file   = ", char (object%filename)
        else if (object%reading) then
            write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
        else
            write (u, "(3x,A)") "[closed]"
        end if
        write (u, "(3x,A,L1)") "Recover beams      = ", object%recover_beams
        write (u, "(3x,A,L1)") "Alpha_s from file = ", &
            object%use_alphas_from_file
        write (u, "(3x,A,L1)") "Scale from file   = ", &
            object%use_scale_from_file
        write (u, "(3x,A,L1)") "Process as run ID = ", &
            object%proc_as_run_id
        write (u, "(3x,A,I0)") "LCIO run ID       = ", &
            object%lcio_run_id
        write (u, "(3x,A,A,A)") "File extension    = '", &
            char (object%extension), "'"
        if (allocated (object%proc_num_id)) then

```

```

        write (u, "(3x,A)") "Numerical process IDs:"
        do i = 1, size (object%proc_num_id)
            write (u, "(5x,I0,': ',I0)") i, object%proc_num_id(i)
        end do
    end if
end subroutine eio_lcio_write

```

Finalizer: close any open file.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: final => eio_lcio_final

<EIO LCIO: procedures>+≡
    subroutine eio_lcio_final (object)
        class(eio_lcio_t), intent(inout) :: object
        if (allocated (object%proc_num_id)) deallocate (object%proc_num_id)
        if (object%writing) then
            write (msg_buffer, "(A,A,A)") "Events: closing LCIO file '", &
                char (object%filename), "'"
            call msg_message ()
            call lcio_writer_close (object%lcio_writer)
            object%writing = .false.
        else if (object%reading) then
            write (msg_buffer, "(A,A,A)") "Events: closing LCIO file '", &
                char (object%filename), "'"
            call msg_message ()
            call lcio_reader_close (object%lcio_reader)
            object%reading = .false.
        end if
    end subroutine eio_lcio_final

```

Split event file: increment the counter, close the current file, open a new one.

If the file needs a header, repeat it for the new file.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: split_out => eio_lcio_split_out

<EIO LCIO: procedures>+≡
    subroutine eio_lcio_split_out (eio)
        class(eio_lcio_t), intent(inout) :: eio
        if (eio%split) then
            eio%split_index = eio%split_index + 1
            call eio%set_filename ()
            write (msg_buffer, "(A,A,A)") "Events: writing to LCIO file '", &
                char (eio%filename), "'"
            call msg_message ()
            call lcio_writer_close (eio%lcio_writer)
            call lcio_writer_open_out (eio%lcio_writer, eio%filename)
        end if
    end subroutine eio_lcio_split_out

```

Common initialization for input and output.

```

<EIO LCIO: eio lcio: TBP>+≡
    procedure :: common_init => eio_lcio_common_init

```

```

<EIO LCIO: procedures>+=
subroutine eio_lcio_common_init (eio, sample, data, extension)
  class(eio_lcio_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(in), optional :: data
  if (.not. present (data)) &
    call msg_bug ("LCIO initialization: missing data")
  eio%data = data
  if (data%n_beam /= 2) &
    call msg_fatal ("LCIO: defined for scattering processes only")
  if (data%unweighted) then
    select case (data%norm_mode)
    case (NORM_UNIT)
    case default; call msg_fatal &
      ("LCIO: normalization for unweighted events must be '1'")
    end select
  else
    call msg_fatal ("LCIO: events must be unweighted")
  end if
  eio%n_alt = data%n_alt
  eio%sample = sample
  if (present (extension)) then
    eio%extension = extension
  end if
  call eio%set_filename ()
  allocate (eio%proc_num_id (data%n_proc), source = data%proc_num_id)
end subroutine eio_lcio_common_init

```

Initialize event writing.

```

<EIO LCIO: eio lcio: TBP>+=
procedure :: init_out => eio_lcio_init_out
<EIO LCIO: procedures>+=
subroutine eio_lcio_init_out (eio, sample, data, success, extension)
  class(eio_lcio_t), intent(inout) :: eio
  type(string_t), intent(in) :: sample
  type(string_t), intent(in), optional :: extension
  type(event_sample_data_t), intent(in), optional :: data
  logical, intent(out), optional :: success
  call eio%set_splitting (data)
  call eio%common_init (sample, data, extension)
  write (msg_buffer, "(A,A,A)") "Events: writing to LCIO file '", &
    char (eio%filename), ""
  call msg_message ()
  eio%writing = .true.
  call lcio_writer_open_out (eio%lcio_writer, eio%filename)
  call lcio_run_header_init (eio%lcio_run_hdr)
  call lcio_run_header_write (eio%lcio_writer, eio%lcio_run_hdr)
  if (present (success)) success = .true.
end subroutine eio_lcio_init_out

```

Initialize event reading. For input, we do not (yet) support split event files.

```

<EIO LCIO: eio lcio: TBP>+=

```

```

    procedure :: init_in => eio_lcio_init_in
<EIO LCIO: procedures>+=
    subroutine eio_lcio_init_in (eio, sample, data, success, extension)
        class(eio_lcio_t), intent(inout) :: eio
        type(string_t), intent(in) :: sample
        type(string_t), intent(in), optional :: extension
        type(event_sample_data_t), intent(inout), optional :: data
        logical, intent(out), optional :: success
        logical :: exist
        eio%split = .false.
        call eio%common_init (sample, data, extension)
        write (msg_buffer, "(A,A,A)") "Events: reading from LCIO file '", &
            char (eio%filename), "'"
        call msg_message ()
        inquire (file = char (eio%filename), exist = exist)
        if (.not. exist) call msg_fatal ("Events: LCIO file not found.")
        eio%reading = .true.
        call lcio_open_file (eio%lcio_reader, eio%filename)
        if (present (success)) success = .true.
    end subroutine eio_lcio_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO LCIO: eio lcio: TBP>+=
    procedure :: switch_inout => eio_lcio_switch_inout
<EIO LCIO: procedures>+=
    subroutine eio_lcio_switch_inout (eio, success)
        class(eio_lcio_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        call msg_bug ("LCIO: in-out switch not supported")
        if (present (success)) success = .false.
    end subroutine eio_lcio_switch_inout

```

Output an event to the allocated LCIO writer.

[WK 21-03-10]: Disable all output of sqme and alt-weight event parameters. Due to the fact that LCIO can only store single-precision values, we not just lose precision, but also can run into overflows (events with ISR).

```

<EIO LCIO: eio lcio: TBP>+=
    procedure :: output => eio_lcio_output
<EIO LCIO: procedures>+=
    subroutine eio_lcio_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_lcio_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        integer, intent(in) :: i_prc
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        type(particle_set_t), pointer :: pset_ptr
        real(default) :: sqme_prc, weight
        integer :: i
        if (present (passed)) then
            if (.not. passed) return

```

```

end if
if (eio%writing) then
  pset_ptr => event%get_particle_set_ptr ()
  if (eio%proc_as_run_id) then
    call lcio_event_init (eio%lcio_event, &
      proc_id = eio%proc_num_id (i_prc), &
      event_id = event%get_index (), &
      run_id = eio%proc_num_id (i_prc))
  else
    call lcio_event_init (eio%lcio_event, &
      proc_id = eio%proc_num_id (i_prc), &
      event_id = event%get_index (), &
      run_id = eio%lcio_run_id)
  end if
  call lcio_event_from_particle_set (eio%lcio_event, pset_ptr)
  call lcio_event_set_weight (eio%lcio_event, event%weight_prc)
  call lcio_event_set_sqrts (eio%lcio_event, event%get_sqrts ())
  call lcio_event_set_sqme (eio%lcio_event, event%get_sqme_prc ())
  call lcio_event_set_scale (eio%lcio_event, event%get_fac_scale ())
  call lcio_event_set_alpha_qcd (eio%lcio_event, event%get_alpha_s ())
  call lcio_event_set_xsec (eio%lcio_event, eio%data%cross_section(i_prc), &
    eio%data%error(i_prc))
  call lcio_event_set_polarization (eio%lcio_event, &
    event%get_polarization ())
  call lcio_event_set_beam_file (eio%lcio_event, &
    event%get_beam_file ())
  call lcio_event_set_process_name (eio%lcio_event, &
    event%get_process_name ())
  do i = 1, eio%n_alt
    sqme_prc = event%get_sqme_alt(i)
    weight = event%get_weight_alt(i)
    call lcio_event_set_alt_sqme (eio%lcio_event, sqme_prc, i)
    call lcio_event_set_alt_weight (eio%lcio_event, weight, i)
  end do
  call lcio_event_write (eio%lcio_writer, eio%lcio_event)
  call maybe_transfer_event_to_handle (eio%lcio_event, &
    event_handle, .true.)
  call lcio_event_final (eio%lcio_event, .true.)
else
  call eio%write ()
  call msg_fatal ("LCIO file is not open for writing")
end if
end subroutine eio_lcio_output

```

Input an event.

[WK 22-04-21] We do no longer fix the `i_mci` and `i_term` indices to 1, this can now be done by `simulation_recalculate`.

(EIO LCIO: eio lcio: TBP)+≡

```

  procedure :: input_i_prc => eio_lcio_input_i_prc
  procedure :: input_event => eio_lcio_input_event

```

(EIO LCIO: procedures)+≡

```

  subroutine eio_lcio_input_i_prc (eio, i_prc, iostat)
  class(eio_lcio_t), intent(inout) :: eio

```

```

integer, intent(out) :: i_prc
integer, intent(out) :: iostat
logical :: ok
integer :: i, proc_num_id
iostat = 0
call lcio_read_event (eio%lcio_reader, eio%lcio_event, ok)
if (.not. ok) then
    iostat = -1
    return
end if
proc_num_id = lcio_event_get_process_id (eio%lcio_event)
i_prc = 0
FIND_I_PRC: do i = 1, size (eio%proc_num_id)
    if (eio%proc_num_id(i) == proc_num_id) then
        i_prc = i
        exit FIND_I_PRC
    end if
end do FIND_I_PRC
if (i_prc == 0) call err_index
contains
subroutine err_index
    call msg_error ("LCIO: reading events: undefined process ID " &
        // char (str (proc_num_id)) // ", aborting read")
    iostat = 1
end subroutine err_index
end subroutine eio_lcio_input_i_prc

subroutine eio_lcio_input_event (eio, event, iostat, event_handle)
    class(eio_lcio_t), intent(inout) :: eio
    class(generic_event_t), intent(inout), target :: event
    integer, intent(out) :: iostat
    class(event_handle_t), intent(inout), optional :: event_handle
    iostat = 0
    call event%reset_contents ()
    call event%select (0, 0, 1)
    call event%set_index (lcio_event_get_event_index (eio%lcio_event))
    call lcio_to_event (event, eio%lcio_event, eio%fallback_model, &
        recover_beams = eio%recover_beams, &
        use_alpha_s = eio%use_alphas_from_file, &
        use_scale = eio%use_scale_from_file)
    call maybe_transfer_event_to_handle (eio%lcio_event, &
        event_handle, .false.)
    call lcio_event_final (eio%lcio_event, .false.)
end subroutine eio_lcio_input_event

```

If an `event_handle` is in the argument list, and it is of the correct HepMC type, do not destroy the event but transfer it to the handle (i.e., the enclosed C pointer). Nullify the original pointer, so the event does not get destroyed.

(*EIO LCIO: procedures*) +=

```

subroutine maybe_transfer_event_to_handle (lcio_event, event_handle, delete)
    type(lcio_event_t), intent(inout) :: lcio_event
    class(event_handle_t), intent(inout), optional :: event_handle
    logical, intent(in) :: delete

```



```

    if (present (event_handle)) then
      select type (event_handle)
      type is (lcio_event_t)
        call lcio_event_final (event_handle, delete) ! just in case
        event_handle = lcio_event
        call lcio_event_nullify (lcio_event) ! avoid destructor call
      end select
    end if
  end subroutine maybe_transfer_event_to_handle

```

```

<EIO LCIO: eio lcio: TBP>+≡
  procedure :: skip => eio_lcio_skip

<EIO LCIO: procedures>+≡
  subroutine eio_lcio_skip (eio, iostat)
    class(eio_lcio_t), intent(inout) :: eio
    integer, intent(out) :: iostat
    iostat = 0
  end subroutine eio_lcio_skip

```

18.18.4 Unit tests

Test module, followed by the corresponding implementation module.

```

<eio_lcio.ut.f90>≡
  <File header>

  module eio_lcio_ut
    use unit_tests
    use eio_lcio_uti

    <Standard module head>

    <EIO LCIO: public test>

    contains

    <EIO LCIO: test driver>

  end module eio_lcio_ut

<eio_lcio.uti.f90>≡
  <File header>

  module eio_lcio_uti

    <Use kinds>
    <Use strings>
    use io_units
    use model_data
    use particles
    use event_base
    use eio_data
    use eio_base

```

```

use hep_events
use lcio_interface

use eio_lcio

use eio_base_ut, only: eio_prepare_test, eio_cleanup_test
use eio_base_ut, only: eio_prepare_fallback_model, eio_cleanup_fallback_model

<Standard module head>

<EIO LCIO: test declarations>

contains

<EIO LCIO: tests>

end module eio_lcio_utl
API: driver for the unit tests below.
<EIO LCIO: public test>≡
    public :: eio_lcio_test
<EIO LCIO: test driver>≡
    subroutine eio_lcio_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <EIO LCIO: execute tests>
    end subroutine eio_lcio_test

```

Test I/O methods

We test the implementation of all I/O methods.

```

<EIO LCIO: execute tests>≡
    call test (eio_lcio_1, "eio_lcio_1", &
        "write event contents", &
        u, results)
<EIO LCIO: test declarations>≡
    public :: eio_lcio_1
<EIO LCIO: tests>≡
    subroutine eio_lcio_1 (u)
        integer, intent(in) :: u
        class(generic_event_t), pointer :: event
        type(event_sample_data_t) :: data
        class(eio_t), allocatable :: eio
        type(particle_set_t), pointer :: pset_ptr
        type(string_t) :: sample
        integer :: u_file, iostat
        character(215) :: buffer

        write (u, "(A)")  "* Test output: eio_lcio_1"
        write (u, "(A)")  "* Purpose: write a LCIO file"
        write (u, "(A)")

```

```

write (u, "(A)")  "* Initialize test process"

call eio_prepare_test (event)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_lcio_1"

allocate (eio_lcio_t :: eio)
select type (eio)
type is (eio_lcio_t)
    call eio%set_parameters ()
end select

call eio%init_out (sample, data)

call event%generate (1, [0._default, 0._default])
call event%set_index (77)
call event%pacify_particle_set ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()

write (u, "(A)")
write (u, "(A)")  "* Reset data"
write (u, "(A)")

deallocate (eio)
allocate (eio_lcio_t :: eio)

select type (eio)
type is (eio_lcio_t)
    call eio%set_parameters ()
end select
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write LCIO file contents to ASCII file"
write (u, "(A)")

```

```

select type (eio)
type is (eio_lcio_t)
  call lcio_event_init (eio%lcio_event, &
    proc_id = 42, &
    event_id = event%get_index ())
  pset_ptr => event%get_particle_set_ptr ()
  call lcio_event_from_particle_set &
    (eio%lcio_event, pset_ptr)
  call write_lcio_event (eio%lcio_event, var_str ("test_file.slcio"))
  call lcio_event_final (eio%lcio_event, .true.)
end select

write (u, "(A)")
write (u, "(A)")  "* Read in ASCII contents of LCIO file"
write (u, "(A)")

u_file = free_unit ()
open (u_file, file = "test_file.slcio", &
  action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat) buffer
  if (iostat /= 0) exit
  if (trim (buffer) == "") cycle
  if (buffer(1:12) == " - timestamp") cycle
  if (buffer(1:6) == " date:") cycle
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio_cleanup_test (event)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lcio_1"

end subroutine eio_lcio_1

```

Test also the reading of LCIO events.

```

<EIO LCIO: execute tests>+≡
  call test (eio_lcio_2, "eio_lcio_2", &
    "read event contents", &
    u, results)

<EIO LCIO: test declarations>+≡
  public :: eio_lcio_2

<EIO LCIO: tests>+≡
  subroutine eio_lcio_2 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: fallback_model
    class(generic_event_t), pointer :: event
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio

```

```

type(string_t) :: sample
integer :: iostat, i_prc

write (u, "(A)")  "* Test output: eio_lcio_2"
write (u, "(A)")  "* Purpose: read a LCIO event"
write (u, "(A)")

write (u, "(A)")  "* Initialize test process"

allocate (fallback_model)
call eio_prepare_fallback_model (fallback_model)
call eio_prepare_test (event)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
data%cross_section(1) = 100
data%error(1) = 1
data%total_cross_section = sum (data%cross_section)

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_lcio_2"

allocate (eio_lcio_t :: eio)
select type (eio)
type is (eio_lcio_t)
    call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%set_index (88)
call event%evaluate_expressions ()
call event%pacify_particle_set ()

call eio%output (event, i_prc = 1)
call eio%write (u)
call eio%final ()
deallocate (eio)

call event%reset_contents ()
call event%reset_index ()

write (u, "(A)")
write (u, "(A)")  "* Initialize"
write (u, "(A)")

```

```

allocate (eio_lcio_t :: eio)
select type (eio)
type is (eio_lcio_t)
    call eio%set_parameters (recover_beams = .false.)
end select
call eio%set_fallback_model (fallback_model)

call data%init (1)
data%n_beam = 2
data%unweighted = .true.
data%norm_mode = NORM_UNIT
data%pdg_beam = 25
data%energy_beam = 500
data%proc_num_id = [42]
call data%write (u)
write (u, *)

write (u, "(A)")  "* Initialize"
write (u, "(A)")

call eio%init_in (sample, data)
call eio%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read event"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)

select type (eio)
type is (eio_lcio_t)
    write (u, "(A,I0,A,I0)")  "Found process #", i_prc, &
        " with ID = ", eio%proc_num_id(i_prc)
end select

call eio%input_event (event, iostat)
call event%select (1, 1, 1)
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Read closing"
write (u, "(A)")

call eio%input_i_prc (i_prc, iostat)
write (u, "(A,I0)")  "iostat = ", iostat

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()

call eio_cleanup_test (event)
call eio_cleanup_fallback_model (fallback_model)

```

```
deallocate (fallback_model)

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_lcio_2"

end subroutine eio_lcio_2
```

Chapter 19

Phase Space

The abstract representation of a type that parameterizes phase space, with methods for construction and evaluation.

phs_base Abstract phase-space representation.

A simple implementation:

phs_none This implements a non-functional dummy module for the phase space. A process which uses this module cannot be integrated. The purpose of this module is to provide a placeholder for processes which do not require phase-space evaluation. They may still allow for evaluating matrix elements.

phs_single Parameterize the phase space of a single particle, i.e., the solid angle. This is useful only for very restricted problems, but it avoids the complexity of a generic approach in those trivial cases.

The standard implementation is called *wood* phase space. It consists of several auxiliary modules and the actual implementation module.

mappings Generate invariant masses and decay angles from given random numbers (or the inverse operation). Each mapping pertains to a particular node in a phase-space tree. Different mappings account for uniform distributions, resonances, zero-mass behavior, and so on.

phs_trees Phase space parameterizations for scattering processes are defined recursively as if there was an initial particle decaying. This module sets up a representation in terms of abstract trees, where each node gets a unique binary number. Each tree is stored as an array of branches, where integers indicate the connections. This emulates pointers in a transparent way. Real pointers would also be possible, but seem to be less efficient for this particular case.

phs_forests The type defined by this module collects the decay trees corresponding to a given process and the applicable mappings. To set this up, a file is read which is either written by the user or by the **cascades** module functions. The module also contains the routines that evaluate phase space, i.e., generate momenta from random numbers and back.

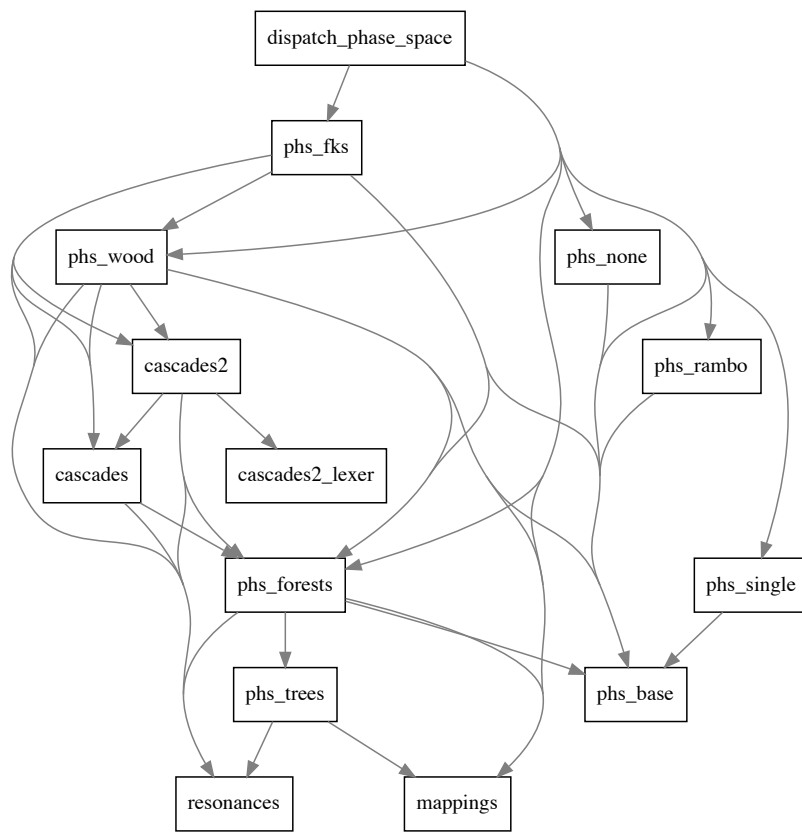


Figure 19.1: Module dependencies in `src/phase_space`.

cascades This module is a pseudo Feynman diagram generator with the particular purpose of finding the phase space parameterizations best suited for a given process. It uses a model file to set up the possible vertices, generates all possible diagrams, identifies resonances and singularities, and simplifies the list by merging equivalent diagrams and dropping irrelevant ones. This process can be controlled at several points by user-defined parameters. Note that it depends on the particular values of particle masses, so it cannot be done before reading the input file.

phs_wood Make the functionality available in form of an implementation of the abstract phase-space type.

phs_fks Phase-space parameterization with modifications for the FKS scheme.

19.1 Abstract phase-space module

In this module we define an abstract base type (and a trivial test implementation) for multi-channel phase-space parameterizations.

```
<phs_base.f90>≡  
  <File header>  
  
  module phs_base  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use constants, only: TWOPI, TWOPI4  
    use string_utils, only: split_string  
    use format_defs, only: FMT_19  
    use numeric_utils  
    use diagnostics  
    use md5  
    use physics_defs  
    use lorentz  
    use model_data  
    use flavors  
    use process_constants  
  
    <Standard module head>  
  
    <PHS base: public>  
  
    <PHS base: types>  
  
    <PHS base: interfaces>  
  
    contains  
  
    <PHS base: procedures>  
  
  end module phs_base
```

19.1.1 Phase-space channels

The kinematics configuration may generate multiple parameterizations of phase space. Some of those have specific properties, such as a resonance in the s channel.

Channel properties

This is the abstract type for the channel properties. We need them as a data transfer container, so everything is public and transparent.

```
<PHS base: public>≡  
  public :: channel_prop_t  
  
<PHS base: types>≡  
  type, abstract :: channel_prop_t
```

```

contains
  procedure (channel_prop_to_string), deferred :: to_string
  generic :: operator (==) => is_equal
  procedure (channel_eq), deferred :: is_equal
end type channel_prop_t

```

```

<PHS base: interfaces>≡
abstract interface
  function channel_prop_to_string (object) result (string)
  import
    class(channel_prop_t), intent(in) :: object
    type(string_t) :: string
  end function channel_prop_to_string
end interface

```

```

<PHS base: interfaces>+≡
abstract interface
  function channel_eq (prop1, prop2) result (flag)
  import
    class(channel_prop_t), intent(in) :: prop1, prop2
    logical :: flag
  end function channel_eq
end interface

```

Here is a resonance as a channel property. Mass and width are stored here in physical units.

```

<PHS base: public>+≡
public :: resonance_t

<PHS base: types>+≡
type, extends (channel_prop_t) :: resonance_t
  real(default) :: mass = 0
  real(default) :: width = 0
contains
  procedure :: to_string => resonance_to_string
  procedure :: is_equal => resonance_is_equal
end type resonance_t

```

Print mass and width.

```

<PHS base: procedures>≡
function resonance_to_string (object) result (string)
  class(resonance_t), intent(in) :: object
  type(string_t) :: string
  character(32) :: buffer
  string = "resonant: m ="
  write (buffer, "(" // FMT_19 // ")") object%mass
  string = string // trim (buffer) // " GeV, w ="
  write (buffer, "(" // FMT_19 // ")") object%width
  string = string // trim (buffer) // " GeV"
end function resonance_to_string

```

Equality.

```

(PHS base: procedures)+≡
function resonance_is_equal (prop1, prop2) result (flag)
  class(resonance_t), intent(in) :: prop1
  class(channel_prop_t), intent(in) :: prop2
  logical :: flag
  select type (prop2)
  type is (resonance_t)
    flag = prop1%mass == prop2%mass .and. prop1%width == prop2%width
  class default
    flag = .false.
  end select
end function resonance_is_equal

```

This is the limiting case of a resonance, namely an on-shell particle. We just store the mass in physical units.

```

(PHS base: public)+≡
public :: on_shell_t

(PHS base: types)+≡
type, extends (channel_prop_t) :: on_shell_t
  real(default) :: mass = 0
contains
  procedure :: to_string => on_shell_to_string
  procedure :: is_equal => on_shell_is_equal
end type on_shell_t

```

Print mass and width.

```

(PHS base: procedures)+≡
function on_shell_to_string (object) result (string)
  class(on_shell_t), intent(in) :: object
  type(string_t) :: string
  character(32) :: buffer
  string = "on shell: m ="
  write (buffer, "(" // FMT_19 // ")") object%mass
  string = string // trim (buffer) // " GeV"
end function on_shell_to_string

```

Equality.

```

(PHS base: procedures)+≡
function on_shell_is_equal (prop1, prop2) result (flag)
  class(on_shell_t), intent(in) :: prop1
  class(channel_prop_t), intent(in) :: prop2
  logical :: flag
  select type (prop2)
  type is (on_shell_t)
    flag = prop1%mass == prop2%mass
  class default
    flag = .false.
  end select
end function on_shell_is_equal

```

Channel equivalences

This type describes an equivalence. The current channel is equivalent to channel `c`. The equivalence involves a permutation `perm` of integration dimensions and, within each integration dimension, a mapping `mode`.

```
<PHS base: types>+≡
  type :: phs_equivalence_t
    integer :: c = 0
    integer, dimension(:), allocatable :: perm
    integer, dimension(:), allocatable :: mode
  contains
    <PHS base: phs equivalence: TBP>
  end type phs_equivalence_t
```

The mapping modes are

```
<PHS base: types>+≡
  integer, parameter, public :: &
    EQ_IDENTITY = 0, EQ_INVERT = 1, EQ_SYMMETRIC = 2, EQ_INVARIANT = 3
```

In particular, if a channel is equivalent to itself in the `EQ_SYMMETRIC` mode, the integrand can be assumed to be symmetric w.r.t. a reflection $x \rightarrow 1 - x$ of the corresponding integration variable.

These are the associated tags, for output:

```
<PHS base: types>+≡
  character, dimension(0:3), parameter :: TAG = ["+", "-", ":", "x"]
```

Write an equivalence.

```
<PHS base: phs equivalence: TBP>≡
  procedure :: write => phs_equivalence_write

<PHS base: procedures>+≡
  subroutine phs_equivalence_write (object, unit)
    class(phs_equivalence_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, j
    u = given_output_unit (unit)
    write (u, "(5x,'=',1x,I0,1x)", advance = "no") object%c
    if (allocated (object%perm)) then
      write (u, "(A)", advance = "no") "("
      do j = 1, size (object%perm)
        if (j > 1) write (u, "(1x)", advance = "no")
        write (u, "(I0,A1)", advance = "no") &
          object%perm(j), TAG(object%mode(j))
      end do
      write (u, "(A)") ")"
    else
      write (u, "(A)")
    end if
  end subroutine phs_equivalence_write
```

Initialize an equivalence. This allocates the `perm` and `mode` arrays with equal size.

```

(PHS base: phs equivalence: TBP)+≡
  procedure :: init => phs_equivalence_init

(PHS base: procedures)+≡
  subroutine phs_equivalence_init (eq, n_dim)
    class(phs_equivalence_t), intent(out) :: eq
    integer, intent(in) :: n_dim
    allocate (eq%perm (n_dim), source = 0)
    allocate (eq%mode (n_dim), source = EQ_IDENTITY)
  end subroutine phs_equivalence_init

```

Channel objects

The channel entry holds (optionally) specific properties.

`sf_channel` is the structure-function channel that corresponds to this phase-space channel. The structure-function channel may be set up with a specific mapping that depends on the phase-space channel properties. (The default setting is to leave the properties empty.)

```

(PHS base: public)+≡
  public :: phs_channel_t

(PHS base: types)+≡
  type :: phs_channel_t
    class(channel_prop_t), allocatable :: prop
    integer :: sf_channel = 1
    type(phs_equivalence_t), dimension(:), allocatable :: eq
  contains
    (PHS base: phs channel: TBP)
  end type phs_channel_t

```

Output.

```

(PHS base: phs channel: TBP)≡
  procedure :: write => phs_channel_write

(PHS base: procedures)+≡
  subroutine phs_channel_write (object, unit)
    class(phs_channel_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, j
    u = given_output_unit (unit)
    write (u, "(1x,I0)", advance="no") object%sf_channel
    if (allocated (object%prop)) then
      write (u, "(1x,A)") char (object%prop%to_string ())
    else
      write (u, *)
    end if
    if (allocated (object%eq)) then
      do j = 1, size (object%eq)
        call object%eq(j)%write (u)
      end do
    end if
  end subroutine

```

```
end subroutine phs_channel_write
```

Identify the channel with an s-channel resonance.

```
<PHS base: phs channel: TBP>+≡
  procedure :: set_resonant => channel_set_resonant

<PHS base: procedures>+≡
  subroutine channel_set_resonant (channel, mass, width)
    class(phs_channel_t), intent(inout) :: channel
    real(default), intent(in) :: mass, width
    allocate (resonance_t :: channel%prop)
    select type (prop => channel%prop)
    type is (resonance_t)
      prop%mass = mass
      prop%width = width
    end select
  end subroutine channel_set_resonant
```

Identify the channel with an on-shell particle.

```
<PHS base: phs channel: TBP>+≡
  procedure :: set_on_shell => channel_set_on_shell

<PHS base: procedures>+≡
  subroutine channel_set_on_shell (channel, mass)
    class(phs_channel_t), intent(inout) :: channel
    real(default), intent(in) :: mass
    allocate (on_shell_t :: channel%prop)
    select type (prop => channel%prop)
    type is (on_shell_t)
      prop%mass = mass
    end select
  end subroutine channel_set_on_shell
```

19.1.2 Property collection

We can set up a list of all distinct channel properties for a given set of channels.

```
<PHS base: public>+≡
  public :: phs_channel_collection_t

<PHS base: types>+≡
  type :: prop_entry_t
    integer :: i = 0
    class(channel_prop_t), allocatable :: prop
    type(prop_entry_t), pointer :: next => null ()
  end type prop_entry_t

  type :: phs_channel_collection_t
    integer :: n = 0
    type(prop_entry_t), pointer :: first => null ()
    contains
    <PHS base: phs channel collection: TBP>
  end type phs_channel_collection_t
```


Finalizer for the list.

```

(PHS base: phs_channel_collection: TBP)≡
  procedure :: final => phs_channel_collection_final

(PHS base: procedures)+≡
  subroutine phs_channel_collection_final (object)
    class(phs_channel_collection_t), intent(inout) :: object
    type(prop_entry_t), pointer :: entry
    do while (associated (object%first))
      entry => object%first
      object%first => entry%next
      deallocate (entry)
    end do
  end subroutine phs_channel_collection_final

```

Output.

```

(PHS base: phs_channel_collection: TBP)+≡
  procedure :: write => phs_channel_collection_write

(PHS base: procedures)+≡
  subroutine phs_channel_collection_write (object, unit)
    class(phs_channel_collection_t), intent(in) :: object
    integer, intent(in), optional :: unit
    type(prop_entry_t), pointer :: entry
    integer :: u
    u = given_output_unit (unit)
    entry => object%first
    do while (associated (entry))
      if (allocated (entry%prop)) then
        write (u, "(1x,I0,1x,A)" entry%i, char (entry%prop%to_string ()))
      else
        write (u, "(1x,I0)" entry%i
      end if
      entry => entry%next
    end do
  end subroutine phs_channel_collection_write

```

Push a new property to the stack if it is not yet included. Simultaneously, set the `sf_channel` entry in the phase-space channel object to the index of the matching entry, or the new entry if there was no match.

```

(PHS base: phs_channel_collection: TBP)+≡
  procedure :: push => phs_channel_collection_push

(PHS base: procedures)+≡
  subroutine phs_channel_collection_push (coll, channel)
    class(phs_channel_collection_t), intent(inout) :: coll
    type(phs_channel_t), intent(inout) :: channel
    type(prop_entry_t), pointer :: entry, new
    if (associated (coll%first)) then
      entry => coll%first
    do
      if (allocated (entry%prop)) then
        if (allocated (channel%prop)) then
          if (entry%prop == channel%prop) then

```

```

        channel%sf_channel = entry%i
        return
    end if
    end if
    else if (.not. allocated (channel%prop)) then
        channel%sf_channel = entry%i
        return
    end if
    if (associated (entry%next)) then
        entry => entry%next
    else
        exit
    end if
end do
allocate (new)
entry%next => new
else
    allocate (new)
    coll%first => new
end if
coll%n = coll%n + 1
new%i = coll%n
channel%sf_channel = new%i
if (allocated (channel%prop)) then
    allocate (new%prop, source = channel%prop)
end if
end subroutine phs_channel_collection_push

```

Return the number of collected distinct channels.

```

<PHS base: phs channel collection: TBP>+≡
    procedure :: get_n => phs_channel_collection_get_n

<PHS base: procedures>+≡
    function phs_channel_collection_get_n (coll) result (n)
        class(phs_channel_collection_t), intent(in) :: coll
        integer :: n
        n = coll%n
    end function phs_channel_collection_get_n

```

Return a specific channel (property object).

```

<PHS base: phs channel collection: TBP>+≡
    procedure :: get_entry => phs_channel_collection_get_entry

<PHS base: procedures>+≡
    subroutine phs_channel_collection_get_entry (coll, i, prop)
        class(phs_channel_collection_t), intent(in) :: coll
        integer, intent(in) :: i
        class(channel_prop_t), intent(out), allocatable :: prop
        type(prop_entry_t), pointer :: entry
        integer :: k
        if (i > 0 .and. i <= coll%n) then
            entry => coll%first
            do k = 2, i
                entry => entry%next
            end do
        end if
    end subroutine phs_channel_collection_get_entry

```

```

    end do
    if (allocated (entry%prop)) then
        if (allocated (prop)) deallocate (prop)
        allocate (prop, source = entry%prop)
    end if
else
    call msg_bug ("PHS channel collection: get entry: illegal index")
end if
end subroutine phs_channel_collection_get_entry

```

19.1.3 Kinematics configuration

Here, we store the universal information that is specifically relevant for phase-space generation. It is a subset of the process data, supplemented by basic information on phase-space parameterization channels.

A concrete implementation will contain more data, that describe the phase space in detail.

MD5 sums: the phase space setup depends on the process, it depends on the model parameters (the masses, that is), and on the configuration parameters. (It does not depend on the QCD setup.)

```

<PHS base: public>+≡
    public :: phs_config_t

<PHS base: types>+≡
    type, abstract :: phs_config_t
    ! private
    type(string_t) :: id
    integer :: n_in = 0
    integer :: n_out = 0
    integer :: n_tot = 0
    integer :: n_state = 0
    integer :: n_par = 0
    integer :: n_channel = 0
    real(default) :: sqrts = 0
    logical :: sqrts_fixed = .true.
    logical :: lab_is_cm = .true.
    logical :: azimuthal_dependence = .false.
    integer, dimension(:), allocatable :: dim_flat
    logical :: provides_equivalences = .false.
    logical :: provides_chains = .false.
    logical :: vis_channels = .false.
    integer, dimension(:), allocatable :: chain
    class(model_data_t), pointer :: model => null ()
    type(flavor_t), dimension(:,:), allocatable :: flv
    type(phs_channel_t), dimension(:), allocatable :: channel
    character(32) :: md5sum_process = ""
    character(32) :: md5sum_model_par = ""
    character(32) :: md5sum_phs_config = ""
    integer :: nlo_type
contains
    <PHS base: phs config: TBP>
end type phs_config_t

```

Finalizer, deferred.

```

<PHS base: phs config: TBP>≡
    procedure (phs_config_final), deferred :: final

<PHS base: interfaces>+≡
    abstract interface
        subroutine phs_config_final (object)
            import
            class(phs_config_t), intent(inout) :: object
        end subroutine phs_config_final
    end interface

```

Output. We provide an implementation for the output of the base-type contents and an interface for the actual write method.

```

<PHS base: phs config: TBP>+≡
    procedure (phs_config_write), deferred :: write
    procedure :: base_write => phs_config_write

<PHS base: procedures>+≡
    subroutine phs_config_write (object, unit, include_id)
        class(phs_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: include_id
        integer :: u, i, j
        integer :: n_tot_flv
        logical :: use_id
        n_tot_flv = object%n_tot
        u = given_output_unit (unit)
        use_id = .true.; if (present (include_id)) use_id = include_id
        if (use_id) write (u, "(3x,A,A,A)") "ID          = ", char (object%id), ""
        write (u, "(3x,A,I0)") "n_in          = ", object%n_in
        write (u, "(3x,A,I0)") "n_out          = ", object%n_out
        write (u, "(3x,A,I0)") "n_tot          = ", object%n_tot
        write (u, "(3x,A,I0)") "n_state        = ", object%n_state
        write (u, "(3x,A,I0)") "n_par          = ", object%n_par
        write (u, "(3x,A,I0)") "n_channel      = ", object%n_channel
        write (u, "(3x,A," // FMT_19 // ")") "sqrts          = ", object%sqrts
        write (u, "(3x,A,L1)") "s_fixed        = ", object%sqrts_fixed
        write (u, "(3x,A,L1)") "lab_is_cm      = ", object%lab_is_cm
        write (u, "(3x,A,L1)") "azim.dep.     = ", object%azimuthal_dependence
        if (allocated (object%dim_flat)) then
            write (u, "(3x,A,I0)") "flat dim.     = ", object%dim_flat
        end if
        write (u, "(1x,A)") "Flavor combinations:"
        do i = 1, object%n_state
            write (u, "(3x,I0,':')", advance="no") i
            ! do j = 1, object%n_tot
            do j = 1, n_tot_flv
                write (u, "(1x,A)", advance="no") char (object%flv(j,i)%get_name ())
            end do
            write (u, "(A)")
        end do
        if (allocated (object%channel)) then

```

```

        write (u, "(1x,A)") "Phase-space / structure-function channels:"
        do i = 1, object%n_channel
            write (u, "(3x,I0,':')", advance="no") i
            call object%channel(i)%write (u)
        end do
    end if
    if (object%md5sum_process /= "") then
        write (u, "(3x,A,A,A)") "MD5 sum (process) = '", &
            object%md5sum_process, "'"
    end if
    if (object%md5sum_model_par /= "") then
        write (u, "(3x,A,A,A)") "MD5 sum (model par) = '", &
            object%md5sum_model_par, "'"
    end if
    if (object%md5sum_phs_config /= "") then
        write (u, "(3x,A,A,A)") "MD5 sum (phs config) = '", &
            object%md5sum_phs_config, "'"
    end if
end subroutine phs_config_write

```

Similarly, a basic initializer and an interface. The model pointer is taken as an argument; we may verify that this has the expected model name.

The intent is `inout`. We want to be able to set parameters in advance.

(PHS base: phs config: TBP)+≡

```

    procedure :: init => phs_config_init

```

(PHS base: procedures)+≡

```

subroutine phs_config_init (phs_config, data, model)
    class(phs_config_t), intent(inout) :: phs_config
    type(process_constants_t), intent(in) :: data
    class(model_data_t), intent(in), target :: model
    integer :: i, j
    phs_config%id = data%id
    phs_config%n_in = data%n_in
    phs_config%n_out = data%n_out
    phs_config%n_tot = data%n_in + data%n_out
    phs_config%n_state = data%n_flv
    if (data%model_name == model%get_name ()) then
        phs_config%model => model
    else
        call msg_bug ("phs_config_init: model name mismatch")
    end if
    allocate (phs_config%flv (phs_config%n_tot, phs_config%n_state))
    do i = 1, phs_config%n_state
        do j = 1, phs_config%n_tot
            call phs_config%flv(j,i)%init (data%flv_state(j,i), &
                phs_config%model)
        end do
    end do
    phs_config%md5sum_process = data%md5sum
end subroutine phs_config_init

```

WK 2018-04-05: This procedure appears to be redundant?

```

<XXX PHS base: phs config: TBP>≡
  procedure :: set_component_index => phs_config_set_component_index

<XXX PHS base: procedures>≡
  subroutine phs_config_set_component_index (phs_config, index)
    class(phs_config_t), intent(inout) :: phs_config
    integer, intent(in) :: index
    type(string_t), dimension(:), allocatable :: id
    type(string_t) :: suffix
    integer :: i, n
    suffix = var_str ('i') // int2string (index)
    call split_string (phs_config%id, var_str ('_'), id)
    phs_config%id = var_str ('')
    n = size (id) - 1
    do i = 1, n
      phs_config%id = phs_config%id // id(i) // var_str ('_')
    end do
    phs_config%id = phs_config%id // suffix
  end subroutine phs_config_set_component_index

```

This procedure should complete the phase-space configuration. We need the `sqrts` value as overall scale, which is known only after the beams have been defined. The procedure should determine the number of channels, their properties (if any), and allocate and fill the `channel` array accordingly.

```

<PHS base: phs config: TBP>+≡
  procedure (phs_config_configure), deferred :: configure

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_config_configure (phs_config, sqrts, &
      sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, ignore_mismatch, &
      nlo_type, subdir)
    import
    class(phs_config_t), intent(inout) :: phs_config
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: sqrts_fixed
    logical, intent(in), optional :: lab_is_cm
    logical, intent(in), optional :: azimuthal_dependence
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    integer, intent(in), optional :: nlo_type
    type(string_t), intent(in), optional :: subdir
  end subroutine phs_config_configure
  end interface

```

Manually assign structure-function channel indices to the phase-space channel objects. (Used by a test routine.)

```

<PHS base: phs config: TBP>+≡
  procedure :: set_sf_channel => phs_config_set_sf_channel

<PHS base: procedures>+≡
  subroutine phs_config_set_sf_channel (phs_config, sf_channel)
    class(phs_config_t), intent(inout) :: phs_config
    integer, dimension(:), intent(in) :: sf_channel

```

```

    phs_config%channel%sf_channel = sf_channel
end subroutine phs_config_set_sf_channel

```

Collect new channels not yet in the collection from this phase-space configuration object. At the same time, assign structure-function channels.

```

<PHS base: phs config: TBP>+≡
    procedure :: collect_channels => phs_config_collect_channels

<PHS base: procedures>+≡
    subroutine phs_config_collect_channels (phs_config, coll)
        class(phs_config_t), intent(inout) :: phs_config
        type(phs_channel_collection_t), intent(inout) :: coll
        integer :: c
        do c = 1, phs_config%n_channel
            call coll%push (phs_config%channel(c))
        end do
    end subroutine phs_config_collect_channels

```

Compute the MD5 sum. We abuse the `write` method. In type implementations, `write` should only display information that is relevant for the MD5 sum. The data include the process MD5 sum which is taken from the process constants, and the MD5 sum of the model parameters. This may change, so it is computed here.

```

<PHS base: phs config: TBP>+≡
    procedure :: compute_md5sum => phs_config_compute_md5sum

<PHS base: procedures>+≡
    subroutine phs_config_compute_md5sum (phs_config, include_id)
        class(phs_config_t), intent(inout) :: phs_config
        logical, intent(in), optional :: include_id
        integer :: u
        phs_config%md5sum_model_par = phs_config%model%get_parameters_md5sum ()
        phs_config%md5sum_phs_config = ""
        u = free_unit ()
        open (u, status = "scratch", action = "readwrite")
        call phs_config%write (u, include_id)
        rewind (u)
        phs_config%md5sum_phs_config = md5sum (u)
        close (u)
    end subroutine phs_config_compute_md5sum

```

Print an informative message after phase-space configuration.

```

<PHS base: phs config: TBP>+≡
    procedure (phs_startup_message), deferred :: startup_message
    procedure :: base_startup_message => phs_startup_message

<PHS base: procedures>+≡
    subroutine phs_startup_message (phs_config, unit)
        class(phs_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        write (msg_buffer, "(A,3(1x,I0,1x,A))") &
            "Phase space:", &
            phs_config%n_channel, "channels,", &

```

```

        phs_config%n_par, "dimensions"
    call msg_message (unit = unit)
end subroutine phs_startup_message

```

This procedure should be implemented such that the phase-space configuration object allocates a phase-space instance of matching type.

```

<PHS base: phs config: TBP>+≡
    procedure (phs_config_allocate_instance), nopass, deferred :: &
        allocate_instance

<PHS base: interfaces>+≡
    abstract interface
        subroutine phs_config_allocate_instance (phs)
            import
            class(phs_t), intent(inout), pointer :: phs
        end subroutine phs_config_allocate_instance
    end interface

```

19.1.4 Extract data

Return the number of MC input parameters.

```

<PHS base: phs config: TBP>+≡
    procedure :: get_n_par => phs_config_get_n_par

<PHS base: procedures>+≡
    function phs_config_get_n_par (phs_config) result (n)
        class(phs_config_t), intent(in) :: phs_config
        integer :: n
        n = phs_config%n_par
    end function phs_config_get_n_par

```

Return dimensions (parameter indices) for which the phase-space dimension is flat, so integration and event generation can be simplified.

```

<PHS base: phs config: TBP>+≡
    procedure :: get_flat_dimensions => phs_config_get_flat_dimensions

<PHS base: procedures>+≡
    function phs_config_get_flat_dimensions (phs_config) result (dim_flat)
        class(phs_config_t), intent(in) :: phs_config
        integer, dimension(:), allocatable :: dim_flat
        if (allocated (phs_config%dim_flat)) then
            allocate (dim_flat (size (phs_config%dim_flat)))
            dim_flat = phs_config%dim_flat
        else
            allocate (dim_flat (0))
        end if
    end function phs_config_get_flat_dimensions

```

Return the number of phase-space channels.

```

<PHS base: phs config: TBP>+≡
    procedure :: get_n_channel => phs_config_get_n_channel

```



```

<PHS base: procedures>+≡
function phs_config_get_n_channel (phs_config) result (n)
  class(phs_config_t), intent(in) :: phs_config
  integer :: n
  n = phs_config%n_channel
end function phs_config_get_n_channel

```

Return the structure-function channel that corresponds to the phase-space channel *c*. If the channel array is not allocated (which happens if there is no structure function), return zero.

```

<PHS base: phs config: TBP>+≡
  procedure :: get_sf_channel => phs_config_get_sf_channel

<PHS base: procedures>+≡
function phs_config_get_sf_channel (phs_config, c) result (c_sf)
  class(phs_config_t), intent(in) :: phs_config
  integer, intent(in) :: c
  integer :: c_sf
  if (allocated (phs_config%channel)) then
    c_sf = phs_config%channel(c)%sf_channel
  else
    c_sf = 0
  end if
end function phs_config_get_sf_channel

```

Return the mass(es) of the incoming particle(s). We take the first flavor combination in the array, assuming that masses must be degenerate among flavors.

```

<PHS base: phs config: TBP>+≡
  procedure :: get_masses_in => phs_config_get_masses_in

<PHS base: procedures>+≡
subroutine phs_config_get_masses_in (phs_config, m)
  class(phs_config_t), intent(in) :: phs_config
  real(default), dimension(:), intent(out) :: m
  integer :: i
  do i = 1, phs_config%n_in
    m(i) = phs_config%flv(i,1)%get_mass ()
  end do
end subroutine phs_config_get_masses_in

```

Return the MD5 sum of the configuration.

```

<PHS base: phs config: TBP>+≡
  procedure :: get_md5sum => phs_config_get_md5sum

<PHS base: procedures>+≡
function phs_config_get_md5sum (phs_config) result (md5sum)
  class(phs_config_t), intent(in) :: phs_config
  character(32) :: md5sum
  md5sum = phs_config%md5sum_phs_config
end function phs_config_get_md5sum

```

19.1.5 Phase-space point instance

The `phs_t` object holds the workspace for phase-space generation. In the base object, we have the MC input parameters `r` and the Jacobian factor `f`, for each channel, and the incoming and outgoing momenta.

Note: The `active_channel` array is not used yet, all elements are initialized with `.true..` It should be touched by the integrator if it decides to drop irrelevant channels.

```

(PHS base: public)+≡
    public :: phs_t

(PHS base: types)+≡
    type, abstract :: phs_t
        class(phs_config_t), pointer :: config => null ()
        logical :: r_defined = .false.
        integer :: selected_channel = 0
        logical, dimension(:), allocatable :: active_channel
        real(default), dimension(:,:), allocatable :: r
        real(default), dimension(:), allocatable :: f
        real(default), dimension(:), allocatable :: m_in
        real(default), dimension(:), allocatable :: m_out
        real(default) :: flux = 0
        real(default) :: volume = 0
        type(lorentz_transformation_t) :: lt_cm_to_lab
        logical :: p_defined = .false.
        real(default) :: sqrts_hat = 0
        type(vector4_t), dimension(:), allocatable :: p
        logical :: q_defined = .false.
        type(vector4_t), dimension(:), allocatable :: q
    contains
        (PHS base: phs: TBP)
    end type phs_t

```

Output. Since phase space may get complicated, we include a `verbose` option for the abstract `write` procedure.

```

(PHS base: phs: TBP)≡
    procedure (phs_write), deferred :: write

(PHS base: interfaces)+≡
    abstract interface
        subroutine phs_write (object, unit, verbose)
            import
            class(phs_t), intent(in) :: object
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: verbose
        end subroutine phs_write
    end interface

```

This procedure can be called to print the contents of the base type.

```

(PHS base: phs: TBP)+≡
    procedure :: base_write => phs_base_write

```

```

<PHS base: procedures>+≡
subroutine phs_base_write (object, unit)
  class(phs_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u, c, i
  u = given_output_unit (unit)
  write (u, "(1x,A)", advance="no") "Partonic phase space: parameters"
  if (object%r_defined) then
    write (u, *)
  else
    write (u, "(1x,A)") "[undefined]"
  end if
  write (u, "(3x,A,999(1x," // FMT_19 // "))") "m_in   =", object%m_in
  write (u, "(3x,A,999(1x," // FMT_19 // "))") "m_out   =", object%m_out
  write (u, "(3x,A," // FMT_19 // ")") "Flux    =", object%flux
  write (u, "(3x,A," // FMT_19 // ")") "Volume  =", object%volume
  if (allocated (object%f)) then
    do c = 1, size (object%r, 2)
      write (u, "(1x,A,IO,A)", advance="no") "Channel #", c, ":"
      if (c == object%selected_channel) then
        write (u, "(1x,A)") "[selected]"
      else
        write (u, *)
      end if
      write (u, "(3x,A)", advance="no") "r ="
      do i = 1, size (object%r, 1)
        write (u, "(1x,F9.7)", advance="no") object%r(i,c)
      end do
      write (u, *)
      write (u, "(3x,A,1x,ES13.7)") "f =", object%f(c)
    end do
  end if
  write (u, "(1x,A)") "Partonic phase space: momenta"
  if (object%p_defined) then
    write (u, "(3x,A," // FMT_19 // ")") "sqrts  =", object%sqrts_hat
  end if
  write (u, "(1x,A)", advance="no") "Incoming:"
  if (object%p_defined) then
    write (u, *)
  else
    write (u, "(1x,A)") "[undefined]"
  end if
  if (allocated (object%p)) then
    do i = 1, size (object%p)
      call vector4_write (object%p(i), u)
    end do
  end if
  write (u, "(1x,A)", advance="no") "Outgoing:"
  if (object%q_defined) then
    write (u, *)
  else
    write (u, "(1x,A)") "[undefined]"
  end if
  if (allocated (object%q)) then

```

```

do i = 1, size (object%q)
  call vector4_write (object%q(i), u)
end do
end if
if (object%p_defined .and. .not. object%config%lab_is_cm) then
  write (u, "(1x,A)") "Transformation c.m -> lab frame"
  call lorentz_transformation_write (object%lt_cm_to_lab, u)
end if
end subroutine phs_base_write

```

Finalizer. The base type does not need it, but extensions may.

```

<PHS base: phs: TBP>+≡
  procedure (phs_final), deferred :: final

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_final (object)
      import
      class(phs_t), intent(inout) :: object
    end subroutine phs_final
  end interface

```

Initializer. Everything should be contained in the `process_data` configuration object, so we can require a universal interface.

```

<PHS base: phs: TBP>+≡
  procedure (phs_init), deferred :: init

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_init (phs, phs_config)
      import
      class(phs_t), intent(out) :: phs
      class(phs_config_t), intent(in), target :: phs_config
    end subroutine phs_init
  end interface

```

The base version will just allocate the arrays. It should be called at the beginning of the implementation of `phs_init`.

```

<PHS base: phs: TBP>+≡
  procedure :: base_init => phs_base_init

<PHS base: procedures>+≡
  subroutine phs_base_init (phs, phs_config)
    class(phs_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
    real(default), dimension(phs_config%n_in) :: m_in
    real(default), dimension(phs_config%n_out) :: m_out
    phs%config => phs_config
    allocate (phs%active_channel (phs%config%n_channel))
    phs%active_channel = .true.
    allocate (phs%r (phs%config%n_par, phs%config%n_channel)); phs%r = 0
    allocate (phs%f (phs%config%n_channel)); phs%f = 0
    allocate (phs%p (phs%config%n_in))

```

```

!!! !!! !!! Workaround for gfortran 5.0 ICE
m_in = phs_config%flv(:phs_config%n_in, 1)%get_mass ()
m_out = phs_config%flv(phs_config%n_in+1:, 1)%get_mass ()
allocate (phs%m_in (phs%config%n_in), source = m_in)
!!! allocate (phs%m_in (phs%config%n_in), &
!!! source = phs_config%flv(:phs_config%n_in, 1)%get_mass ())
allocate (phs%q (phs%config%n_out))
allocate (phs%m_out (phs%config%n_out), source = m_out)
!!! allocate (phs%m_out (phs%config%n_out), &
!!! source = phs_config%flv(phs_config%n_in+1:, 1)%get_mass ())
call phs%compute_flux ()
end subroutine phs_base_init

```

Manually select a channel.

```

<PHS base: phs: TBP>+=
  procedure :: select_channel => phs_base_select_channel

<PHS base: procedures>+=
  subroutine phs_base_select_channel (phs, channel)
    class(phs_t), intent(inout) :: phs
    integer, intent(in), optional :: channel
    if (present (channel)) then
      phs%selected_channel = channel
    else
      phs%selected_channel = 0
    end if
  end subroutine phs_base_select_channel

```

Set incoming momenta. Assume that array shapes match. If requested, compute the Lorentz transformation from the c.m. to the lab frame and apply that transformation to the incoming momenta.

In the c.m. frame, the sum of three-momenta is zero. In a scattering process, the z axis is the direction of the first beam, the second beam is along the negative z axis. The transformation from the c.m. to the lab frame is a rotation from the z axis to the boost axis followed by a boost, such that the c.m. momenta are transformed into the lab-frame momenta. In a decay process, we just boost along the flight direction, without rotation.

```

<PHS base: phs: TBP>+=
  procedure :: set_incoming_momenta => phs_set_incoming_momenta

<PHS base: procedures>+=
  subroutine phs_set_incoming_momenta (phs, p)
    class(phs_t), intent(inout) :: phs
    type(vector4_t), dimension(:), intent(in) :: p
    type(vector4_t) :: p0, p1
    type(lorentz_transformation_t) :: lt0
    integer :: i
    phs%p = p
    if (phs%config%lab_is_cm) then
      phs%sqrts_hat = phs%config%sqrts
      phs%p = p
      phs%lt_cm_to_lab = identity
    else

```

```

p0 = sum (p)
if (phs%config%sqrts_fixed) then
  phs%sqrts_hat = phs%config%sqrts
else
  phs%sqrts_hat = p0 ** 1
end if
lt0 = boost (p0, phs%sqrts_hat)
select case (phs%config%n_in)
case (1)
  phs%lt_cm_to_lab = lt0
case (2)
  p1 = inverse (lt0) * p(1)
  phs%lt_cm_to_lab = lt0 * rotation_to_2nd (3, space_part (p1))
end select
phs%p = inverse (phs%lt_cm_to_lab) * p
end if
phs%p_defined = .true.
end subroutine phs_set_incoming_momenta

```

Set outgoing momenta. Assume that array shapes match. The incoming momenta must be known, so we can apply the Lorentz transformation from c.m. to lab (inverse) to the momenta.

```

<PHS base: phs: TBP>+≡
  procedure :: set_outgoing_momenta => phs_set_outgoing_momenta
<PHS base: procedures>+≡
  subroutine phs_set_outgoing_momenta (phs, q)
    class(phs_t), intent(inout) :: phs
    type(vector4_t), dimension(:), intent(in) :: q
    integer :: i
    if (phs%p_defined) then
      if (phs%config%lab_is_cm) then
        phs%q = q
      else
        phs%q = inverse (phs%lt_cm_to_lab) * q
      end if
      phs%q_defined = .true.
    end if
  end subroutine phs_set_outgoing_momenta

```

Return outgoing momenta. Apply the c.m. to lab transformation if necessary.

```

<PHS base: phs: TBP>+≡
  procedure :: get_outgoing_momenta => phs_get_outgoing_momenta
<PHS base: procedures>+≡
  subroutine phs_get_outgoing_momenta (phs, q)
    class(phs_t), intent(in) :: phs
    type(vector4_t), dimension(:), intent(out) :: q
    if (phs%p_defined .and. phs%q_defined) then
      if (phs%config%lab_is_cm) then
        q = phs%q
      else
        q = phs%lt_cm_to_lab * phs%q
      end if
    end if
  end subroutine phs_get_outgoing_momenta

```

```

        else
            q = vector4_null
        end if
    end subroutine phs_get_outgoing_momenta

<PHS base: phs: TBP>+=
    procedure :: lab_is_cm => phs_lab_is_cm

<PHS base: procedures>+=
    function phs_lab_is_cm (phs) result (lab_is_cm)
        logical :: lab_is_cm
        class(phs_t), intent(in) :: phs
        lab_is_cm = phs%config%lab_is_cm
    end function phs_lab_is_cm

<PHS base: phs: TBP>+=
    procedure :: get_n_tot => phs_get_n_tot

<PHS base: procedures>+=
    elemental function phs_get_n_tot (phs) result (n_tot)
        integer :: n_tot
        class(phs_t), intent(in) :: phs
        n_tot = phs%config%n_tot
    end function phs_get_n_tot

<PHS base: phs: TBP>+=
    procedure :: set_lorentz_transformation => phs_set_lorentz_transformation

<PHS base: procedures>+=
    subroutine phs_set_lorentz_transformation (phs, lt)
        class(phs_t), intent(inout) :: phs
        type(lorentz_transformation_t), intent(in) :: lt
        phs%lt_cm_to_lab = lt
    end subroutine phs_set_lorentz_transformation

<PHS base: phs: TBP>+=
    procedure :: get_lorentz_transformation => phs_get_lorentz_transformation

<PHS base: procedures>+=
    function phs_get_lorentz_transformation (phs) result (lt)
        type(lorentz_transformation_t) :: lt
        class(phs_t), intent(in) :: phs
        lt = phs%lt_cm_to_lab
    end function phs_get_lorentz_transformation

Return the input parameter array for a channel.

<PHS base: phs: TBP>+=
    procedure :: get_mcpair => phs_get_mcpair

```

```

<PHS base: procedures>+≡
subroutine phs_get_mcpair (phs, c, r)
  class(phs_t), intent(in) :: phs
  integer, intent(in) :: c
  real(default), dimension(:), intent(out) :: r
  if (phs%r_defined) then
    r = phs%r(:,c)
  else
    r = 0
  end if
end subroutine phs_get_mcpair

```

Return the Jacobian factor for a channel.

```

<PHS base: phs: TBP>+≡
  procedure :: get_f => phs_get_f
<PHS base: procedures>+≡
function phs_get_f (phs, c) result (f)
  class(phs_t), intent(in) :: phs
  integer, intent(in) :: c
  real(default) :: f
  if (phs%r_defined) then
    f = phs%f(c)
  else
    f = 0
  end if
end function phs_get_f

```

Return the overall factor, which is the product of the flux factor for the incoming partons and the phase-space volume for the outgoing partons.

```

<PHS base: phs: TBP>+≡
  procedure :: get_overall_factor => phs_get_overall_factor
<PHS base: procedures>+≡
function phs_get_overall_factor (phs) result (f)
  class(phs_t), intent(in) :: phs
  real(default) :: f
  f = phs%flux * phs%volume
end function phs_get_overall_factor

```

Compute flux factor. We do this during initialization (when the incoming momenta `p` are undefined), unless `sqrts` is variable. We do this again once for each phase-space point, but then we skip the calculation if `sqrts` is fixed.

There are three different flux factors.

1. For a decaying massive particle, the factor is

$$f = (2\pi)^4/(2M) \quad (19.1)$$

2. For a $2 \rightarrow n$ scattering process with $n > 1$, the factor is

$$f = (2\pi)^4/(2\sqrt{\lambda}) \quad (19.2)$$

where for massless incoming particles, $\sqrt{\lambda} = s$.

3. For a $2 \rightarrow 1$ on-shell production process, the factor includes an extra $1/(2\pi)^3$ factor and a $1/m^2$ factor from the phase-space delta function $\delta(x_1x_2 - m^2/s)$, which originate from the one-particle phase space that we integrate out.

$$f = 2\pi/(2sm^2) \quad (19.3)$$

The delta function is handled by the structure-function parameterization.

```

<PHS base: phs: TBP>+=
  procedure :: compute_flux => phs_compute_flux
  procedure :: compute_base_flux => phs_compute_flux

<PHS base: procedures>+=
  subroutine phs_compute_flux (phs)
    class(phs_t), intent(inout) :: phs
    real(default) :: s_hat, lda
    select case (phs%config%n_in)
    case (1)
      if (.not. phs%p_defined) then
        phs%flux = twopi4 / (2 * phs%m_in(1))
      end if
    case (2)
      if (phs%p_defined) then
        if (phs%config%sqrts_fixed) then
          return
        else
          s_hat = sum (phs%p) ** 2
        end if
      else
        if (phs%config%sqrts_fixed) then
          s_hat = phs%config%sqrts ** 2
        else
          return
        end if
      end if
    select case (phs%config%n_out)
    case (2:)
      lda = lambda (s_hat, phs%m_in(1) ** 2, phs%m_in(2) ** 2)
      if (lda > 0) then
        phs%flux = conv * twopi4 / (2 * sqrt (lda))
      else
        phs%flux = 0
      end if
    case (1)
      phs%flux = conv * twopi &
        / (2 * phs%config%sqrts ** 2 * phs%m_out(1) ** 2)
    case default
      phs%flux = 0
    end select
  end select
end subroutine phs_compute_flux

```

Evaluate the phase-space point for a particular channel and compute momenta, Jacobian, and phase-space volume. This is, of course, deferred to the imple-

mentation.

```

<PHS base: phs: TBP>+≡
  procedure (phs_evaluate_selected_channel), deferred :: &
    evaluate_selected_channel

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_evaluate_selected_channel (phs, c_in, r_in)
      import
      class(phs_t), intent(inout) :: phs
      integer, intent(in) :: c_in
      real(default), dimension(:), intent(in) :: r_in
    end subroutine phs_evaluate_selected_channel
  end interface

```

Compute the inverse mappings to completely fill the **r** and **f** arrays, for the non-selected channels.

```

<PHS base: phs: TBP>+≡
  procedure (phs_evaluate_other_channels), deferred :: &
    evaluate_other_channels

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_evaluate_other_channels (phs, c_in)
      import
      class(phs_t), intent(inout) :: phs
      integer, intent(in) :: c_in
    end subroutine phs_evaluate_other_channels
  end interface

```

Inverse evaluation. If all momenta are known, we compute the inverse mappings to fill the **r** and **f** arrays.

```

<PHS base: phs: TBP>+≡
  procedure (phs_inverse), deferred :: inverse

<PHS base: interfaces>+≡
  abstract interface
    subroutine phs_inverse (phs)
      import
      class(phs_t), intent(inout) :: phs
    end subroutine phs_inverse
  end interface

```

```

<PHS base: phs: TBP>+≡
  procedure :: get_sqrts => phs_get_sqrts

<PHS base: procedures>+≡
  function phs_get_sqrts (phs) result (sqrts)
    real(default) :: sqrts
    class(phs_t), intent(in) :: phs
    sqrts = phs%config%sqrts
  end function phs_get_sqrts

```

Uniform angular distribution

These procedures implement the uniform angular distribution, generated from two parameters x_1 and x_2 :

$$\cos \theta = 1 - 2x_1, \quad \phi = 2\pi x_2 \quad (19.4)$$

We generate a rotation (Lorentz transformation) which rotates the positive z axis into this point on the unit sphere. This rotation is applied to the \mathbf{p} momenta, which are assumed to be back-to-back, on-shell, and with the correct mass.

We do not compute a Jacobian (constant). The uniform distribution is assumed to be normalized.

<PHS base: public>+≡

```
public :: compute_kinematics_solid_angle
```

<PHS base: procedures>+≡

```
subroutine compute_kinematics_solid_angle (p, q, x)
  type(vector4_t), dimension(2), intent(in) :: p
  type(vector4_t), dimension(2), intent(out) :: q
  real(default), dimension(2), intent(in) :: x
  real(default) :: ct, st, phi
  type(lorentz_transformation_t) :: rot
  integer :: i
  ct = 1 - 2*x(1)
  st = sqrt (1 - ct**2)
  phi = twopi * x(2)
  rot = rotation (phi, 3) * rotation (ct, st, 2)
  do i = 1, 2
    q(i) = rot * p(i)
  end do
end subroutine compute_kinematics_solid_angle
```

This is the inverse transformation. We assume that the outgoing momenta are rotated versions of the incoming momenta, back-to-back. Thus, we determine the angles from $q(1)$ alone. \mathbf{p} is unused.

<PHS base: public>+≡

```
public :: inverse_kinematics_solid_angle
```

<PHS base: procedures>+≡

```
subroutine inverse_kinematics_solid_angle (p, q, x)
  type(vector4_t), dimension(:), intent(in) :: p
  type(vector4_t), dimension(2), intent(in) :: q
  real(default), dimension(2), intent(out) :: x
  real(default) :: ct, phi
  ct = polar_angle_ct (q(1))
  phi = azimuthal_angle (q(1))
  x(1) = (1 - ct) / 2
  x(2) = phi / twopi
end subroutine inverse_kinematics_solid_angle
```

19.1.6 Auxiliary stuff

The `pacify` subroutine, which is provided by the Lorentz module, has the purpose of setting numbers to zero which are (by comparing with a `tolerance` parameter) considered equivalent with zero. This is useful for numerical checks.

```
<PHS base: public>+≡
    public :: pacify

<PHS base: interfaces>+≡
    interface pacify
        module procedure pacify_phs
    end interface pacify

<PHS base: procedures>+≡
    subroutine pacify_phs (phs)
        class(phs_t), intent(inout) :: phs
        if (phs%p_defined) then
            call pacify (phs%p, 30 * epsilon (1._default) * phs%config%sqrts)
            call pacify (phs%lt_cm_to_lab, 30 * epsilon (1._default))
        end if
        if (phs%q_defined) then
            call pacify (phs%q, 30 * epsilon (1._default) * phs%config%sqrts)
        end if
    end subroutine pacify_phs
```

19.1.7 Unit tests

Test module, followed by the corresponding implementation module.

```
<phs_base_ut.f90>≡
<File header>

    module phs_base_ut
        use unit_tests
        use phs_base_util

<Standard module head>

<PHS base: public test>

<PHS base: public test auxiliary>

    contains

<PHS base: test driver>

    end module phs_base_ut

<phs_base_util.f90>≡
<File header>

    module phs_base_util

<Use kinds>
```

```

    <Use strings>
    use diagnostics
    use io_units
    use format_defs, only: FMT_19
    use physics_defs, only: BORN
    use lorentz
    use flavors
    use model_data
    use process_constants

    use phs_base

    <Standard module head>

    <PHS base: public test auxiliary>

    <PHS base: test declarations>

    <PHS base: test types>

contains

    <PHS base: tests>

    <PHS base: test auxiliary>

end module phs_base_util

API: driver for the unit tests below.
<PHS base: public test>≡
    public :: phs_base_test
<PHS base: test driver>≡
    subroutine phs_base_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS base: execute tests>
    end subroutine phs_base_test

```

Test process data

We provide a procedure that initializes a test case for the process constants. This set of process data contains just the minimal contents that we need for the phase space. The rest is left uninitialized.

```

<PHS base: public test auxiliary>≡
    public :: init_test_process_data
<PHS base: test auxiliary>≡
    subroutine init_test_process_data (id, data)
        type(process_constants_t), intent(out) :: data
        type(string_t), intent(in), optional :: id
        if (present (id)) then
            data%id = id
        else

```

```

        data%id = "testproc"
    end if
    data%model_name = "Test"
    data%n_in = 2
    data%n_out = 2
    data%n_flv = 1
    allocate (data%flv_state (data%n_in + data%n_out, data%n_flv))
    data%flv_state = 25
end subroutine init_test_process_data

```

This is the variant for a decay process.

```

<PHS base: public test auxiliary>+≡
    public :: init_test_decay_data

<PHS base: test auxiliary>+≡
    subroutine init_test_decay_data (id, data)
        type(process_constants_t), intent(out) :: data
        type(string_t), intent(in), optional :: id
        if (present (id)) then
            data%id = id
        else
            data%id = "testproc"
        end if
        data%model_name = "Test"
        data%n_in = 1
        data%n_out = 2
        data%n_flv = 1
        allocate (data%flv_state (data%n_in + data%n_out, data%n_flv))
        data%flv_state(:,1) = [25, 6, -6]
    end subroutine init_test_decay_data

```

Test kinematics configuration

This is a trivial implementation of the `phs_config_t` configuration object.

```

<PHS base: public test auxiliary>+≡
    public :: phs_test_config_t

<PHS base: test types>≡
    type, extends (phs_config_t) :: phs_test_config_t
        logical :: create_equivalences = .false.
    contains
        procedure :: final => phs_test_config_final
        procedure :: write => phs_test_config_write
        procedure :: configure => phs_test_config_configure
        procedure :: startup_message => phs_test_config_startup_message
        procedure, nopass :: allocate_instance => phs_test_config_allocate_instance
    end type phs_test_config_t

```

The finalizer is empty.

```

<PHS base: test auxiliary>+≡
    subroutine phs_test_config_final (object)
        class(phs_test_config_t), intent(inout) :: object
    end subroutine

```

```
end subroutine phs_test_config_final
```

The `lab_is_cm` parameter is not tested here; we defer this to the `phs.single` implementation.

(PHS base: test auxiliary)+≡

```
subroutine phs_test_config_write (object, unit, include_id)
  class(phs_test_config_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: include_id
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Partonic phase-space configuration:"
  call object%base_write (unit)
end subroutine phs_test_config_write

subroutine phs_test_config_configure (phs_config, sqrts, &
  sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
  ignore_mismatch, nlo_type, subdir)
  class(phs_test_config_t), intent(inout) :: phs_config
  real(default), intent(in) :: sqrts
  logical, intent(in), optional :: sqrts_fixed
  logical, intent(in), optional :: lab_is_cm
  logical, intent(in), optional :: azimuthal_dependence
  logical, intent(in), optional :: rebuild
  logical, intent(in), optional :: ignore_mismatch
  integer, intent(in), optional :: nlo_type
  type(string_t), intent(in), optional :: subdir
  phs_config%n_channel = 2
  phs_config%n_par = 2
  phs_config%sqrts = sqrts
  if (.not. present (nlo_type)) &
    phs_config%nlo_type = BORN
  if (present (sqrts_fixed)) then
    phs_config%sqrts_fixed = sqrts_fixed
  end if
  if (present (lab_is_cm)) then
    phs_config%lab_is_cm = lab_is_cm
  end if
  if (present (azimuthal_dependence)) then
    phs_config%azimuthal_dependence = azimuthal_dependence
  end if
  if (allocated (phs_config%channel)) deallocate (phs_config%channel)
  allocate (phs_config%channel (phs_config%n_channel))
  if (phs_config%create_equivalences) then
    call setup_test_equivalences (phs_config)
    call setup_test_channel_props (phs_config)
  end if
  call phs_config%compute_md5sum ()
end subroutine phs_test_config_configure
```

If requested, we make up an arbitrary set of equivalences.

(PHS base: test auxiliary)+≡

```
subroutine setup_test_equivalences (phs_config)
```

```

class(phs_test_config_t), intent(inout) :: phs_config
integer :: i
associate (channel => phs_config%channel(1))
  allocate (channel%eq (2))
  do i = 1, size (channel%eq)
    call channel%eq(i)%init (phs_config%n_par)
  end do
  associate (eq => channel%eq(1))
    eq%c = 1; eq%perm = [1, 2]; eq%mode = [EQ_IDENTITY, EQ_SYMMETRIC]
  end associate
  associate (eq => channel%eq(2))
    eq%c = 2; eq%perm = [2, 1]; eq%mode = [EQ_INVARIANT, EQ_IDENTITY]
  end associate
end associate
end subroutine setup_test_equivalences

```

Ditto, for channel properties.

```

<PHS base: test auxiliary>+≡
subroutine setup_test_channel_props (phs_config)
  class(phs_test_config_t), intent(inout) :: phs_config
  associate (channel => phs_config%channel(2))
    call channel%set_resonant (140._default, 3.1415_default)
  end associate
end subroutine setup_test_channel_props

```

Startup message

```

<PHS base: test auxiliary>+≡
subroutine phs_test_config_startup_message (phs_config, unit)
  class(phs_test_config_t), intent(in) :: phs_config
  integer, intent(in), optional :: unit
  call phs_config%base_startup_message (unit)
  write (msg_buffer, "(A)") "Phase space: Test"
  call msg_message (unit = unit)
end subroutine phs_test_config_startup_message

```

The instance type that matches `phs_test_config_t` is `phs_test_t`.

```

<PHS base: test auxiliary>+≡
subroutine phs_test_config_allocate_instance (phs)
  class(phs_t), intent(inout), pointer :: phs
  allocate (phs_test_t :: phs)
end subroutine phs_test_config_allocate_instance

```

Test kinematics implementation

This implementation of kinematics generates a simple two-particle configuration from the incoming momenta. The incoming momenta must be in the c.m. system, all masses equal.

There are two channels: one generates $\cos\theta$ and ϕ uniformly, in the other channel we map the r_1 parameter which belongs to $\cos\theta$.

We should store the mass parameter that we need.

```

<PHS base: public test auxiliary>+≡

```



```

    public :: phs_test_t
<PHS base: test types>+≡
    type, extends (phs_t) :: phs_test_t
        real(default) :: m = 0
        real(default), dimension(:), allocatable :: x
    contains
        <PHS base: phs test: TBP>
    end type phs_test_t

```

Output. The specific data are displayed only if `verbose` is set.

```

<PHS base: phs test: TBP>≡
    procedure :: write => phs_test_write

<PHS base: test auxiliary>+≡
    subroutine phs_test_write (object, unit, verbose)
        class(phs_test_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u
        logical :: verb
        u = given_output_unit (unit)
        verb = .false.; if (present (verbose)) verb = verbose
        if (verb) then
            write (u, "(1x,A)") "Partonic phase space: data"
            write (u, "(3x,A," // FMT_19 // ")") "m = ", object%m
        end if
        call object%base_write (u)
    end subroutine phs_test_write

```

The finalizer is empty.

```

<PHS base: phs test: TBP>+≡
    procedure :: final => phs_test_final

<PHS base: test auxiliary>+≡
    subroutine phs_test_final (object)
        class(phs_test_t), intent(inout) :: object
    end subroutine phs_test_final

```

Initialization: set the mass value.

```

<PHS base: phs test: TBP>+≡
    procedure :: init => phs_test_init

<PHS base: test auxiliary>+≡
    subroutine phs_test_init (phs, phs_config)
        class(phs_test_t), intent(out) :: phs
        class(phs_config_t), intent(in), target :: phs_config
        call phs%base_init (phs_config)
        phs%m = phs%config%flv(1,1)%get_mass ()
        allocate (phs%x (phs_config%n_par), source = 0._default)
    end subroutine phs_test_init

```

Evaluation. In channel 1, we uniformly generate $\cos\theta$ and ϕ , with Jacobian normalized to one. In channel 2, we prepend a mapping $r_1 \rightarrow r_1^{(1/3)}$ with Jacobian $f = 3r_1^2$.

The component `x` is allocated in the first subroutine, used and deallocated in the second one.

```

(PHS base: phs test: TBP)+≡
  procedure :: evaluate_selected_channel => phs_test_evaluate_selected_channel
  procedure :: evaluate_other_channels => phs_test_evaluate_other_channels

(PHS base: test auxiliary)+≡
  subroutine phs_test_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_test_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    real(default), intent(in), dimension(:) :: r_in
    if (phs%p_defined) then
      call phs%select_channel (c_in)
      phs%r(:,c_in) = r_in
      select case (c_in)
        case (1)
          phs%x = r_in
        case (2)
          phs%x(1) = r_in(1) ** (1 / 3._default)
          phs%x(2) = r_in(2)
      end select
      call compute_kinematics_solid_angle (phs%p, phs%q, phs%x)
      phs%volume = 1
      phs%q_defined = .true.
    end if
  end subroutine phs_test_evaluate_selected_channel

  subroutine phs_test_evaluate_other_channels (phs, c_in)
    class(phs_test_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    integer :: c, n_channel
    if (phs%p_defined) then
      n_channel = phs%config%n_channel
      do c = 1, n_channel
        if (c /= c_in) then
          call inverse_kinematics_solid_angle (phs%p, phs%q, phs%x)
          select case (c)
            case (1)
              phs%r(:,c) = phs%x
            case (2)
              phs%r(1,c) = phs%x(1) ** 3
              phs%r(2,c) = phs%x(2)
          end select
        end if
      end do
      phs%f(1) = 1
      if (phs%r(1,2) /= 0) then
        phs%f(2) = 1 / (3 * phs%r(1,2) ** (2/3._default))
      else
        phs%f(2) = 0
      end if
    end if
  end subroutine phs_test_evaluate_other_channels

```

```

        phs%r_defined = .true.
    end if
end subroutine phs_test_evaluate_other_channels

```

Inverse evaluation.

```

<PHS base: phs test: TBP>+=
    procedure :: inverse => phs_test_inverse

<PHS base: test auxiliary>+=
    subroutine phs_test_inverse (phs)
        class(phs_test_t), intent(inout) :: phs
        integer :: c, n_channel
        real(default), dimension(:), allocatable :: x
        if (phs%p_defined .and. phs%q_defined) then
            call phs%select_channel ()
            n_channel = phs%config%n_channel
            allocate (x (phs%config%n_par))
            do c = 1, n_channel
                call inverse_kinematics_solid_angle (phs%p, phs%q, x)
                select case (c)
                case (1)
                    phs%r(:,c) = x
                case (2)
                    phs%r(1,c) = x(1) ** 3
                    phs%r(2,c) = x(2)
                end select
            end do
            phs%f(1) = 1
            if (phs%r(1,2) /= 0) then
                phs%f(2) = 1 / (3 * phs%r(1,2) ** (2/3._default))
            else
                phs%f(2) = 0
            end if
            phs%volume = 1
            phs%r_defined = .true.
        end if
    end subroutine phs_test_inverse

```

Phase-space configuration data

Construct and display a test phase-space configuration object.

```

<PHS base: execute tests>=
    call test (phs_base_1, "phs_base_1", &
        "phase-space configuration", &
        u, results)

<PHS base: test declarations>=
    public :: phs_base_1

<PHS base: tests>=
    subroutine phs_base_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model

```

```

type(process_constants_t) :: process_data
class(phs_config_t), allocatable :: phs_data

write (u, "(A)")  "* Test output: phs_base_1"
write (u, "(A)")  "*   Purpose: initialize and display &
                    &test phase-space configuration data"
write (u, "(A)")

call model%init_test ()

write (u, "(A)")  "* Initialize a process and a matching &
                    &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_base_1"), process_data)

allocate (phs_test_config_t :: phs_data)
call phs_data%init (process_data, model)

call phs_data%write (u)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_1"

end subroutine phs_base_1

```

Phase space evaluation

Compute kinematics for given parameters, also invert the calculation.

```

<PHS base: execute tests>+≡
    call test (phs_base_2, "phs_base_2", &
                "phase-space evaluation", &
                u, results)

<PHS base: test declarations>+≡
    public :: phs_base_2

<PHS base: tests>+≡
    subroutine phs_base_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(process_constants_t) :: process_data
        real(default) :: sqrts, E
        class(phs_config_t), allocatable, target :: phs_data
        class(phs_t), pointer :: phs => null ()
        type(vector4_t), dimension(2) :: p, q

        write (u, "(A)")  "* Test output: phs_base_2"
        write (u, "(A)")  "*   Purpose: test simple two-channel phase space"
        write (u, "(A)")

```

```

call model%init_test ()
call flv%init (25, model)

write (u, "(A)")  "* Initialize a process and a matching &
                    &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_base_2"), process_data)

allocate (phs_test_config_t :: phs_data)
call phs_data%init (process_data, model)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
select type (phs)
type is (phs_test_t)
    call phs%init (phs_data)
end select

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

E = sqrts / 2
p(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point in channel 1 &
                    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point in channel 2 &
                    &for x = 0.125, 0.125"

```

```

write (u, "(A)")

call phs%evaluate_selected_channel (2, [0.125_default, 0.125_default])
call phs%evaluate_other_channels (2)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrt_s = 1000._default
select type (phs_data)
type is (phs_test_config_t)
    call phs_data%configure (sqrt_s)
end select

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_2"

end subroutine phs_base_2

```

Phase-space equivalences

Construct a test phase-space configuration which contains channel equivalences.

```

<PHS base: execute tests>+≡
    call test (phs_base_3, "phs_base_3", &
        "channel equivalences", &
        u, results)

<PHS base: test declarations>+≡
    public :: phs_base_3

<PHS base: tests>+≡
    subroutine phs_base_3 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model

```

```

type(process_constants_t) :: process_data
class(phs_config_t), allocatable :: phs_data

write (u, "(A)")  "* Test output: phs_base_3"
write (u, "(A)")  "*   Purpose: construct phase-space configuration data &
                    &with equivalences"
write (u, "(A)")

call model%init_test ()

write (u, "(A)")  "* Initialize a process and a matching &
                    &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_base_3"), process_data)

allocate (phs_test_config_t :: phs_data)
call phs_data%init (process_data, model)
select type (phs_data)
type is (phs_test_config_t)
    phs_data%create_equivalences = .true.
end select

call phs_data%configure (1000._default)
call phs_data%write (u)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_3"

end subroutine phs_base_3

```

MD5 sum checks

Construct a test phase-space configuration, compute and compare MD5 sums.

```

<PHS base: execute tests>+≡
    call test (phs_base_4, "phs_base_4", &
               "MD5 sum", &
               u, results)

<PHS base: test declarations>+≡
    public :: phs_base_4

<PHS base: tests>+≡
    subroutine phs_base_4 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        class(phs_config_t), allocatable :: phs_data

        write (u, "(A)")  "* Test output: phs_base_4"
        write (u, "(A)")  "*   Purpose: compute and compare MD5 sums"
    end subroutine

```

```

write (u, "(A)")

call model%init_test ()

write (u, "(A)")  "* Model parameters"
write (u, "(A)")

call model%write (unit = u, &
  show_parameters = .true., &
  show_particles = .false., show_vertices = .false.)

write (u, "(A)")
write (u, "(A)")  "* Initialize a process and a matching &
  &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_base_4"), process_data)
process_data%md5sum = "test_process_data_m6sum_12345678"

allocate (phs_test_config_t :: phs_data)
call phs_data%init (process_data, model)

call phs_data%compute_md5sum ()
call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Modify model parameter"
write (u, "(A)")

call model%set_par (var_str ("ms"), 100._default)
call model%write (show_parameters = .true., &
  show_particles = .false., show_vertices = .false.)

write (u, "(A)")
write (u, "(A)")  "* PHS configuration"
write (u, "(A)")

call phs_data%compute_md5sum ()
call phs_data%write (u)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_4"

end subroutine phs_base_4

```

Phase-space channel collection

Set up an array of various phase-space channels and collect them in a list.

(PHS base: execute tests) +≡


```

call test (phs_base_5, "phs_base_5", &
          "channel collection", &
          u, results)
<PHS base: test declarations>+≡
public :: phs_base_5
<PHS base: tests>+≡
subroutine phs_base_5 (u)
  integer, intent(in) :: u
  type(phs_channel_t), dimension(:), allocatable :: channel
  type(phs_channel_collection_t) :: coll
  integer :: i, n

  write (u, "(A)")  "* Test output: phs_base_5"
  write (u, "(A)")  "* Purpose: collect channel properties"
  write (u, "(A)")

  write (u, "(A)")  "* Set up an array of channels"
  write (u, "(A)")

  n = 6

  allocate (channel (n))
  call channel(2)%set_resonant (75._default, 3._default)
  call channel(4)%set_resonant (130._default, 1._default)
  call channel(5)%set_resonant (75._default, 3._default)
  call channel(6)%set_on_shell (33._default)

  do i = 1, n
    write (u, "(1x,I0)", advance="no") i
    call channel(i)%write (u)
  end do

  write (u, "(A)")
  write (u, "(A)")  "* Collect distinct properties"
  write (u, "(A)")

  do i = 1, n
    call coll%push (channel(i))
  end do

  write (u, "(1x,A,I0)") "n = ", coll%get_n ()
  write (u, "(A)")

  call coll%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Channel array with collection index assigned"
  write (u, "(A)")

  do i = 1, n
    write (u, "(1x,I0)", advance="no") i
    call channel(i)%write (u)
  end do

```

```
write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call coll%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_base_5"

end subroutine phs_base_5
```

19.2 Dummy phase space

This module implements a dummy phase space module for cases where the program structure demands the existence of a phase-space module, but no phase space integration is performed.

```
<phs_none.f90>≡  
  <File header>  
  
  module phs_none  
  
    <Use kinds>  
    <Use strings>  
    use io_units, only: given_output_unit  
    use diagnostics, only: msg_message, msg_fatal  
    use phs_base, only: phs_config_t, phs_t  
  
    <Standard module head>  
  
    <PHS none: public>  
  
    <PHS none: types>  
  
    contains  
  
    <PHS none: procedures>  
  
  end module phs_none
```

19.2.1 Configuration

Nothing to configure, but we provide the type and methods.

```
<PHS none: public>≡  
  public :: phs_none_config_t  
  
<PHS none: types>≡  
  type, extends (phs_config_t) :: phs_none_config_t  
  contains  
  <PHS none: phs none config: TBP>  
  end type phs_none_config_t
```

The finalizer is empty.

```
<PHS none: phs none config: TBP>≡  
  procedure :: final => phs_none_config_final  
  
<PHS none: procedures>≡  
  subroutine phs_none_config_final (object)  
    class(phs_none_config_t), intent(inout) :: object  
  end subroutine phs_none_config_final
```

Output. No contents, just an informative line.

```
<PHS none: phs none config: TBP>+≡  
  procedure :: write => phs_none_config_write
```

```

<PHS none: procedures>+≡
  subroutine phs_none_config_write (object, unit, include_id)
    class(phs_none_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: include_id
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Partonic phase-space configuration: non-functional dummy"
  end subroutine phs_none_config_write

```

Configuration: we have to implement this method, but it obviously does nothing.

```

<PHS none: phs none config: TBP>+≡
  procedure :: configure => phs_none_config_configure

<PHS none: procedures>+≡
  subroutine phs_none_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, ignore_mismatch, &
    nlo_type, subdir)
    class(phs_none_config_t), intent(inout) :: phs_config
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: sqrts_fixed
    logical, intent(in), optional :: lab_is_cm
    logical, intent(in), optional :: azimuthal_dependence
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    integer, intent(in), optional :: nlo_type
    type(string_t), intent(in), optional :: subdir
  end subroutine phs_none_config_configure

```

Startup message, after configuration is complete.

```

<PHS none: phs none config: TBP>+≡
  procedure :: startup_message => phs_none_config_startup_message

<PHS none: procedures>+≡
  subroutine phs_none_config_startup_message (phs_config, unit)
    class(phs_none_config_t), intent(in) :: phs_config
    integer, intent(in), optional :: unit
    call msg_message ("Phase space: none")
  end subroutine phs_none_config_startup_message

```

Allocate an instance: the actual phase-space object.

```

<PHS none: phs none config: TBP>+≡
  procedure, nopass :: allocate_instance => phs_none_config_allocate_instance

<PHS none: procedures>+≡
  subroutine phs_none_config_allocate_instance (phs)
    class(phs_t), intent(inout), pointer :: phs
    allocate (phs_none_t :: phs)
  end subroutine phs_none_config_allocate_instance

```

19.2.2 Kinematics implementation

This is considered as empty, but we have to implement the minimal set of methods.

```
<PHS none: public>+≡
    public :: phs_none_t
<PHS none: types>+≡
    type, extends (phs_t) :: phs_none_t
    contains
    <PHS none: phs none: TBP>
    end type phs_none_t
```

Output.

```
<PHS none: phs none: TBP>≡
    procedure :: write => phs_none_write
<PHS none: procedures>+≡
    subroutine phs_none_write (object, unit, verbose)
        class(phs_none_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u
        u = given_output_unit (unit)
        write (u, "(A)") "Partonic phase space: none"
    end subroutine phs_none_write
```

The finalizer is empty.

```
<PHS none: phs none: TBP>+≡
    procedure :: final => phs_none_final
<PHS none: procedures>+≡
    subroutine phs_none_final (object)
        class(phs_none_t), intent(inout) :: object
    end subroutine phs_none_final
```

Initialization, trivial.

```
<PHS none: phs none: TBP>+≡
    procedure :: init => phs_none_init
<PHS none: procedures>+≡
    subroutine phs_none_init (phs, phs_config)
        class(phs_none_t), intent(out) :: phs
        class(phs_config_t), intent(in), target :: phs_config
        call phs%base_init (phs_config)
    end subroutine phs_none_init
```

Evaluation. This must not be called at all.

```
<PHS none: phs none: TBP>+≡
    procedure :: evaluate_selected_channel => phs_none_evaluate_selected_channel
    procedure :: evaluate_other_channels => phs_none_evaluate_other_channels
```

```

<PHS none: procedures>+≡
  subroutine phs_none_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_none_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    real(default), intent(in), dimension(:) :: r_in
    call msg_fatal ("Phase space: attempt to evaluate with the 'phs_none' method")
  end subroutine phs_none_evaluate_selected_channel

  subroutine phs_none_evaluate_other_channels (phs, c_in)
    class(phs_none_t), intent(inout) :: phs
    integer, intent(in) :: c_in
  end subroutine phs_none_evaluate_other_channels

```

Inverse evaluation, likewise.

```

<PHS none: phs none: TBP>+≡
  procedure :: inverse => phs_none_inverse

<PHS none: procedures>+≡
  subroutine phs_none_inverse (phs)
    class(phs_none_t), intent(inout) :: phs
    call msg_fatal ("Phase space: attempt to evaluate inverse with the 'phs_none' method")
  end subroutine phs_none_inverse

```

19.2.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<phs_none_ut.f90>≡
  <File header>

  module phs_none_ut
    use unit_tests
    use phs_none_ut_i

    <Standard module head>

    <PHS none: public test>

    contains

    <PHS none: test driver>

  end module phs_none_ut

<phs_none_ut_i.f90>≡
  <File header>

  module phs_none_ut_i

    <Use kinds>
    <Use strings>
    use flavors
    use lorentz
    use model_data

```

```

use process_constants
use phs_base

use phs_none

use phs_base_ut, only: init_test_process_data, init_test_decay_data

<Standard module head>

<PHS none: test declarations>

contains

<PHS none: tests>

end module phs_none_ut
API: driver for the unit tests below.
<PHS none: public test>≡
public :: phs_none_test
<PHS none: test driver>≡
subroutine phs_none_test (u, results)
integer, intent(in) :: u
type(test_results_t), intent(inout) :: results
<PHS none: execute tests>
end subroutine phs_none_test

```

Phase-space configuration data

Construct and display a test phase-space configuration object. Also check the azimuthal dependence flag.

```

<PHS none: execute tests>≡
call test (phs_none_1, "phs_none_1", &
"phase-space configuration dummy", &
u, results)
<PHS none: test declarations>≡
public :: phs_none_1
<PHS none: tests>≡
subroutine phs_none_1 (u)
integer, intent(in) :: u
type(model_data_t), target :: model
type(process_constants_t) :: process_data
class(phs_config_t), allocatable :: phs_data
real(default) :: sqrts

write (u, "(A)")  "* Test output: phs_none_1"
write (u, "(A)")  "* Purpose: display &
&phase-space configuration data"
write (u, "(A)")

allocate (phs_none_config_t :: phs_data)

```

```

call phs_data%init (process_data, model)

sqrts = 1000._default
call phs_data%configure (sqrts, azimuthal_dependence=.false.)

call phs_data%write (u)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_none_1"

end subroutine phs_none_1

```


19.3 Single-particle phase space

This module implements the phase space for a single particle, i.e., the solid angle, in a straightforward parameterization with a single channel. The phase-space implementation may be used either for $1 \rightarrow 2$ decays or for $2 \rightarrow 2$ scattering processes, so the number of incoming particles is the only free parameter in the configuration. In the latter case, we should restrict its use to non-resonant s-channel processes, because there is no mapping of the scattering angle.

(We might extend this later to account for generic $2 \rightarrow 2$ situations, e.g., account for a Coulomb singularity or detect an s-channel resonance structure that requires matching structure-function mappings.)

This is derived from the `phs_test` implementation in the `phs_base` module above, even more simplified, but intended for actual use.

```
<phs_single.f90>≡  
  <File header>  
  
  module phs_single  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use constants  
    use numeric_utils  
    use diagnostics  
    use os_interface  
    use lorentz  
    use physics_defs  
    use model_data  
    use flavors  
    use process_constants  
    use phs_base  
  
    <Standard module head>  
  
    <PHS single: public>  
  
    <PHS single: types>  
  
    contains  
  
    <PHS single: procedures>  
  
  end module phs_single
```

19.3.1 Configuration

```
<PHS single: public>≡  
  public :: phs_single_config_t  
  
<PHS single: types>≡  
  type, extends (phs_config_t) :: phs_single_config_t  
  contains  
  <PHS single: phs single config: TBP>
```

```
end type phs_single_config_t
```

The finalizer is empty.

```
<PHS single: phs single config: TBP>≡
  procedure :: final => phs_single_config_final

<PHS single: procedures>≡
  subroutine phs_single_config_final (object)
    class(phs_single_config_t), intent(inout) :: object
  end subroutine phs_single_config_final
```

Output.

```
<PHS single: phs single config: TBP>+≡
  procedure :: write => phs_single_config_write

<PHS single: procedures>+≡
  subroutine phs_single_config_write (object, unit, include_id)
    class(phs_single_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: include_id
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Partonic phase-space configuration (single-particle):"
    call object%base_write (unit)
  end subroutine phs_single_config_write
```

Configuration: there is only one channel and two parameters. The second parameter is the azimuthal angle, which may be a flat dimension.

```
<PHS single: phs single config: TBP>+≡
  procedure :: configure => phs_single_config_configure

<PHS single: procedures>+≡
  subroutine phs_single_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, ignore_mismatch, &
    nlo_type, subdir)
    class(phs_single_config_t), intent(inout) :: phs_config
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: sqrts_fixed
    logical, intent(in), optional :: lab_is_cm
    logical, intent(in), optional :: azimuthal_dependence
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    integer, intent(in), optional :: nlo_type
    type(string_t), intent(in), optional :: subdir
    if (.not. present (nlo_type)) &
      phs_config%nlo_type = BORN
    if (phs_config%n_out == 2) then
      phs_config%n_channel = 1
      phs_config%n_par = 2
      phs_config%sqrts = sqrts
      if (present (sqrts_fixed)) phs_config%sqrts_fixed = sqrts_fixed
      if (present (lab_is_cm)) phs_config%lab_is_cm = lab_is_cm
      if (present (azimuthal_dependence)) then
```

```

        phs_config%azimuthal_dependence = azimuthal_dependence
        if (.not. azimuthal_dependence) then
            allocate (phs_config%dim_flat (1))
            phs_config%dim_flat(1) = 2
        end if
    end if
    if (allocated (phs_config%channel)) deallocate (phs_config%channel)
    allocate (phs_config%channel (1))
    call phs_config%compute_md5sum ()
else
    call msg_fatal ("Single-particle phase space requires n_out = 2")
end if
end subroutine phs_single_config_configure

```

Startup message, after configuration is complete.

```

<PHS single: phs single config: TBP>+≡
    procedure :: startup_message => phs_single_config_startup_message

<PHS single: procedures>+≡
    subroutine phs_single_config_startup_message (phs_config, unit)
        class(phs_single_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        call phs_config%base_startup_message (unit)
        write (msg_buffer, "(A,2(1x,I0,1x,A))") &
            "Phase space: single-particle"
        call msg_message (unit = unit)
    end subroutine phs_single_config_startup_message

```

Allocate an instance: the actual phase-space object.

```

<PHS single: phs single config: TBP>+≡
    procedure, nopass :: allocate_instance => phs_single_config_allocate_instance

<PHS single: procedures>+≡
    subroutine phs_single_config_allocate_instance (phs)
        class(phs_t), intent(inout), pointer :: phs
        allocate (phs_single_t :: phs)
    end subroutine phs_single_config_allocate_instance

```

19.3.2 Kinematics implementation

We generate $\cos\theta$ and ϕ uniformly, covering the solid angle.

Note: The incoming momenta must be in the c.m. system.

```

<PHS single: public>+≡
    public :: phs_single_t

<PHS single: types>+≡
    type, extends (phs_t) :: phs_single_t
        contains
        <PHS single: phs single: TBP>
    end type phs_single_t

```

Output. The `verbose` setting is irrelevant, we just display the contents of the base object.

```

<PHS single: phs single: TBP>≡
  procedure :: write => phs_single_write

<PHS single: procedures>+≡
  subroutine phs_single_write (object, unit, verbose)
    class(phs_single_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    call object%base_write (u)
  end subroutine phs_single_write

```

The finalizer is empty.

```

<PHS single: phs single: TBP>+≡
  procedure :: final => phs_single_final

<PHS single: procedures>+≡
  subroutine phs_single_final (object)
    class(phs_single_t), intent(inout) :: object
  end subroutine phs_single_final

```

Initialization. We allocate arrays (`base_init`) and adjust the phase-space volume. The massless two-particle phase space volume is

$$\Phi_2 = \frac{1}{4(2\pi)^5} = 2.55294034614 \times 10^{-5} \quad (19.5)$$

For a decay with nonvanishing masses (m_3, m_4), there is a correction factor

$$\Phi_2(m)/\Phi_2(0) = \frac{1}{\hat{s}} \lambda^{1/2}(\hat{s}, m_3^2, m_4^2). \quad (19.6)$$

For a scattering process with nonvanishing masses, the correction factor is

$$\Phi_2(m)/\Phi_2(0) = \frac{1}{\hat{s}^2} \lambda^{1/2}(\hat{s}, m_1^2, m_2^2) \lambda^{1/2}(\hat{s}, m_3^2, m_4^2). \quad (19.7)$$

If the energy is fixed, this is constant. Otherwise, we have to account for varying \hat{s} .

```

<PHS single: phs single: TBP>+≡
  procedure :: init => phs_single_init

<PHS single: procedures>+≡
  subroutine phs_single_init (phs, phs_config)
    class(phs_single_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
    call phs%base_init (phs_config)
    phs%volume = 1 / (4 * twopi5)
    call phs%compute_factor ()
  end subroutine phs_single_init

```

Compute the correction factor for nonzero masses. We do this during initialization (when the incoming momenta \mathbf{p} are undefined), unless `sqrts` is variable. We do this again once for each phase-space point, but then we skip the calculation if `sqrts` is fixed.

```

<PHS single: phs single: TBP>+≡
  procedure :: compute_factor => phs_single_compute_factor

<PHS single: procedures>+≡
  subroutine phs_single_compute_factor (phs)
    class(phs_single_t), intent(inout) :: phs
    real(default) :: s_hat
    select case (phs%config%n_in)
    case (1)
      if (.not. phs%p_defined) then
        if (sum (phs%m_out) < phs%m_in(1)) then
          s_hat = phs%m_in(1) ** 2
          phs%f(1) = 1 / s_hat &
            * sqrt (lambda (s_hat, phs%m_out(1)**2, phs%m_out(2)**2))
        else
          print *, "m_in = ", phs%m_in
          print *, "m_out = ", phs%m_out
          call msg_fatal ("Decay is kinematically forbidden")
        end if
      end if
    case (2)
      if (phs%config%sqrts_fixed) then
        if (phs%p_defined) return
        s_hat = phs%config%sqrts ** 2
      else
        if (.not. phs%p_defined) return
        s_hat = sum (phs%p) ** 2
      end if
      if (sum (phs%m_in)**2 < s_hat .and. sum (phs%m_out)**2 < s_hat) then
        phs%f(1) = 1 / s_hat * &
          ( lambda (s_hat, phs%m_in (1)**2, phs%m_in (2)**2) &
            * lambda (s_hat, phs%m_out(1)**2, phs%m_out(2)**2) ) &
          ** 0.25_default
      else
        phs%f(1) = 0
      end if
    end select
  end subroutine phs_single_compute_factor

```

Evaluation. We uniformly generate $\cos\theta$ and ϕ , with Jacobian normalized to one.

There is only a single channel, so the second subroutine does nothing.

Note: the current implementation works for elastic scattering only.

```

<PHS single: phs single: TBP>+≡
  procedure :: evaluate_selected_channel => phs_single_evaluate_selected_channel
  procedure :: evaluate_other_channels => phs_single_evaluate_other_channels

<PHS single: procedures>+≡
  subroutine phs_single_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_single_t), intent(inout) :: phs

```

```

integer, intent(in) :: c_in
real(default), intent(in), dimension(:) :: r_in
if (phs%p_defined) then
  call phs%select_channel (c_in)
  phs%r(:,c_in) = r_in
  select case (phs%config%n_in)
  case (2)
    if (all (phs%m_in == phs%m_out)) then
      call compute_kinematics_solid_angle (phs%p, phs%q, r_in)
    else
      call msg_bug ("PHS single: inelastic scattering not implemented")
    end if
  case (1)
    call compute_kinematics_solid_angle (phs%decay_p (), phs%q, r_in)
  end select
  call phs%compute_factor ()
  phs%q_defined = .true.
  phs%r_defined = .true.
end if
end subroutine phs_single_evaluate_selected_channel

subroutine phs_single_evaluate_other_channels (phs, c_in)
  class(phs_single_t), intent(inout) :: phs
  integer, intent(in) :: c_in
end subroutine phs_single_evaluate_other_channels

```

Auxiliary: split a decaying particle at rest into the decay products, aligned along the z axis.

```

<PHS single: phs single: TBP>+≡
  procedure :: decay_p => phs_single_decay_p

<PHS single: procedures>+≡
  function phs_single_decay_p (phs) result (p)
    class(phs_single_t), intent(in) :: phs
    type(vector4_t), dimension(2) :: p
    real(default) :: k
    real(default), dimension(2) :: E
    k = sqrt (lambda (phs%m_in(1) ** 2, phs%m_out(1) ** 2, phs%m_out(2) ** 2)) &
      / (2 * phs%m_in(1))
    E = sqrt (phs%m_out ** 2 + k ** 2)
    p(1) = vector4_moving (E(1), k, 3)
    p(2) = vector4_moving (E(2), -k, 3)
  end function phs_single_decay_p

```

Inverse evaluation.

```

<PHS single: phs single: TBP>+≡
  procedure :: inverse => phs_single_inverse

<PHS single: procedures>+≡
  subroutine phs_single_inverse (phs)
    class(phs_single_t), intent(inout) :: phs
    real(default), dimension(:), allocatable :: x
    if (phs%p_defined .and. phs%q_defined) then
      call phs%select_channel ()
    end if
  end subroutine phs_single_inverse

```

```

        allocate (x (phs%config%n_par))
        call inverse_kinematics_solid_angle (phs%p, phs%q, x)
        phs%r(:,1) = x
        call phs%compute_factor ()
        phs%r_defined = .true.
    end if
end subroutine phs_single_inverse

```

19.3.3 Unit tests

Test module, followed by the corresponding implementation module.

`<phs_single_ut.f90>`≡

<File header>

```

module phs_single_ut
  use unit_tests
  use phs_single_ut

```

<Standard module head>

<PHS single: public test>

contains

<PHS single: test driver>

```

end module phs_single_ut

```

`<phs_single_util.f90>`≡

<File header>

```

module phs_single_util

```

<Use kinds>

<Use strings>

```

  use flavors
  use lorentz
  use model_data
  use process_constants
  use phs_base

```

```

  use phs_single

```

```

  use phs_base_ut, only: init_test_process_data, init_test_decay_data

```

<Standard module head>

<PHS single: test declarations>

contains

<PHS single: tests>

```

    end module phs_single_util
API: driver for the unit tests below.
<PHS single: public test>≡
    public :: phs_single_test
<PHS single: test driver>≡
    subroutine phs_single_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS single: execute tests>
    end subroutine phs_single_test

```

Phase-space configuration data

Construct and display a test phase-space configuration object. Also check the azimuthal dependence flag.

```

<PHS single: execute tests>≡
    call test (phs_single_1, "phs_single_1", &
        "phase-space configuration", &
        u, results)
<PHS single: test declarations>≡
    public :: phs_single_1
<PHS single: tests>≡
    subroutine phs_single_1 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        class(phs_config_t), allocatable :: phs_data
        real(default) :: sqrts

        write (u, "(A)")  "* Test output: phs_single_1"
        write (u, "(A)")  "* Purpose: initialize and display &
            &phase-space configuration data"
        write (u, "(A)")

        call model%init_test ()

        write (u, "(A)")  "* Initialize a process and a matching &
            &phase-space configuration"
        write (u, "(A)")

        call init_test_process_data (var_str ("phs_single_1"), process_data)

        allocate (phs_single_config_t :: phs_data)
        call phs_data%init (process_data, model)

        sqrts = 1000._default
        call phs_data%configure (sqrts, azimuthal_dependence=.false.)

        call phs_data%write (u)
    end subroutine phs_single_1

```



```

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: phs_single_1"

end subroutine phs_single_1

```

Phase space evaluation

Compute kinematics for given parameters, also invert the calculation.

```

<PHS single: execute tests>+≡
  call test (phs_single_2, "phs_single_2", &
    "phase-space evaluation", &
    u, results)

<PHS single: test declarations>+≡
  public :: phs_single_2

<PHS single: tests>+≡
  subroutine phs_single_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(process_constants_t) :: process_data
    real(default) :: sqrts, E
    class(phs_config_t), allocatable, target :: phs_data
    class(phs_t), pointer :: phs => null ()
    type(vector4_t), dimension(2) :: p, q

    write (u, "(A)")  "** Test output: phs_single_2"
    write (u, "(A)")  "** Purpose: test simple two-channel phase space"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)

    write (u, "(A)")  "** Initialize a process and a matching &
      &phase-space configuration"
    write (u, "(A)")

    call init_test_process_data (var_str ("phs_single_2"), process_data)

    allocate (phs_single_config_t :: phs_data)
    call phs_data%init (process_data, model)

    sqrts = 1000._default
    call phs_data%configure (sqrts)

    call phs_data%write (u)

    write (u, "(A)")
    write (u, "(A)")  "** Initialize the phase-space instance"
    write (u, "(A)")

```

```

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

E = sqrt(s) / 2
p(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = vector4_moving (E,-sqrt (E**2 - flv%get_mass ()**2), 3)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrt(s) = 1000._default
call phs_data%configure (sqrt(s))

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_single_2"

```

```
end subroutine phs_single_2
```

Phase space for non-c.m. system

Compute kinematics for given parameters, also invert the calculation. Since this will involve cancellations, we call `pacify` to eliminate numerical noise.

```
<PHS single: execute tests>+≡
  call test (phs_single_3, "phs_single_3", &
    "phase-space evaluation in lab frame", &
    u, results)

<PHS single: test declarations>+≡
  public :: phs_single_3

<PHS single: tests>+≡
  subroutine phs_single_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(process_constants_t) :: process_data
    real(default) :: sqrts, E
    class(phs_config_t), allocatable, target :: phs_data
    class(phs_t), pointer :: phs => null ()
    type(vector4_t), dimension(2) :: p, q
    type(lorentz_transformation_t) :: lt

    write (u, "(A)")  "* Test output: phs_single_3"
    write (u, "(A)")  "* Purpose: test simple two-channel phase space"
    write (u, "(A)")  "*           without c.m. kinematics assumption"
    write (u, "(A)")

    call model%init_test ()
    call flv%init (25, model)

    write (u, "(A)")  "* Initialize a process and a matching &
      &phase-space configuration"
    write (u, "(A)")

    call init_test_process_data (var_str ("phs_single_3"), process_data)

    allocate (phs_single_config_t :: phs_data)
    call phs_data%init (process_data, model)

    sqrts = 1000._default
    call phs_data%configure (sqrts, lab_is_cm=.false., sqrts_fixed=.false.)

    call phs_data%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Initialize the phase-space instance"
    write (u, "(A)")
```

```

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta in lab system"
write (u, "(A)")

lt = boost (0.1_default, 1) * boost (0.3_default, 3)

E = sqrts / 2
p(1) = lt * vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = lt * vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

call vector4_write (p(1), u)
call vector4_write (p(2), u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%set_incoming_momenta (p)
call phs%compute_flux ()

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call pacify (phs)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract outgoing momenta in lab system"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
call vector4_write (q(1), u)
call vector4_write (q(2), u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

```

```

call phs%inverse ()
call pacify (phs)
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_single_3"

end subroutine phs_single_3

```

Decay Phase space evaluation

Compute kinematics for given parameters, also invert the calculation. This time, implement a decay process.

```

<PHS single: execute tests>+≡
  call test (phs_single_4, "phs_single_4", &
    "decay phase-space evaluation", &
    u, results)

<PHS single: test declarations>+≡
  public :: phs_single_4

<PHS single: tests>+≡
  subroutine phs_single_4 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t) :: flv
    type(process_constants_t) :: process_data
    class(phs_config_t), allocatable, target :: phs_data
    class(phs_t), pointer :: phs => null ()
    type(vector4_t), dimension(1) :: p
    type(vector4_t), dimension(2) :: q

    write (u, "(A)")  "* Test output: phs_single_4"
    write (u, "(A)")  "* Purpose: test simple two-channel phase space"
    write (u, "(A)")

    call model%init_test ()

    call model%set_par (var_str ("ff"), 0.4_default)
    call model%set_par (var_str ("mf"), &
      model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))
    call flv%init (25, model)

    write (u, "(A)")  "* Initialize a decay and a matching &
      &phase-space configuration"
    write (u, "(A)")

```

```

call init_test_decay_data (var_str ("phs_single_4"), process_data)

allocate (phs_single_config_t :: phs_data)
call phs_data%init (process_data, model)

call phs_data%configure (flv%get_mass ())

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

p(1) = vector4_at_rest (flv%get_mass ())

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs_data%configure (flv%get_mass ())

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

```

```
call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_single_4"

end subroutine phs_single_4
```

19.4 Flat RAMBO phase space

This module implements the flat RAMBO phase space for massless and massive particles using the minimal d.o.f $3n - 4$ in a straightforward parameterization with a single channel. We generate n mass systems M_i with $M_0 = \sqrt{s}$ and $M_n = 0$. We let each mass system decay $1 \rightarrow 2$ in a four-momentum conserving way. The four-momenta of the two particles are generated back-to-back where we map the d.o.f. to energy, azimuthal and polar angle. The particle momenta are then boosted to CMS by an appropriate boost using the kinematics of the parent mass system.

```
<phs_rambo.f90>≡  
<File header>  
  
module phs_rambo  
  
  <Use kinds>  
  <Use strings>  
    use io_units  
    use constants  
    use numeric_utils  
    use format_defs, only: FMT_19  
    use permutations, only: factorial  
    use diagnostics  
    use os_interface  
    use lorentz  
    use physics_defs  
    use model_data  
    use flavors  
    use process_constants  
    use phs_base  
  
  <Standard module head>  
  
  <PHS rambo: parameters>  
  
  <PHS rambo: types>  
  
  <PHS rambo: public>  
  
  contains  
  
  <PHS rambo: procedures>  
  
end module phs_rambo
```

19.4.1 Configuration

```
<PHS rambo: public>≡  
  public :: phs_rambo_config_t  
  
<PHS rambo: types>≡  
  type, extends (phs_config_t) :: phs_rambo_config_t  
  contains
```



```

    <PHS rambo: phs rambo config: TBP>
end type phs_rambo_config_t

```

The finalizer is empty.

```

    <PHS rambo: phs rambo config: TBP>≡
    procedure :: final => phs_rambo_config_final

    <PHS rambo: procedures>≡
    subroutine phs_rambo_config_final (object)
        class(phs_rambo_config_t), intent(inout) :: object
    end subroutine phs_rambo_config_final

```

Output.

```

    <PHS rambo: phs rambo config: TBP>+≡
    procedure :: write => phs_rambo_config_write

    <PHS rambo: procedures>+≡
    subroutine phs_rambo_config_write (object, unit, include_id)
        class(phs_rambo_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: include_id
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Partonic, flat phase-space configuration (RAMBO):"
        call object%base_write (unit)
    end subroutine phs_rambo_config_write

```

Configuration: there is only one channel and $3n - 4$ parameters.

```

    <PHS rambo: phs rambo config: TBP>+≡
    procedure :: configure => phs_rambo_config_configure

    <PHS rambo: procedures>+≡
    subroutine phs_rambo_config_configure (phs_config, sqrts, &
        sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, ignore_mismatch, &
        nlo_type, subdir)
        class(phs_rambo_config_t), intent(inout) :: phs_config
        real(default), intent(in) :: sqrts
        logical, intent(in), optional :: sqrts_fixed
        logical, intent(in), optional :: lab_is_cm
        logical, intent(in), optional :: azimuthal_dependence
        logical, intent(in), optional :: rebuild
        logical, intent(in), optional :: ignore_mismatch
        integer, intent(in), optional :: nlo_type
        type(string_t), intent(in), optional :: subdir
        if (.not. present (nlo_type)) &
            phs_config%nlo_type = BORN
        if (phs_config%n_out < 2) then
            call msg_fatal ("RAMBO phase space requires n_out >= 2")
        end if
        phs_config%n_channel = 1
        phs_config%n_par = 3 * phs_config%n_out - 4
        phs_config%sqrts = sqrts
        if (present (sqrts_fixed)) phs_config%sqrts_fixed = sqrts_fixed
        if (present (lab_is_cm)) phs_config%lab_is_cm = lab_is_cm
    end subroutine phs_rambo_config_configure

```

```

        if (allocated (phs_config%channel)) deallocate (phs_config%channel)
        allocate (phs_config%channel (1))
        call phs_config%compute_md5sum ()
    end subroutine phs_rambo_config_configure

```

Startup message, after configuration is complete.

```

<PHS rambo: phs rambo config: TBP>+≡
    procedure :: startup_message => phs_rambo_config_startup_message

<PHS rambo: procedures>+≡
    subroutine phs_rambo_config_startup_message (phs_config, unit)
        class(phs_rambo_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        call phs_config%base_startup_message (unit)
        write (msg_buffer, "(A,2(1x,IO,1x,A))") &
            "Phase space: flat (RAMBO)"
        call msg_message (unit = unit)
    end subroutine phs_rambo_config_startup_message

```

Allocate an instance: the actual phase-space object.

```

<PHS rambo: phs rambo config: TBP>+≡
    procedure, nopass :: allocate_instance => phs_rambo_config_allocate_instance

<PHS rambo: procedures>+≡
    subroutine phs_rambo_config_allocate_instance (phs)
        class(phs_t), intent(inout), pointer :: phs
        allocate (phs_rambo_t :: phs)
    end subroutine phs_rambo_config_allocate_instance

```

19.4.2 Kinematics implementation

We generate $n - 2$ mass systems M_i with $M_0 = \sqrt{s}$ and $M_n = 0...$

Note: The incoming momenta must be in the c.m. system.

```

<PHS rambo: public>+≡
    public :: phs_rambo_t

<PHS rambo: types>+≡
    type, extends (phs_t) :: phs_rambo_t
        real(default), dimension(:), allocatable :: k
        real(default), dimension(:), allocatable :: m
        contains
        <PHS rambo: phs rambo: TBP>
    end type phs_rambo_t

```

Output.

```

<PHS rambo: phs rambo: TBP>≡
    procedure :: write => phs_rambo_write

```

```

<PHS rambo: procedures>+≡
  subroutine phs_rambo_write (object, unit, verbose)
    class(phs_rambo_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    u = given_output_unit (unit)
    call object%base_write (u)
    write (u, "(1X,A)") "Intermediate masses (massless):"
    write (u, "(3X,999(" // FMT_19 // "))") object%k
    write (u, "(1X,A)") "Intermediate masses (massive):"
    write (u, "(3X,999(" // FMT_19 // "))") object%m
  end subroutine phs_rambo_write

```

The finalizer is empty.

```

<PHS rambo: phs rambo: TBP>+≡
  procedure :: final => phs_rambo_final

<PHS rambo: procedures>+≡
  subroutine phs_rambo_final (object)
    class(phs_rambo_t), intent(inout) :: object
  end subroutine phs_rambo_final

```

Initialization. We allocate arrays (base_init) and adjust the phase-space volume. The energy dependent factor of s^{n-2} is applied later.

```

<PHS rambo: phs rambo: TBP>+≡
  procedure :: init => phs_rambo_init

<PHS rambo: procedures>+≡
  subroutine phs_rambo_init (phs, phs_config)
    class(phs_rambo_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
    call phs%base_init (phs_config)
    associate (n => phs%config%n_out)
      select case (n)
      case (1)
        if (sum (phs%m_out) > phs%m_in (1)) then
          print *, "m_in = ", phs%m_in
          print *, "m_out = ", phs%m_out
          call msg_fatal ("[phs_rambo_init] Decay is kinematically forbidden.")
        end if
      end select
      allocate (phs%k(n), source = 0._default)
      allocate (phs%m(n), source = 0._default)
      phs%volume = 1. / (twopi)**(3 * n) &
        * (pi / 2.)**(n - 1) / (factorial(n - 1) * factorial(n - 2))
    end associate
  end subroutine phs_rambo_init

```

Evaluation. There is only one channel for RAMBO, so the second subroutine does nothing.

Note: the current implementation works for elastic scattering only.

```

<PHS rambo: phs rambo: TBP>+≡

```

```

procedure :: evaluate_selected_channel => phs_rambo_evaluate_selected_channel
procedure :: evaluate_other_channels => phs_rambo_evaluate_other_channels

<PHS rambo: procedures>+≡
subroutine phs_rambo_evaluate_selected_channel (phs, c_in, r_in)
  class(phs_rambo_t), intent(inout) :: phs
  integer, intent(in) :: c_in
  real(default), intent(in), dimension(:) :: r_in
  type(vector4_t), dimension(2) :: p_rest, p_boosted
  type(vector4_t) :: q
  real(default), dimension(2) :: r_angle
  integer :: i
  if (.not. phs%p_defined) return
  call phs%select_channel (c_in)
  phs%r(:,c_in) = r_in
  associate (n => phs%config%n_out, m => phs%m)
    call phs%generate_intermediates (r_in(:n - 2))
    q = sum (phs%p)
    do i = 2, n
      r_angle(1) = r_in(n - 5 + 2 * i)
      r_angle(2) = r_in(n - 4 + 2 * i)
      call phs%decay_intermediate (i, r_angle, p_rest)
      p_boosted = boost(q, m(i - 1)) * p_rest
      q = p_boosted(1)
      phs%q(i - 1) = p_boosted(2)
    end do
    phs%q(n) = q
  end associate
  phs%q_defined = .true.
  phs%r_defined = .true.
end subroutine phs_rambo_evaluate_selected_channel

subroutine phs_rambo_evaluate_other_channels (phs, c_in)
  class(phs_rambo_t), intent(inout) :: phs
  integer, intent(in) :: c_in
end subroutine phs_rambo_evaluate_other_channels

```

Decay intermediate mass system M_{i-1} into a on-shell particle with mass m_{i-1} and subsequent intermediate mass system with fixed M_i .

```

<PHS rambo: phs rambo: TBP>+≡
  procedure, private :: decay_intermediate => phs_rambo_decay_intermediate

<PHS rambo: procedures>+≡
subroutine phs_rambo_decay_intermediate (phs, i, r_angle, p)
  class(phs_rambo_t), intent(in) :: phs
  integer, intent(in) :: i
  real(default), dimension(2), intent(in) :: r_angle
  type(vector4_t), dimension(2), intent(out) :: p
  real(default) :: k_abs, cos_theta, phi
  type(vector3_t) :: k
  real(default), dimension(2) :: E
  cos_theta = 2. * r_angle(1) - 1.
  phi = twopi * r_angle(2)
  if (phi > pi) phi = phi - twopi
  k_abs = sqrt (lambda (phs%m(i - 1)**2, phs%m(i)**2, phs%m_out(i - 1)**2)) &

```

```

      / (2. * phs%m(i - 1))
k = k_abs * [cos(phi) * sqrt(1. - cos_theta**2), &
            sin(phi) * sqrt(1. - cos_theta**2), cos_theta]
E(1) = sqrt (phs%m(i)**2 + k_abs**2)
E(2) = sqrt (phs%m_out(i - 1)**2 + k_abs**2)
p(1) = vector4_moving (E(1), -k)
p(2) = vector4_moving (E(2), k)
end subroutine phs_rambo_decay_intermediate

```

Generate intermediate masses.

```

(PHS rambo: parameters)≡
  integer, parameter :: BISECT_MAX_ITERATIONS = 1000
  real(default), parameter :: BISECT_MIN_PRECISION = tiny_10
(PHS rambo: phs rambo: TBP)+≡
  procedure, private :: generate_intermediates => phs_rambo_generate_intermediates
  procedure, private :: invert_intermediates => phs_rambo_invert_intermediates
(PHS rambo: procedures)+≡
  subroutine phs_rambo_generate_intermediates (phs, r)
    class(phs_rambo_t), intent(inout) :: phs
    real(default), dimension(:), intent(in) :: r
    integer :: i, j
    associate (n => phs%config%n_out, k => phs%k, m => phs%m)
      m(1) = invariant_mass (sum (phs%p))
      m(n) = phs%m_out (n)
      call calculate_k (r)
      do i = 2, n - 1
        m(i) = k(i) + sum (phs%m_out (i:n))
      end do
      ! Massless volume times reweighting for massive volume
      phs%f(1) = k(1)**(2 * n - 4) &
        * 8. * rho(m(n - 1), phs%m_out(n), phs%m_out(n - 1))
      do i = 2, n - 1
        phs%f(1) = phs%f(1) * &
          rho(m(i - 1), m(i), phs%m_out(i - 1)) / &
          rho(k(i - 1), k(i), 0._default) * &
          M(i) / K(i)
      end do
    end associate
contains
  subroutine calculate_k (r)
    real(default), dimension(:), intent(in) :: r
    real(default), dimension(:), allocatable :: u
    integer :: i
    associate (n => phs%config%n_out, k => phs%k, m => phs%m)
      k = 0
      k(1) = m(1) - sum(phs%m_out(1:n))
      allocate (u(2:n - 1), source=0._default)
      call solve_for_u (r, u)
      do i = 2, n - 1
        k(i) = sqrt (u(i) * k(i - 1)**2)
      end do
    end associate
  end subroutine calculate_k

```

```

subroutine solve_for_u (r, u)
  real(default), dimension(phs%config%n_out - 2), intent(in) :: r
  real(default), dimension(2:phs%config%n_out - 1), intent(out) :: u
  integer :: i, j
  real(default) :: f, f_mid, xl, xr, xmid
  associate (n => phs%config%n_out)
    do i = 2, n - 1
      xl = 0
      xr = 1
      if (r(i - 1) == 1 .or. r(i - 1) == 0) then
        u(i) = r(i - 1)
      else
        do j = 1, BISECT_MAX_ITERATIONS
          xmid = (xl + xr) / 2.
          f = f_rambo (xl, n - i) - r(i - 1)
          f_mid = f_rambo (xmid, n - i) - r(i - 1)
          if (f * f_mid > 0) then
            xl = xmid
          else
            xr = xmid
          end if
          if (abs(xl - xr) < BISECT_MIN_PRECISION) exit
        end do
        u(i) = xmid
      end if
    end do
  end associate
end subroutine solve_for_u

real(default) function f_rambo(u, n)
  real(default), intent(in) :: u
  integer, intent(in) :: n
  f_rambo = (n + 1) * u**n - n * u**(n + 1)
end function f_rambo

real(default) function rho (M1, M2, m)
  real(default), intent(in) :: M1, M2, m
  real(default) :: MP, MM
  rho = sqrt ((M1**2 - (M2 + m)**2) * (M1**2 - (M2 - m)**2))
  ! MP = (M1 - (M2 + m)) * (M1 + (M2 + m))
  ! MM = (M1 - (M2 - m)) * (M1 + (M2 - m))
  ! rho = sqrt (MP) * sqrt (MM)
  rho = rho / (8._default * M1**2)
end function rho

end subroutine phs_rambo_generate_intermediates

subroutine phs_rambo_invert_intermediates (phs)
  class(phs_rambo_t), intent(inout) :: phs
  real(default) :: u
  integer :: i
  associate (n => phs%config%n_out, k => phs%k, m => phs%m)
    k = m
  end associate
end subroutine

```

```

do i = 1, n - 1
  k(i) = k(i) - sum (phs%m_out(i:n))
end do
do i = 2, n - 1
  u = (k(i) / k(i - 1))**2
  phs%r(i - 1, 1) = (n + 1 - i) * u**(n - i) &
    - (n - i) * u**(n + 1 - i)
end do
end associate
end subroutine phs_rambo_invert_intermediates

```

Inverse evaluation.

<PHS rambo: phs rambo: TBP>+≡

```
procedure :: inverse => phs_rambo_inverse
```

<PHS rambo: procedures>+≡

```

subroutine phs_rambo_inverse (phs)
  class(phs_rambo_t), intent(inout) :: phs
  type(vector4_t), dimension(:), allocatable :: q
  type(vector4_t) :: p
  type(lorentz_transformation_t) :: L
  real(default) :: phi, cos_theta
  integer :: i
  if (.not. (phs%p_defined .and. phs%q_defined)) return
  call phs%select_channel ()
  associate (n => phs%config%n_out, m => phs%m)
    allocate(q(n))
    m(1) = invariant_mass (sum (phs%p))
    q(1) = vector4_at_rest (m(1))
    q(n) = phs%q(n)
    do i = 2, n - 1
      q(i) = q(i) + sum (phs%q(i:n))
      m(i) = invariant_mass (q(i))
    end do
    call phs%invert_intermediates ()
    do i = 2, n
      L = inverse (boost (q(i - 1), m(i - 1)))
      p = L * phs%q(i - 1)
      phi = azimuthal_angle (p); cos_theta = polar_angle_ct (p)
      phs%r(n - 5 + 2 * i, 1) = (cos_theta + 1.) / 2.
      phs%r(n - 4 + 2 * i, 1) = phi / twopi
    end do
  end associate
  phs%r_defined = .true.
end subroutine phs_rambo_inverse

```

19.4.3 Unit tests

Test module, followed by the corresponding implementation module.

<phs_rambo_ut.f90>≡

<File header>

```
module phs_rambo_ut
```

```

    use unit_tests
    use phs_rambo_ut

    <Standard module head>

    <PHS rambo: public test>

contains

    <PHS rambo: test driver>

end module phs_rambo_ut
<phs_rambo_ut.f90>≡
    <File header>

module phs_rambo_ut

    <Use kinds>
    <Use strings>
    use flavors
    use lorentz
    use model_data
    use process_constants
    use phs_base

    use phs_rambo

    use phs_base_ut, only: init_test_process_data, init_test_decay_data

    <Standard module head>

    <PHS rambo: test declarations>

contains

    <PHS rambo: tests>

end module phs_rambo_ut
API: driver for the unit tests below.
<PHS rambo: public test>≡
    public :: phs_rambo_test
<PHS rambo: test driver>≡
    subroutine phs_rambo_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS rambo: execute tests>
    end subroutine phs_rambo_test

```

Phase-space configuration data

Construct and display a test phase-space configuration object. Also check the azimuthal dependence flag.


```

<PHS rambo: execute tests>≡
  call test (phs_rambo_1, "phs_rambo_1", &
    "phase-space configuration", &
    u, results)
<PHS rambo: test declarations>≡
  public :: phs_rambo_1
<PHS rambo: tests>≡
  subroutine phs_rambo_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    class(phs_config_t), allocatable :: phs_data
    real(default) :: sqrts

    write (u, "(A)")  "* Test output: phs_rambo_1"
    write (u, "(A)")  "*   Purpose: initialize and display &
      &phase-space configuration data"
    write (u, "(A)")

    call model%init_test ()

    write (u, "(A)")  "* Initialize a process and a matching &
      &phase-space configuration"
    write (u, "(A)")

    call init_test_process_data (var_str ("phs_rambo_1"), process_data)

    allocate (phs_rambo_config_t :: phs_data)
    call phs_data%init (process_data, model)

    sqrts = 1000._default
    call phs_data%configure (sqrts)

    call phs_data%write (u)

    call phs_data%final ()
    call model%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: phs_rambo_1"

  end subroutine phs_rambo_1

```

Phase space evaluation

Compute kinematics for given parameters, also invert the calculation.

```

<PHS rambo: execute tests>+≡
  call test (phs_rambo_2, "phs_rambo_2", &
    "phase-space evaluation", &
    u, results)
<PHS rambo: test declarations>+≡
  public :: phs_rambo_2

```

<PHS rambo: tests>+≡

```

subroutine phs_rambo_2 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(flavor_t) :: flv
  type(process_constants_t) :: process_data
  real(default) :: sqrts, E
  class(phs_config_t), allocatable, target :: phs_data
  class(phs_t), pointer :: phs => null ()
  type(vector4_t), dimension(2) :: p, q

  write (u, "(A)")  "* Test output: phs_rambo_2"
  write (u, "(A)")  "* Purpose: test simple two-channel phase space"
  write (u, "(A)")

  call model%init_test ()
  call flv%init (25, model)

  write (u, "(A)")  "* Initialize a process and a matching &
    &phase-space configuration"
  write (u, "(A)")

  call init_test_process_data (var_str ("phs_rambo_2"), process_data)

  allocate (phs_rambo_config_t :: phs_data)
  call phs_data%init (process_data, model)

  sqrts = 1000._default
  call phs_data%configure (sqrts)

  call phs_data%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Initialize the phase-space instance"
  write (u, "(A)")

  call phs_data%allocate_instance (phs)
  call phs%init (phs_data)

  call phs%write (u, verbose=.true.)

  write (u, "(A)")
  write (u, "(A)")  "* Set incoming momenta"
  write (u, "(A)")

  E = sqrts / 2
  p(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
  p(2) = vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

  call phs%set_incoming_momenta (p)
  call phs%compute_flux ()
  call phs%write (u)

  write (u, "(A)")

```

```

write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_rambo_2"

end subroutine phs_rambo_2

```

Phase space for non-c.m. system

Compute kinematics for given parameters, also invert the calculation. Since this will involve cancellations, we call `pacify` to eliminate numerical noise.

```

<PHS rambo: execute tests>+≡
  call test (phs_rambo_3, "phs_rambo_3", &
    "phase-space evaluation in lab frame", &
    u, results)

<PHS rambo: test declarations>+≡
  public :: phs_rambo_3

<PHS rambo: tests>+≡
  subroutine phs_rambo_3 (u)
    integer, intent(in) :: u

```

```

type(model_data_t), target :: model
type(flavor_t) :: flv
type(process_constants_t) :: process_data
real(default) :: sqrts, E
class(phs_config_t), allocatable, target :: phs_data
class(phs_t), pointer :: phs => null ()
type(vector4_t), dimension(2) :: p, q
type(lorentz_transformation_t) :: lt

write (u, "(A)")  "* Test output: phs_rambo_3"
write (u, "(A)")  "* Purpose: phase-space evaluation in lab frame"
write (u, "(A)")

call model%init_test ()
call flv%init (25, model)

write (u, "(A)")  "* Initialize a process and a matching &
                  &phase-space configuration"
write (u, "(A)")

call init_test_process_data (var_str ("phs_rambo_3"), process_data)

allocate (phs_rambo_config_t :: phs_data)
call phs_data%init (process_data, model)

sqrts = 1000._default
call phs_data%configure (sqrts, lab_is_cm=.false., sqrts_fixed=.false.)

call phs_data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta in lab system"
write (u, "(A)")

lt = boost (0.1_default, 1) * boost (0.3_default, 3)

E = sqrts / 2
p(1) = lt * vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = lt * vector4_moving (E, -sqrt (E**2 - flv%get_mass ()**2), 3)

call vector4_write (p(1), u)
call vector4_write (p(2), u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &

```

```

        &for x = 0.5, 0.125"
write (u, "(A)")

call phs%set_incoming_momenta (p)
call phs%compute_flux ()

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call pacify (phs)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract outgoing momenta in lab system"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
call vector4_write (q(1), u)
call vector4_write (q(2), u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call pacify (phs)
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_rambo_3"

end subroutine phs_rambo_3

```

Decay Phase space evaluation

Compute kinematics for given parameters, also invert the calculation. This time, implement a decay process.

```

<PHS rambo: execute tests>+≡
    call test (phs_rambo_4, "phs_rambo_4", &
        "decay phase-space evaluation", &
        u, results)

<PHS rambo: test declarations>+≡
    public :: phs_rambo_4

<PHS rambo: tests>+≡
    subroutine phs_rambo_4 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(process_constants_t) :: process_data
        class(phs_config_t), allocatable, target :: phs_data
        class(phs_t), pointer :: phs => null ()
        type(vector4_t), dimension(1) :: p
        type(vector4_t), dimension(2) :: q

        write (u, "(A)")  "* Test output: phs_rambo_4"
        write (u, "(A)")  "* Purpose: test simple two-channel phase space"
        write (u, "(A)")

        call model%init_test ()

        call model%set_par (var_str ("ff"), 0.4_default)
        call model%set_par (var_str ("mf"), &
            model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))
        call flv%init (25, model)

        write (u, "(A)")  "* Initialize a decay and a matching &
            &phase-space configuration"
        write (u, "(A)")

        call init_test_decay_data (var_str ("phs_rambo_4"), process_data)

        allocate (phs_rambo_config_t :: phs_data)
        call phs_data%init (process_data, model)

        call phs_data%configure (flv%get_mass ())

        call phs_data%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Initialize the phase-space instance"
        write (u, "(A)")

        call phs_data%allocate_instance (phs)
        call phs%init (phs_data)

        call phs%write (u, verbose=.true.)

        write (u, "(A)")
        write (u, "(A)")  "* Set incoming momenta"
        write (u, "(A)")

```

```

p(1) = vector4_at_rest (flv%get_mass ())

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
    &for x = 0.5, 0.125"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.5_default, 0.125_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
deallocate (phs)
call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs_data%configure (flv%get_mass ())

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_rambo_4"

end subroutine phs_rambo_4

```

19.5 Resonance Handler

For various purposes (e.g., shower histories), we should extract the set of resonances and resonant channels from a phase-space tree set. A few methods do kinematics calculations specifically for those resonance data.

```
<resonances.f90>≡  
  <File header>  
  
  module resonances  
  
    <Use kinds>  
    <Use strings>  
    <Use debug>  
    use string_utils, only: str  
    use format_utils, only: write_indent  
    use io_units  
    use diagnostics  
    use lorentz  
    use constants, only: one  
    use model_data, only: model_data_t  
    use flavors, only: flavor_t  
  
    <Standard module head>  
  
    <Resonances: public>  
  
    <Resonances: parameters>  
  
    <Resonances: types>  
  
    contains  
  
    <Resonances: procedures>  
  
  end module resonances
```

19.5.1 Decay products (contributors)

This stores the indices of the particles that contribute to a resonance, i.e., the decay products.

```
<Resonances: public>≡  
  public :: resonance_contributors_t  
  
<Resonances: types>≡  
  type :: resonance_contributors_t  
    integer, dimension(:), allocatable :: c  
    contains  
    <Resonances: resonance contributors: TBP>  
  end type resonance_contributors_t
```

Equality (comparison)

```
<Resonances: resonance contributors: TBP>≡  
  procedure, private :: resonance_contributors_equal
```



```

generic :: operator(==) => resonance_contributors_equal
<Resonances: procedures>≡
  elemental function resonance_contributors_equal (c1, c2) result (equal)
    logical :: equal
    class(resonance_contributors_t), intent(in) :: c1, c2
    equal = allocated (c1%c) .and. allocated (c2%c)
    if (equal) equal = size (c1%c) == size (c2%c)
    if (equal) equal = all (c1%c == c2%c)
  end function resonance_contributors_equal

```

Assignment

```

<Resonances: resonance_contributors: TBP>+≡
  procedure, private :: resonance_contributors_assign
  generic :: assignment(=) => resonance_contributors_assign

<Resonances: procedures>+≡
  pure subroutine resonance_contributors_assign (contributors_out, contributors_in)
    class(resonance_contributors_t), intent(inout) :: contributors_out
    class(resonance_contributors_t), intent(in) :: contributors_in
    if (allocated (contributors_out%c)) deallocate (contributors_out%c)
    if (allocated (contributors_in%c)) then
      allocate (contributors_out%c (size (contributors_in%c)))
      contributors_out%c = contributors_in%c
    end if
  end subroutine resonance_contributors_assign

```

19.5.2 Resonance info object

This data structure augments the set of resonance contributors by a flavor object, such that we can perform calculations that take into account the particle properties, including mass and width.

Avoiding nameclash with similar but different `resonance_t` of `phs_base`:

```

<Resonances: public>+≡
  public :: resonance_info_t

<Resonances: types>+≡
  type :: resonance_info_t
    type(flavor_t) :: flavor
    type(resonance_contributors_t) :: contributors
  contains
    <Resonances: resonance_info: TBP>
  end type resonance_info_t

<Resonances: resonance_info: TBP>≡
  procedure :: copy => resonance_info_copy

<Resonances: procedures>+≡
  subroutine resonance_info_copy (resonance_in, resonance_out)
    class(resonance_info_t), intent(in) :: resonance_in
    type(resonance_info_t), intent(out) :: resonance_out
    resonance_out%flavor = resonance_in%flavor
    if (allocated (resonance_in%contributors%c)) then

```

```

        associate (c => resonance_in%contributors%c)
        allocate (resonance_out%contributors%c (size (c)))
        resonance_out%contributors%c = c
    end associate
end if
end subroutine resonance_info_copy

```

<Resonances: resonance info: TBP>+≡

```

    procedure :: write => resonance_info_write

```

<Resonances: procedures>+≡

```

    subroutine resonance_info_write (resonance, unit, verbose)
    class(resonance_info_t), intent(in) :: resonance
    integer, optional, intent(in) :: unit
    logical, optional, intent(in) :: verbose
    integer :: u, i
    logical :: verb
    u = given_output_unit (unit); if (u < 0) return
    verb = .true.; if (present (verbose)) verb = verbose
    if (verb) then
        write (u, '(A)', advance='no') "Resonance contributors: "
    else
        write (u, '(1x)', advance="no")
    end if
    if (allocated (resonance%contributors%c)) then
        do i = 1, size(resonance%contributors%c)
            write (u, '(I0,1X)', advance='no') resonance%contributors%c(i)
        end do
    else if (verb) then
        write (u, "(A)", advance="no") "[not allocated]"
    end if
    if (resonance%flavor%is_defined ()) call resonance%flavor%write (u)
    write (u, '(A)')
end subroutine resonance_info_write

```

Create a resonance-info object. The particle info may be available in term of a flavor object or as a PDG code; in the latter case we have to require a model data object that provides mass and width information.

<Resonances: resonance info: TBP>+≡

```

    procedure, private :: resonance_info_init_pdg
    procedure, private :: resonance_info_init_flv
    generic :: init => resonance_info_init_pdg, resonance_info_init_flv

```

<Resonances: procedures>+≡

```

    subroutine resonance_info_init_pdg (resonance, mom_id, pdg, model, n_out)
    class(resonance_info_t), intent(out) :: resonance
    integer, intent(in) :: mom_id
    integer, intent(in) :: pdg, n_out
    class(model_data_t), intent(in), target :: model
    type(flavor_t) :: flv
    if (debug_on) call msg_debug (D_PHASESPACE, "resonance_info_init_pdg")
    call flv%init (pdg, model)
    call resonance%init (mom_id, flv, n_out)
end subroutine resonance_info_init_pdg

```

```

subroutine resonance_info_init_flv (resonance, mom_id, flv, n_out)
  class(resonance_info_t), intent(out) :: resonance
  integer, intent(in) :: mom_id
  type(flavor_t), intent(in) :: flv
  integer, intent(in) :: n_out
  integer :: i
  logical, dimension(n_out) :: contrib
  integer, dimension(n_out) :: tmp
  if (debug_on) call msg_debug (D_PHASESPACE, "resonance_info_init_flv")
  resonance%flavor = flv
  do i = 1, n_out
    tmp(i) = i
  end do
  contrib = btest (mom_id, tmp - 1)
  allocate (resonance%contributors%c (count (contrib)))
  resonance%contributors%c = pack (tmp, contrib)
end subroutine resonance_info_init_flv

```

```

⟨Resonances: resonance info: TBP⟩+≡
  procedure, private :: resonance_info_equal
  generic :: operator(==) => resonance_info_equal

⟨Resonances: procedures⟩+≡
  elemental function resonance_info_equal (r1, r2) result (equal)
    logical :: equal
    class(resonance_info_t), intent(in) :: r1, r2
    equal = r1%flavor == r2%flavor .and. r1%contributors == r2%contributors
  end function resonance_info_equal

```

With each resonance region we associate a Breit-Wigner function

$$P = \frac{M_{res}^4}{(s - M_{res}^2)^2 + \Gamma_{res}^2 M_{res}^2},$$

where s denotes the invariant mass of the outgoing momenta originating from this resonance. Note that the M_{res}^4 in the nominator makes the mapping a dimensionless quantity.

```

⟨Resonances: resonance info: TBP⟩+≡
  procedure :: mapping => resonance_info_mapping

⟨Resonances: procedures⟩+≡
  function resonance_info_mapping (resonance, s) result (bw)
    real(default) :: bw
    class(resonance_info_t), intent(in) :: resonance
    real(default), intent(in) :: s
    real(default) :: m, gamma
    if (resonance%flavor%is_defined ()) then
      m = resonance%flavor%get_mass ()
      gamma = resonance%flavor%get_width ()
      bw = m**4 / ((s - m**2)**2 + gamma**2 * m**2)
    else
      bw = one
    end if
  end function

```

```
end function resonance_info_mapping
```

Used for building a resonance tree below.

```
<Resonances: resonance info: TBP>+≡
  procedure, private :: get_n_contributors => resonance_info_get_n_contributors
  procedure, private :: contains => resonance_info_contains

<Resonances: procedures>+≡
  elemental function resonance_info_get_n_contributors (resonance) result (n)
    class(resonance_info_t), intent(in) :: resonance
    integer :: n
    if (allocated (resonance%contributors%c)) then
      n = size (resonance%contributors%c)
    else
      n = 0
    end if
  end function resonance_info_get_n_contributors

  elemental function resonance_info_contains (resonance, c) result (flag)
    class(resonance_info_t), intent(in) :: resonance
    integer, intent(in) :: c
    logical :: flag
    if (allocated (resonance%contributors%c)) then
      flag = any (resonance%contributors%c == c)
    else
      flag = .false.
    end if
  end function resonance_info_contains
```

19.5.3 Resonance history object

This data structure stores a set of resonances, i.e., the resonances that appear in a particular Feynman graph or, in the context of phase space, phase space diagram.

```
<Resonances: public>+≡
  public :: resonance_history_t

<Resonances: types>+≡
  type :: resonance_history_t
    type(resonance_info_t), dimension(:), allocatable :: resonances
    integer :: n_resonances = 0
  contains
    <Resonances: resonance history: TBP>
  end type resonance_history_t
```

Clear the resonance history. Assuming that there are no pointer-allocated parts, a straightforward `intent(out)` will do.

```
<Resonances: resonance history: TBP>≡
  procedure :: clear => resonance_history_clear
```

```

<Resonances: procedures>+≡
  subroutine resonance_history_clear (res_hist)
    class(resonance_history_t), intent(out) :: res_hist
  end subroutine resonance_history_clear

<Resonances: resonance history: TBP>+≡
  procedure :: copy => resonance_history_copy

<Resonances: procedures>+≡
  subroutine resonance_history_copy (res_hist_in, res_hist_out)
    class(resonance_history_t), intent(in) :: res_hist_in
    type(resonance_history_t), intent(out) :: res_hist_out
    integer :: i
    res_hist_out%n_resonances = res_hist_in%n_resonances
    allocate (res_hist_out%resonances (size (res_hist_in%resonances)))
    do i = 1, size (res_hist_in%resonances)
      call res_hist_in%resonances(i)%copy (res_hist_out%resonances(i))
    end do
  end subroutine resonance_history_copy

<Resonances: resonance history: TBP>+≡
  procedure :: write => resonance_history_write

<Resonances: procedures>+≡
  subroutine resonance_history_write (res_hist, unit, verbose, indent)
    class(resonance_history_t), intent(in) :: res_hist
    integer, optional, intent(in) :: unit
    logical, optional, intent(in) :: verbose
    integer, optional, intent(in) :: indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write(u, '(A,I0,A)') "Resonance history with ", &
      res_hist%n_resonances, " resonances:"
    do i = 1, res_hist%n_resonances
      call write_indent (u, indent)
      write (u, "(2x)", advance="no")
      call res_hist%resonances(i)%write (u, verbose)
    end do
  end subroutine resonance_history_write

```

Assignment. Indirectly calls type-bound assignment for the contributors.

Strictly speaking, this is redundant. But NAGfor 6.208 intrinsic assignment crashes under certain conditions.

```

<Resonances: resonance history: TBP>+≡
  procedure, private :: resonance_history_assign
  generic :: assignment(=) => resonance_history_assign

<Resonances: procedures>+≡
  subroutine resonance_history_assign (res_hist_out, res_hist_in)
    class(resonance_history_t), intent(out) :: res_hist_out
    class(resonance_history_t), intent(in) :: res_hist_in
    if (allocated (res_hist_in%resonances)) then
      res_hist_out%resonances = res_hist_in%resonances
    end if
  end subroutine resonance_history_assign

```

```

        res_hist_out%n_resonances = res_hist_in%n_resonances
    end if
end subroutine resonance_history_assign

```

Equality. If this turns out to slow down the program, we should change the implementation or use hash codes.

```

<Resonances: resonance history: TBP>+≡
    procedure, private :: resonance_history_equal
    generic :: operator(==) => resonance_history_equal

<Resonances: procedures>+≡
    elemental function resonance_history_equal (rh1, rh2) result (equal)
        logical :: equal
        class(resonance_history_t), intent(in) :: rh1, rh2
        integer :: i
        equal = .false.
        if (rh1%n_resonances == rh2%n_resonances) then
            do i = 1, rh1%n_resonances
                if (.not. rh1%resonances(i) == rh2%resonances(i)) then
                    return
                end if
            end do
            equal = .true.
        end if
    end function resonance_history_equal

```

Check if a resonance history is a strict superset of another one. This is true if the first one is nonempty and the second one is empty. Otherwise, we check if each entry of the second argument appears in the first one.

```

<Resonances: resonance history: TBP>+≡
    procedure, private :: resonance_history_contains
    generic :: operator(.contains.) => resonance_history_contains

<Resonances: procedures>+≡
    elemental function resonance_history_contains (rh1, rh2) result (flag)
        logical :: flag
        class(resonance_history_t), intent(in) :: rh1, rh2
        integer :: i
        if (rh1%n_resonances > rh2%n_resonances) then
            flag = .true.
            do i = 1, rh2%n_resonances
                flag = flag .and. any (rh1%resonances == rh2%resonances(i))
            end do
        else
            flag = .false.
        end if
    end function resonance_history_contains

```

Number of entries for dynamically extending the resonance-info array.

```

<Resonances: parameters>≡
    integer, parameter :: n_max_resonances = 10

<Resonances: resonance history: TBP>+≡
    procedure :: add_resonance => resonance_history_add_resonance

```

<Resonances: procedures>+≡

```

subroutine resonance_history_add_resonance (res_hist, resonance)
  class(resonance_history_t), intent(inout) :: res_hist
  type(resonance_info_t), intent(in) :: resonance
  type(resonance_info_t), dimension(:), allocatable :: tmp
  integer :: n, i
  if (debug_on) call msg_debug (D_PHASESPACE, "resonance_history_add_resonance")
  if (.not. allocated (res_hist%resonances)) then
    n = 0
    allocate (res_hist%resonances (1))
  else
    n = res_hist%n_resonances
    allocate (tmp (n))
    do i = 1, n
      call res_hist%resonances(i)%copy (tmp(i))
    end do
    deallocate (res_hist%resonances)
    allocate (res_hist%resonances (n+1))
    do i = 1, n
      call tmp(i)%copy (res_hist%resonances(i))
    end do
    deallocate (tmp)
  end if
  call resonance%copy (res_hist%resonances(n+1))
  res_hist%n_resonances = n + 1
  if (debug_on) call msg_debug &
    (D_PHASESPACE, "res_hist%n_resonances", res_hist%n_resonances)
end subroutine resonance_history_add_resonance

```

<Resonances: resonance history: TBP>+≡

```

procedure :: remove_resonance => resonance_history_remove_resonance

```

<Resonances: procedures>+≡

```

subroutine resonance_history_remove_resonance (res_hist, i_res)
  class(resonance_history_t), intent(inout) :: res_hist
  integer, intent(in) :: i_res
  type(resonance_info_t), dimension(:), allocatable :: tmp_1, tmp_2
  integer :: i, j, n
  n = res_hist%n_resonances
  res_hist%n_resonances = n - 1
  if (res_hist%n_resonances == 0) then
    deallocate (res_hist%resonances)
  else
    if (i_res > 1) allocate (tmp_1(1:i_res-1))
    if (i_res < n) allocate (tmp_2(i_res+1:n))
    if (allocated (tmp_1)) then
      do i = 1, i_res - 1
        call res_hist%resonances(i)%copy (tmp_1(i))
      end do
    end if
    if (allocated (tmp_2)) then
      do i = i_res + 1, n
        call res_hist%resonances(i)%copy (tmp_2(i))
      end do
    end if
  end if

```

```

end if
deallocate (res_hist%resonances)
allocate (res_hist%resonances (res_hist%n_resonances))
j = 1
if (allocated (tmp_1)) then
  do i = 1, i_res - 1
    call tmp_1(i)%copy (res_hist%resonances(j))
    j = j + 1
  end do
  deallocate (tmp_1)
end if
if (allocated (tmp_2)) then
  do i = i_res + 1, n
    call tmp_2(i)%copy (res_hist%resonances(j))
    j = j + 1
  end do
  deallocate (tmp_2)
end if
end if
end subroutine resonance_history_remove_resonance

```

<Resonances: resonance history: TBP>+≡

```

procedure :: add_offset => resonance_history_add_offset

```

<Resonances: procedures>+≡

```

subroutine resonance_history_add_offset (res_hist, n)
  class(resonance_history_t), intent(inout) :: res_hist
  integer, intent(in) :: n
  integer :: i_res
  do i_res = 1, res_hist%n_resonances
    associate (contributors => res_hist%resonances(i_res)%contributors%c)
      contributors = contributors + n
    end associate
  end do
end subroutine resonance_history_add_offset

```

<Resonances: resonance history: TBP>+≡

```

procedure :: contains_leg => resonance_history_contains_leg

```

<Resonances: procedures>+≡

```

function resonance_history_contains_leg (res_hist, i_leg) result (val)
  logical :: val
  class(resonance_history_t), intent(in) :: res_hist
  integer, intent(in) :: i_leg
  integer :: i_res
  val = .false.
  do i_res = 1, res_hist%n_resonances
    if (any (res_hist%resonances(i_res)%contributors%c == i_leg)) then
      val = .true.
      exit
    end if
  end do
end function resonance_history_contains_leg

```



```

⟨Resonances: resonance history: TBP⟩+≡
  procedure :: mapping => resonance_history_mapping

⟨Resonances: procedures⟩+≡
  function resonance_history_mapping (res_hist, p, i_gluon) result (p_map)
    real(default) :: p_map
    class(resonance_history_t), intent(in) :: res_hist
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in), optional :: i_gluon
    integer :: i_res
    real(default) :: s
    p_map = one
    do i_res = 1, res_hist%n_resonances
      associate (res => res_hist%resonances(i_res))
        s = compute_resonance_mass (p, res%contributors%c, i_gluon)**2
        p_map = p_map * res%mapping (s)
      end associate
    end do
  end function resonance_history_mapping

```

This predicate is true if all resonances in the history have exactly n contributors. For instance, if $n = 2$, all resonances have a two-particle decay.

```

⟨Resonances: resonance history: TBP⟩+≡
  procedure :: only_has_n_contributors => resonance_history_only_has_n_contributors

⟨Resonances: procedures⟩+≡
  function resonance_history_only_has_n_contributors (res_hist, n) result (value)
    logical :: value
    class(resonance_history_t), intent(in) :: res_hist
    integer, intent(in) :: n
    integer :: i_res
    value = .true.
    do i_res = 1, res_hist%n_resonances
      associate (res => res_hist%resonances(i_res))
        value = value .and. size (res%contributors%c) == n
      end associate
    end do
  end function resonance_history_only_has_n_contributors

```

```

⟨Resonances: resonance history: TBP⟩+≡
  procedure :: has_flavor => resonance_history_has_flavor

⟨Resonances: procedures⟩+≡
  function resonance_history_has_flavor (res_hist, flv) result (has_flv)
    logical :: has_flv
    class(resonance_history_t), intent(in) :: res_hist
    type(flavor_t), intent(in) :: flv
    integer :: i
    has_flv = .false.
    do i = 1, res_hist%n_resonances
      has_flv = has_flv .or. res_hist%resonances(i)%flavor == flv
    end do
  end function resonance_history_has_flavor

```

19.5.4 Kinematics

Evaluate the distance from a resonance. The distance is given by $|p^2 - m^2|/(m\Gamma)$. For $\Gamma \ll m$, this is the relative distance from the resonance peak in units of the half-width.

```

⟨Resonances: resonance info: TBP⟩+≡
  procedure :: evaluate_distance => resonance_info_evaluate_distance

⟨Resonances: procedures⟩+≡
  subroutine resonance_info_evaluate_distance (res_info, p, dist)
    class(resonance_info_t), intent(in) :: res_info
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(out) :: dist
    real(default) :: m, w
    type(vector4_t) :: q
    m = res_info%flavor%get_mass ()
    w = res_info%flavor%get_width ()
    q = sum (p(res_info%contributors%c))
    dist = abs (q**2 - m**2) / (m * w)
  end subroutine resonance_info_evaluate_distance

```

Evaluate the array of distances from a resonance history. We assume that the array has been allocated with correct size, namely the number of resonances in this history.

```

⟨Resonances: resonance history: TBP⟩+≡
  procedure :: evaluate_distances => resonance_history_evaluate_distances

⟨Resonances: procedures⟩+≡
  subroutine resonance_history_evaluate_distances (res_hist, p, dist)
    class(resonance_history_t), intent(in) :: res_hist
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), dimension(:), intent(out) :: dist
    integer :: i
    do i = 1, res_hist%n_resonances
      call res_hist%resonances(i)%evaluate_distance (p, dist(i))
    end do
  end subroutine resonance_history_evaluate_distances

```

Use the distance to determine a Gaussian turnoff factor for a resonance. The factor is given by a Gaussian function e^{-d^2/σ^2} , where σ is the **gw** parameter multiplied by the resonance width, and d is the distance (see above). So, for $d = \sigma$, the factor is 0.37, and for $d = 2\sigma$ we get 0.018.

If the **gw** factor is less or equal to zero, return 1.

```

⟨Resonances: resonance info: TBP⟩+≡
  procedure :: evaluate_gaussian => resonance_info_evaluate_gaussian

⟨Resonances: procedures⟩+≡
  function resonance_info_evaluate_gaussian (res_info, p, gw) result (factor)
    class(resonance_info_t), intent(in) :: res_info
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: gw
    real(default) :: factor
    real(default) :: dist, w
    if (gw > 0) then

```

```

        w = res_info%flavor%get_width ()
        call res_info%evaluate_distance (p, dist)
        factor = exp (- (dist / (gw * w)) **2)
    else
        factor = 1
    end if
end function resonance_info_evaluate_gaussian

```

The Gaussian factor of the history is the product of all factors.

```

<Resonances: resonance history: TBP>+≡
    procedure :: evaluate_gaussian => resonance_history_evaluate_gaussian

<Resonances: procedures>+≡
    function resonance_history_evaluate_gaussian (res_hist, p, gw) result (factor)
        class(resonance_history_t), intent(in) :: res_hist
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: gw
        real(default), dimension(:), allocatable :: dist
        real(default) :: factor
        integer :: i
        factor = 1
        do i = 1, res_hist%n_resonances
            factor = factor * res_hist%resonances(i)%evaluate_gaussian (p, gw)
        end do
    end function resonance_history_evaluate_gaussian

```

Use the distances to determine whether the resonance history can qualify as on-shell. The criterion is whether the distance is greater than the number of width values as given by `on_shell_limit`.

```

<Resonances: resonance info: TBP>+≡
    procedure :: is_on_shell => resonance_info_is_on_shell

<Resonances: procedures>+≡
    function resonance_info_is_on_shell (res_info, p, on_shell_limit) &
        result (flag)
        class(resonance_info_t), intent(in) :: res_info
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: on_shell_limit
        logical :: flag
        real(default) :: dist
        call res_info%evaluate_distance (p, dist)
        flag = dist < on_shell_limit
    end function resonance_info_is_on_shell

```

```

<Resonances: resonance history: TBP>+≡
    procedure :: is_on_shell => resonance_history_is_on_shell

<Resonances: procedures>+≡
    function resonance_history_is_on_shell (res_hist, p, on_shell_limit) &
        result (flag)
        class(resonance_history_t), intent(in) :: res_hist
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), intent(in) :: on_shell_limit

```

```

logical :: flag
integer :: i
flag = .true.
do i = 1, res_hist%n_resonances
    flag = flag .and. res_hist%resonances(i)%is_on_shell (p, on_shell_limit)
end do
end function resonance_history_is_on_shell

```

19.5.5 OMega restriction strings

One application of the resonance module is creating restriction strings that can be fed into process definitions with the OMega generator. Since OMega counts the incoming particles first, we have to supply `n_in` as an offset.

```

⟨Resonances: resonance info: TBP⟩+≡
    procedure :: as_omega_string => resonance_info_as_omega_string

⟨Resonances: resonance history: TBP⟩+≡
    procedure :: as_omega_string => resonance_history_as_omega_string

⟨Resonances: procedures⟩+≡
    function resonance_info_as_omega_string (res_info, n_in) result (string)
        class(resonance_info_t), intent(in) :: res_info
        integer, intent(in) :: n_in
        type(string_t) :: string
        integer :: i
        string = ""
        if (allocated (res_info%contributors%c)) then
            do i = 1, size (res_info%contributors%c)
                if (i > 1) string = string // "+"
                string = string // str (res_info%contributors%c(i) + n_in)
            end do
            string = string // "~" // res_info%flavor%get_name ()
        end if
    end function resonance_info_as_omega_string

    function resonance_history_as_omega_string (res_hist, n_in) result (string)
        class(resonance_history_t), intent(in) :: res_hist
        integer, intent(in) :: n_in
        type(string_t) :: string
        integer :: i
        string = ""
        do i = 1, res_hist%n_resonances
            if (i > 1) string = string // " && "
            string = string // res_hist%resonances(i)%as_omega_string (n_in)
        end do
    end function resonance_history_as_omega_string

```

19.5.6 Resonance history as tree

If we want to organize the resonances and their decay products, it can be useful to have them explicitly as a tree structure. We implement this in the tradi-

tional event-record form with the resonances sorted by decreasing number of contributors, and their decay products added as an extra array.

```

<Resonances: public>+≡
    public :: resonance_tree_t

<Resonances: types>+≡
    type :: resonance_branch_t
        integer :: i = 0
        type(flavor_t) :: flv
        integer, dimension(:), allocatable :: r_child
        integer, dimension(:), allocatable :: o_child
    end type resonance_branch_t

    type :: resonance_tree_t
        private
        integer :: n = 0
        type(resonance_branch_t), dimension(:), allocatable :: branch
    contains
        <Resonances: resonance tree: TBP>
    end type resonance_tree_t

<Resonances: resonance tree: TBP>≡
    procedure :: write => resonance_tree_write

<Resonances: procedures>+≡
    subroutine resonance_tree_write (tree, unit, indent)
        class(resonance_tree_t), intent(in) :: tree
        integer, intent(in), optional :: unit, indent
        integer :: u, b, c
        u = given_output_unit (unit)
        call write_indent (u, indent)
        write (u, "(A)", advance="no") "Resonance tree:"
        if (tree%n > 0) then
            write (u, *)
            do b = 1, tree%n
                call write_indent (u, indent)
                write (u, "(2x,'r',I0,':',1x)", advance="no") b
                associate (branch => tree%branch(b))
                    call branch%flv%write (u)
                    write (u, "(1x,'=>')", advance="no")
                    if (allocated (branch%r_child)) then
                        do c = 1, size (branch%r_child)
                            write (u, "(1x,'r',I0)", advance="no") branch%r_child(c)
                        end do
                    end if
                    if (allocated (branch%o_child)) then
                        do c = 1, size (branch%o_child)
                            write (u, "(1x,I0)", advance="no") branch%o_child(c)
                        end do
                    end if
                    write (u, *)
                end associate
            end do
        end if
    end subroutine resonance_tree_write

```

```

    else
        write (u, "(1x,A)" "[empty]"
    end if
end subroutine resonance_tree_write

```

Contents.

```

<Resonances: resonance tree: TBP>+≡
    procedure :: get_n_resonances => resonance_tree_get_n_resonances
    procedure :: get_flv => resonance_tree_get_flv

<Resonances: procedures>+≡
    function resonance_tree_get_n_resonances (tree) result (n)
        class(resonance_tree_t), intent(in) :: tree
        integer :: n
        n = tree%n
    end function resonance_tree_get_n_resonances

    function resonance_tree_get_flv (tree, i) result (flv)
        class(resonance_tree_t), intent(in) :: tree
        integer, intent(in) :: i
        type(flavor_t) :: flv
        flv = tree%branch(i)%flv
    end function resonance_tree_get_flv

```

Return the shifted indices of the resonance children for branch *i*. For a child which is itself a resonance, add `offset_r` to the index value. For the others, add `offset_o`. Combine both in a single array.

```

<Resonances: resonance tree: TBP>+≡
    procedure :: get_children => resonance_tree_get_children

<Resonances: procedures>+≡
    function resonance_tree_get_children (tree, i, offset_r, offset_o) &
        result (child)
        class(resonance_tree_t), intent(in) :: tree
        integer, intent(in) :: i, offset_r, offset_o
        integer, dimension(:), allocatable :: child
        integer :: nr, no
        associate (branch => tree%branch(i))
            nr = size (branch%r_child)
            no = size (branch%o_child)
            allocate (child (nr + no))
            child(1:nr) = branch%r_child + offset_r
            child(nr+1:nr+no) = branch%o_child + offset_o
        end associate
    end function resonance_tree_get_children

```

Transform a resonance history into a resonance tree. Algorithm:

1. Determine a mapping of the resonance array, such that in the new array the resonances are ordered by decreasing number of contributors.
2. Copy the flavor entries to the mapped array.

3. Scan all resonances and, for each one, find a resonance that is its parent. Since the resonances are ordered, later matches overwrite earlier ones. The last match is the correct one. Then scan again and, for each resonance, collect the resonances that have it as parent. This is the set of child resonances.
4. Analogously, scan all outgoing particles that appear in any of the contributors list. Determine their immediate parent as above, and set the child outgoing parents for the resonances, as above.

```

<Resonances: resonance history: TBP>+≡
  procedure :: to_tree => resonance_history_to_tree

<Resonances: procedures>+≡
  subroutine resonance_history_to_tree (res_hist, tree)
    class(resonance_history_t), intent(in) :: res_hist
    type(resonance_tree_t), intent(out) :: tree
    integer :: nr
    integer, dimension(:), allocatable :: r_branch, r_source

    nr = res_hist%n_resonances
    tree%n = nr
    allocate (tree%branch (tree%n), r_branch (tree%n), r_source (tree%n))
    if (tree%n > 0) then
      call find_branch_ordering ()
      call set_flavors ()
      call set_child_resonances ()
      call set_child_outgoing ()
    end if

contains

    subroutine find_branch_ordering ()
      integer, dimension(:), allocatable :: nc_array
      integer :: r, ir, nc
      allocate (nc_array (tree%n))
      nc_array(:) = res_hist%resonances%get_n_contributors ()
      ir = 0
      do nc = maxval (nc_array), minval (nc_array), -1
        do r = 1, nr
          if (nc_array(r) == nc) then
            ir = ir + 1
            r_branch(r) = ir
            r_source(ir) = r
          end if
        end do
      end do
    end subroutine find_branch_ordering

    subroutine set_flavors ()
      integer :: r
      do r = 1, nr
        tree%branch(r_branch(r))%flv = res_hist%resonances(r)%flavor
      end do
    end subroutine set_flavors

```

```

subroutine set_child_resonances ()
  integer, dimension(:), allocatable :: r_child, r_parent
  integer :: r, ir, pr
  allocate (r_parent (nr), source = 0)
  SCAN_RES: do r = 1, nr
    associate (this_res => res_hist%resonances(r))
      SCAN_PARENT: do ir = 1, nr
        pr = r_source(ir)
        if (pr == r) cycle SCAN_PARENT
        if (all (res_hist%resonances(pr)%contains &
          (this_res%contributors%c))) then
          r_parent (r) = pr
        end if
      end do SCAN_PARENT
    end associate
  end do SCAN_RES
  allocate (r_child (nr), source = [(r, r = 1, nr)])
  do r = 1, nr
    ir = r_branch(r)
    tree%branch(ir)%r_child = r_branch (pack (r_child, r_parent == r))
  end do
end subroutine set_child_resonances

subroutine set_child_outgoing ()
  integer, dimension(:), allocatable :: o_child, o_parent
  integer :: o_max, r, o, ir
  o_max = 0
  do r = 1, nr
    associate (this_res => res_hist%resonances(r))
      o_max = max (o_max, maxval (this_res%contributors%c))
    end associate
  end do
  allocate (o_parent (o_max), source=0)
  SCAN_OUT: do o = 1, o_max
    SCAN_PARENT: do ir = 1, nr
      r = r_source(ir)
      associate (this_res => res_hist%resonances(r))
        if (this_res%contains (o)) o_parent(o) = r
      end associate
    end do SCAN_PARENT
  end do SCAN_OUT
  allocate (o_child (o_max), source = [(o, o = 1, o_max)])
  do r = 1, nr
    ir = r_branch(r)
    tree%branch(ir)%o_child = pack (o_child, o_parent == r)
  end do
end subroutine set_child_outgoing

end subroutine resonance_history_to_tree

```


19.5.7 Resonance history set

This is an array of resonance histories. The elements are supposed to be unique. That is, entering a new element is successful only if the element does not already exist.

The current implementation uses a straightforward linear search for comparison. If this should become an issue, we may change the implementation to a hash table. To keep this freedom, the set should be an opaque object. In fact, we expect to use it as a transient data structure. Once the set is complete, we transform it into a contiguous array.

```

<Resonances: public>+≡
    public :: resonance_history_set_t

<Resonances: types>+≡
    type :: index_array_t
        integer, dimension(:), allocatable :: i
    end type index_array_t

    type :: resonance_history_set_t
        private
        logical :: complete = .false.
        integer :: n_filter = 0
        type(resonance_history_t), dimension(:), allocatable :: history
        type(index_array_t), dimension(:), allocatable :: contains_this
        type(resonance_tree_t), dimension(:), allocatable :: tree
        integer :: last = 0
    contains
        <Resonances: resonance history set: TBP>
    end type resonance_history_set_t

```

Display.

The tree-format version of the histories is displayed only upon request.

```

<Resonances: resonance history set: TBP>≡
    procedure :: write => resonance_history_set_write

<Resonances: procedures>+≡
    subroutine resonance_history_set_write (res_set, unit, indent, show_trees)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        logical, intent(in), optional :: show_trees
        logical :: s_trees
        integer :: u, i, j, ind
        u = given_output_unit (unit)
        s_trees = .false.; if (present (show_trees)) s_trees = show_trees
        ind = 0; if (present (indent)) ind = indent
        call write_indent (u, indent)
        write (u, "(A)", advance="no") "Resonance history set:"
        if (res_set%complete) then
            write (u, *)
        else
            write (u, "(1x,A)") "[incomplete]"
        end if
        do i = 1, res_set%last

```

```

write (u, "(1x,I0,1x)", advance="no") i
call res_set%history(i)%write (u, verbose=.false., indent=indent)
if (allocated (res_set%contains_this)) then
  call write_indent (u, indent)
  write (u, "(3x,A)", advance="no") "contained in ("
  do j = 1, size (res_set%contains_this(i)%i)
    if (j>1) write (u, "(',')", advance="no")
    write (u, "(I0)", advance="no") res_set%contains_this(i)%i(j)
  end do
  write (u, "(A)" ) " "
end if
if (s_trees .and. allocated (res_set%tree)) then
  call res_set%tree(i)%write (u, ind + 1)
end if
end do
end subroutine resonance_history_set_write

```

Initialization. The default initial size is 16 elements, to be doubled in size repeatedly as needed.

```

<Resonances: parameters>+≡
  integer, parameter :: resonance_history_set_initial_size = 16

<Resonances: resonance history set: TBP>+≡
  procedure :: init => resonance_history_set_init

<Resonances: procedures>+≡
  subroutine resonance_history_set_init (res_set, n_filter, initial_size)
    class(resonance_history_set_t), intent(out) :: res_set
    integer, intent(in), optional :: n_filter
    integer, intent(in), optional :: initial_size
    if (present (n_filter)) res_set%n_filter = n_filter
    if (present (initial_size)) then
      allocate (res_set%history (initial_size))
    else
      allocate (res_set%history (resonance_history_set_initial_size))
    end if
  end subroutine resonance_history_set_init

```

Enter an entry: append to the array if it does not yet exist, expand as needed. If a `n_filter` value has been provided, enter the resonance only if it fulfils the requirement.

An empty resonance history is entered only if the `trivial` flag is set.

```

<Resonances: resonance history set: TBP>+≡
  procedure :: enter => resonance_history_set_enter

<Resonances: procedures>+≡
  subroutine resonance_history_set_enter (res_set, res_history, trivial)
    class(resonance_history_set_t), intent(inout) :: res_set
    type(resonance_history_t), intent(in) :: res_history
    logical, intent(in), optional :: trivial
    integer :: i, new
    if (res_history%n_resonances == 0) then
      if (present (trivial)) then
        if (.not. trivial) return

```

```

        else
            return
        end if
    end if
    if (res_set%n_filter > 0) then
        if (.not. res_history%only_has_n_contributors (res_set%n_filter)) return
    end if
    do i = 1, res_set%last
        if (res_set%history(i) == res_history) return
    end do
    new = res_set%last + 1
    if (new > size (res_set%history)) call res_set%expand ()
    res_set%history(new) = res_history
    res_set%last = new
end subroutine resonance_history_set_enter

```

Freeze the resonance history set: determine the array that determines in which other resonance histories a particular history is contained.

This can only be done once, and once this is done, no further histories can be entered.

```

<Resonances: resonance history set: TBP>+≡
    procedure :: freeze => resonance_history_set_freeze

<Resonances: procedures>+≡
    subroutine resonance_history_set_freeze (res_set)
        class(resonance_history_set_t), intent(inout) :: res_set
        integer :: i, n, c
        logical, dimension(:), allocatable :: contains_this
        integer, dimension(:), allocatable :: index_array
        n = res_set%last
        allocate (contains_this (n))
        allocate (index_array (n), source = [(i, i=1, n)])
        allocate (res_set%contains_this (n))
        do i = 1, n
            contains_this = resonance_history_contains &
                (res_set%history(1:n), res_set%history(i))
            c = count (contains_this)
            allocate (res_set%contains_this(i)%i (c))
            res_set%contains_this(i)%i = pack (index_array, contains_this)
        end do
        allocate (res_set%tree (n))
        do i = 1, n
            call res_set%history(i)%to_tree (res_set%tree(i))
        end do
        res_set%complete = .true.
    end subroutine resonance_history_set_freeze

```

Determine the histories (in form of their indices in the array) that can be considered on-shell, given a set of momenta and a maximum distance. The distance from the resonance is measured in multiples of the resonance width.

Note that the momentum array must only contain the outgoing particles.

If a particular history is on-shell, but there is another history which contains this and also is on-shell, only the latter is retained.

```

<Resonances: resonance history set: TBP>+≡
  procedure :: determine_on_shell_histories &
    => resonance_history_set_determine_on_shell_histories

<Resonances: procedures>+≡
  subroutine resonance_history_set_determine_on_shell_histories &
    (res_set, p, on_shell_limit, index_array)
    class(resonance_history_set_t), intent(in) :: res_set
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: on_shell_limit
    integer, dimension(:), allocatable, intent(out) :: index_array
    integer :: n, i
    integer, dimension(:), allocatable :: i_array
    if (res_set%complete) then
      n = res_set%last
      allocate (i_array (n), source=0)
      do i = 1, n
        if (res_set%history(i)%is_on_shell (p, on_shell_limit)) i_array(i) = i
      end do
      do i = 1, n
        if (any (i_array(res_set%contains_this(i)%i) /= 0)) then
          i_array(i) = 0
        end if
      end do
      allocate (index_array (count (i_array /= 0)))
      index_array(:) = pack (i_array, i_array /= 0)
    end if
  end subroutine resonance_history_set_determine_on_shell_histories

```

For the selected history, compute the Gaussian turnoff factor. The turnoff parameter is `gw`.

```

<Resonances: resonance history set: TBP>+≡
  procedure :: evaluate_gaussian => resonance_history_set_evaluate_gaussian

<Resonances: procedures>+≡
  function resonance_history_set_evaluate_gaussian (res_set, p, gw, i) &
    result (factor)
    class(resonance_history_set_t), intent(in) :: res_set
    type(vector4_t), dimension(:), intent(in) :: p
    real(default), intent(in) :: gw
    integer, intent(in) :: i
    real(default) :: factor
    factor = res_set%history(i)%evaluate_gaussian (p, gw)
  end function resonance_history_set_evaluate_gaussian

```

Return the number of histories. This is zero if there are none, or if `freeze` has not been called yet.

```

<Resonances: resonance history set: TBP>+≡
  procedure :: get_n_history => resonance_history_set_get_n_history

<Resonances: procedures>+≡
  function resonance_history_set_get_n_history (res_set) result (n)
    class(resonance_history_set_t), intent(in) :: res_set
    integer :: n

```

```

    if (res_set%complete) then
        n = res_set%last
    else
        n = 0
    end if
end function resonance_history_set_get_n_history

```

Return a single history.

```

⟨Resonances: resonance history set: TBP⟩+≡
    procedure :: get_history => resonance_history_set_get_history

⟨Resonances: procedures⟩+≡
    function resonance_history_set_get_history (res_set, i) result (res_history)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in) :: i
        type(resonance_history_t) :: res_history
        if (res_set%complete .and. i <= res_set%last) then
            res_history = res_set%history(i)
        end if
    end function resonance_history_set_get_history

```

Conversion to a plain array, sized correctly.

```

⟨Resonances: resonance history set: TBP⟩+≡
    procedure :: to_array => resonance_history_set_to_array

⟨Resonances: procedures⟩+≡
    subroutine resonance_history_set_to_array (res_set, res_history)
        class(resonance_history_set_t), intent(in) :: res_set
        type(resonance_history_t), dimension(:), allocatable, intent(out) :: res_history
        if (res_set%complete) then
            allocate (res_history (res_set%last))
            res_history(:) = res_set%history(1:res_set%last)
        end if
    end subroutine resonance_history_set_to_array

```

Return a selected history in tree form.

```

⟨Resonances: resonance history set: TBP⟩+≡
    procedure :: get_tree => resonance_history_set_get_tree

⟨Resonances: procedures⟩+≡
    subroutine resonance_history_set_get_tree (res_set, i, res_tree)
        class(resonance_history_set_t), intent(in) :: res_set
        integer, intent(in) :: i
        type(resonance_tree_t), intent(out) :: res_tree
        if (res_set%complete) then
            res_tree = res_set%tree(i)
        end if
    end subroutine resonance_history_set_get_tree

```

Expand: double the size of the array. We do not need this in the API.

```

⟨Resonances: resonance history set: TBP⟩+≡
    procedure, private :: expand => resonance_history_set_expand

```

```

<Resonances: procedures>+≡
  subroutine resonance_history_set_expand (res_set)
    class(resonance_history_set_t), intent(inout) :: res_set
    type(resonance_history_t), dimension(:), allocatable :: history_new
    integer :: s
    s = size (res_set%history)
    allocate (history_new (2 * s))
    history_new(1:s) = res_set%history(1:s)
    call move_alloc (history_new, res_set%history)
  end subroutine resonance_history_set_expand

```

19.5.8 Unit tests

Test module, followed by the corresponding implementation module.

```

<resonances_ut.f90>≡
  <File header>

  module resonances_ut
    use unit_tests
    use resonances_util

  <Standard module head>

  <Resonances: public test>

  contains

  <Resonances: test driver>

  end module resonances_ut

<resonances_util.f90>≡
  <File header>

  module resonances_util

  <Use kinds>
  <Use strings>
    use format_defs, only: FMF_12
    use lorentz, only: vector4_t, vector4_at_rest
    use model_data, only: model_data_t
    use flavors, only: flavor_t

    use resonances, only: resonance_history_t

    use resonances

  <Standard module head>

  <Resonances: test declarations>

  contains

```

<Resonances: tests>

end module resonances_util

API: driver for the unit tests below.

<Resonances: public test>≡

public :: resonances_test

<Resonances: test driver>≡

subroutine resonances_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Resonances: execute tests>

end subroutine resonances_test

Basic operations on a resonance history object.

<Resonances: execute tests>≡

call test (resonances_1, "resonances_1", &
"check resonance history setup", &
u, results)

<Resonances: test declarations>≡

public :: resonances_1

<Resonances: tests>≡

subroutine resonances_1 (u)

integer, intent(in) :: u

type(resonance_info_t) :: res_info

type(resonance_history_t) :: res_history

type(model_data_t), target :: model

write (u, "(A)") "* Test output: resonances_1"

write (u, "(A)") "* Purpose: test resonance history setup"

write (u, "(A)")

write (u, "(A)") "* Read model file"

call model%init_sm_test ()

write (u, "(A)")

write (u, "(A)") "* Empty resonance history"

write (u, "(A)")

call res_history%write (u)

write (u, "(A)")

write (u, "(A)") "* Add resonance"

write (u, "(A)")

call res_info%init (3, -24, model, 5)

call res_history%add_resonance (res_info)

call res_history%write (u)

write (u, "(A)")

write (u, "(A)") "* Add another resonance"

```

write (u, "(A)")

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Remove resonance"
write (u, "(A)")

call res_history%remove_resonance (1)
call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_1"

end subroutine resonances_1

```

Basic operations on a resonance history object.

```

<Resonances: execute tests>+≡
call test (resonances_2, "resonances_2", &
  "check O'Mega restriction strings", &
  u, results)

<Resonances: test declarations>+≡
public :: resonances_2

<Resonances: tests>+≡
subroutine resonances_2 (u)
  integer, intent(in) :: u
  type(resonance_info_t) :: res_info
  type(resonance_history_t) :: res_history
  type(model_data_t), target :: model
  type(string_t) :: restrictions

  write (u, "(A)")  "* Test output: resonances_2"
  write (u, "(A)")  "* Purpose: test O'Mega restrictions strings &
    &for resonance history"
  write (u, "(A)")

  write (u, "(A)")  "* Read model file"

  call model%init_sm_test ()

  write (u, "(A)")
  write (u, "(A)")  "* Empty resonance history"
  write (u, "(A)")

  restrictions = res_history%as_omega_string (2)
  write (u, "(A,A,A)")  "restrictions = '", char (restrictions), "'"

```



```

write (u, "(A)")
write (u, "(A)")  "* Add resonance"
write (u, "(A)")

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
restrictions = res_history%as_omega_string (2)
write (u, "(A,A,A)") "restrictions = ', char (restrictions), "'"

write (u, "(A)")
write (u, "(A)")  "* Add another resonance"
write (u, "(A)")

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
restrictions = res_history%as_omega_string (2)
write (u, "(A,A,A)") "restrictions = ', char (restrictions), "'"

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_2"

end subroutine resonances_2

```

Basic operations on a resonance history set.

```

<Resonances: execute tests>+≡
  call test (resonances_3, "resonances_3", &
    "check resonance history set", &
    u, results)

<Resonances: test declarations>+≡
  public :: resonances_3

<Resonances: tests>+≡
  subroutine resonances_3 (u)
    integer, intent(in) :: u
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(resonance_history_t), dimension(:), allocatable :: res_histories
    type(resonance_history_set_t) :: res_set
    type(model_data_t), target :: model
    integer :: i

    write (u, "(A)")  "* Test output: resonances_3"
    write (u, "(A)")  "* Purpose: test resonance history set"
    write (u, "(A)")

    write (u, "(A)")  "* Read model file"

    call model%init_sm_test ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Initialize resonance history set"
write (u, "(A)")

call res_set%init (initial_size = 2)

write (u, "(A)")  "* Add resonance histories, one at a time"
write (u, "(A)")

call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_info%init (7, 25, model, 5)
call res_history%add_resonance (res_info)

```

```

call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

call res_set%freeze ()

write (u, "(A)")
write (u, "(A)")  "* Result"
write (u, "(A)")

call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Queries"
write (u, "(A)")

write (u, "(A,1x,I0)")  "n_history =", res_set%get_n_history ()

write (u, "(A)")
write (u, "(A)")  "History #2:"

res_history = res_set%get_history (2)
call res_history%write (u, indent=1)
call res_history%clear ()

write (u, "(A)")
write (u, "(A)")  "* Result in array form"

call res_set%to_array (res_histories)
do i = 1, size (res_histories)
    write (u, *)
    call res_histories(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Re-initialize resonance history set with filter n=2"
write (u, "(A)")

call res_set%init (n_filter = 2)

write (u, "(A)")  "* Add resonance histories, one at a time"
write (u, "(A)")

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_info%init (7, 23, model, 5)

```

```

call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

write (u, *)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%write (u)
call res_set%enter (res_history)
call res_history%clear ()

call res_set%freeze ()

write (u, "(A)")
write (u, "(A)")  "* Result"
write (u, "(A)")

call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_3"

end subroutine resonances_3

```

Probe momenta for resonance histories

```

<Resonances: execute tests>+≡
  call test (resonances_4, "resonances_4", &
    "resonance history: distance evaluation", &
    u, results)

<Resonances: test declarations>+≡
  public :: resonances_4

<Resonances: tests>+≡
  subroutine resonances_4 (u)
    integer, intent(in) :: u
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(model_data_t), target :: model
    type(flavor_t) :: fw, fz

```

```

real(default) :: mw, mz, ww, wz
type(vector4_t), dimension(3) :: p
real(default), dimension(2) :: dist
real(default) :: gw, factor
integer :: i

write (u, "(A)")  "* Test output: resonances_4"
write (u, "(A)")  "* Purpose: test resonance history evaluation"
write (u, "(A)")

write (u, "(A)")  "* Read model file"

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* W and Z parameters"
write (u, "(A)")

call fw%init (24, model)
call fz%init (23, model)
mw = fw%get_mass ()
ww = fw%get_width ()
mz = fz%get_mass ()
wz = fz%get_width ()

write (u, "(A,1x," // FMF_12 // ")")  "mW =", mw
write (u, "(A,1x," // FMF_12 // ")")  "wW =", ww
write (u, "(A,1x," // FMF_12 // ")")  "mZ =", mz
write (u, "(A,1x," // FMF_12 // ")")  "wZ =", wz

write (u, "(A)")
write (u, "(A)")  "* Gaussian width parameter"
write (u, "(A)")

gw = 2
write (u, "(A,1x," // FMF_12 // ")")  "gw =", gw

write (u, "(A)")
write (u, "(A)")  "* Setup resonance histories"
write (u, "(A)")

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)

call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Setup zero momenta"
write (u, "(A)")

do i = 1, 3

```

```

        call p(i)%write (u)
    end do

    write (u, "(A)")
    write (u, "(A)")    "* Evaluate distances from resonances"
    write (u, "(A)")

    call res_history%evaluate_distances (p, dist)
    write (u, "(A,1x," // FMF_12 // ")")    "distance (W) =", dist(1)
    write (u, "(A,1x," // FMF_12 // ")")    "m/w (W)      =", mw / ww
    write (u, "(A,1x," // FMF_12 // ")")    "distance (Z) =", dist(2)
    write (u, "(A,1x," // FMF_12 // ")")    "m/w (Z)      =", mz / wz

    write (u, "(A)")
    write (u, "(A)")    "* Evaluate Gaussian turnoff factor"
    write (u, "(A)")

    factor = res_history%evaluate_gaussian (p, gw)
    write (u, "(A,1x," // FMF_12 // ")")    "gaussian fac =", factor

    write (u, "(A)")
    write (u, "(A)")    "* Set momenta on W peak"
    write (u, "(A)")

    p(1) = vector4_at_rest (mw/2)
    p(2) = vector4_at_rest (mw/2)
    do i = 1, 3
        call p(i)%write (u)
    end do

    write (u, "(A)")
    write (u, "(A)")    "* Evaluate distances from resonances"
    write (u, "(A)")

    call res_history%evaluate_distances (p, dist)
    write (u, "(A,1x," // FMF_12 // ")")    "distance (W) =", dist(1)
    write (u, "(A,1x," // FMF_12 // ")")    "distance (Z) =", dist(2)
    write (u, "(A,1x," // FMF_12 // ")")    "expected      =", &
        abs (mz**2 - mw**2) / (mz*wz)

    write (u, "(A)")
    write (u, "(A)")    "* Evaluate Gaussian turnoff factor"
    write (u, "(A)")

    factor = res_history%evaluate_gaussian (p, gw)
    write (u, "(A,1x," // FMF_12 // ")")    "gaussian fac =", factor
    write (u, "(A,1x," // FMF_12 // ")")    "expected      =", &
        exp (- (abs (mz**2 - mw**2) / (mz*wz))**2 / (gw * wz)**2)

    write (u, "(A)")
    write (u, "(A)")    "* Set momenta on both peaks"
    write (u, "(A)")

    p(3) = vector4_at_rest (mz - mw)

```

```

do i = 1, 3
  call p(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Evaluate distances from resonances"
write (u, "(A)")

call res_history%evaluate_distances (p, dist)
write (u, "(A,1x," // FMF_12 // ")")  "distance (W) =", dist(1)
write (u, "(A,1x," // FMF_12 // ")")  "distance (Z) =", dist(2)

write (u, "(A)")
write (u, "(A)")  "* Evaluate Gaussian turnoff factor"
write (u, "(A)")

factor = res_history%evaluate_gaussian (p, gw)
write (u, "(A,1x," // FMF_12 // ")")  "gaussian fac =", factor

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_4"

end subroutine resonances_4

```

Probe on-shell test for resonance histories

```

<Resonances: execute tests>+≡
  call test (resonances_5, "resonances_5", &
    "resonance history: on-shell test", &
    u, results)

<Resonances: test declarations>+≡
  public :: resonances_5

<Resonances: tests>+≡
  subroutine resonances_5 (u)
    integer, intent(in) :: u
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(resonance_history_set_t) :: res_set
    type(model_data_t), target :: model
    type(flavor_t) :: fw, fz
    real(default) :: mw, mz, ww, wz
    real(default) :: on_shell_limit
    integer, dimension(:), allocatable :: on_shell
    type(vector4_t), dimension(4) :: p

    write (u, "(A)")  "* Test output: resonances_5"
    write (u, "(A)")  "* Purpose: resonance history on-shell test"
    write (u, "(A)")

```

```

write (u, "(A)")  "* Read model file"

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* W and Z parameters"
write (u, "(A)")

call fw%init (24, model)
call fz%init (23, model)
mw = fw%get_mass ()
ww = fw%get_width ()
mz = fz%get_mass ()
wz = fz%get_width ()

write (u, "(A,1x," // FMF_12 // ")")  "mW =", mw
write (u, "(A,1x," // FMF_12 // ")")  "wW =", ww
write (u, "(A,1x," // FMF_12 // ")")  "mZ =", mz
write (u, "(A,1x," // FMF_12 // ")")  "wZ =", wz

write (u, "(A)")
write (u, "(A)")  "* On-shell parameter: distance as multiple of width"
write (u, "(A)")

on_shell_limit = 3
write (u, "(A,1x," // FMF_12 // ")")  "on-shell limit =", on_shell_limit

write (u, "(A)")
write (u, "(A)")  "* Setup resonance history set"
write (u, "(A)")

call res_set%init ()

call res_info%init (3, -24, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (12, 24, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (15, 23, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (3, -24, model, 6)
call res_history%add_resonance (res_info)
call res_info%init (15, 23, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)

```



```

call res_history%clear ()

call res_info%init (12, 24, model, 6)
call res_history%add_resonance (res_info)
call res_info%init (15, 23, model, 6)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_set%freeze ()
call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Setup zero momenta"
write (u, "(A)")

call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near W- resonance (2 widths off)"
write (u, "(A)")

p(1) = vector4_at_rest (82.5_default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near W- resonance (4 widths off)"
write (u, "(A)")

p(1) = vector4_at_rest (84.5_default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near Z resonance"
write (u, "(A)")

p(1) = vector4_at_rest (45._default)
p(3) = vector4_at_rest (45._default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near W- and W+ resonances"

```

```

write (u, "(A)")

p(1) = vector4_at_rest (40._default)
p(2) = vector4_at_rest (40._default)
p(3) = vector4_at_rest (40._default)
p(4) = vector4_at_rest (40._default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Setup momenta near W- and Z resonances, &
    &shadowing single resonances"
write (u, "(A)")

p(1) = vector4_at_rest (40._default)
p(2) = vector4_at_rest (40._default)
p(3) = vector4_at_rest (10._default)
p(4) = vector4_at_rest ( 0._default)
call write_momenta (p)

call res_set%determine_on_shell_histories (p, on_shell_limit, on_shell)
call write_on_shell_histories (on_shell)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_5"

contains

subroutine write_momenta (p)
  type(vector4_t), dimension(:), intent(in) :: p
  integer :: i
  do i = 1, size (p)
    call p(i)%write (u)
  end do
end subroutine write_momenta

subroutine write_on_shell_histories (on_shell)
  integer, dimension(:), intent(in) :: on_shell
  integer :: i
  write (u, *)
  write (u, "(A)", advance="no")  "on-shell = ("
  do i = 1, size (on_shell)
    if (i > 1) write (u, "(',')", advance="no")
    write (u, "(I0)", advance="no")  on_shell(i)
  end do
  write (u, "(',')'")
end subroutine write_on_shell_histories

```

```
end subroutine resonances_5
```

Organize the resonance history as a tree structure.

```
<Resonances: execute tests>+≡
  call test (resonances_6, "resonances_6", &
    "check resonance history setup", &
    u, results)

<Resonances: test declarations>+≡
  public :: resonances_6

<Resonances: tests>+≡
  subroutine resonances_6 (u)
    integer, intent(in) :: u
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history
    type(resonance_tree_t) :: res_tree
    type(model_data_t), target :: model

    write (u, "(A)")  "* Test output: resonances_6"
    write (u, "(A)")  "* Purpose: retrieve resonance histories as trees"
    write (u, "(A)")

    write (u, "(A)")  "* Read model file"

    call model%init_sm_test ()

    write (u, "(A)")
    write (u, "(A)")  "* Empty resonance history"
    write (u, "(A)")

    call res_history%write (u)

    write (u, "(A)")
    call res_history%to_tree (res_tree)
    call res_tree%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Single resonance"
    write (u, "(A)")

    call res_info%init (3, -24, model, 5)
    call res_history%add_resonance (res_info)
    call res_history%write (u)

    write (u, "(A)")
    call res_history%to_tree (res_tree)
    call res_tree%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Nested resonances"
    write (u, "(A)")

    call res_info%init (7, 23, model, 5)
```

```

call res_history%add_resonance (res_info)
call res_history%write (u)

write (u, "(A)")
call res_history%to_tree (res_tree)
call res_tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Disjunct resonances"
write (u, "(A)")

call res_history%clear ()

call res_info%init (5, 24, model, 7)
call res_history%add_resonance (res_info)

call res_info%init (7, 6, model, 7)
call res_history%add_resonance (res_info)

call res_info%init (80, -24, model, 7)
call res_history%add_resonance (res_info)

call res_info%init (112, -6, model, 7)
call res_history%add_resonance (res_info)

call res_history%write (u)

write (u, "(A)")
call res_history%to_tree (res_tree)
call res_tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonances_6"

end subroutine resonances_6

```

Basic operations on a resonance history set.

```

<Resonances: execute tests>+≡
  call test (resonances_7, "resonances_7", &
    "display tree format of history set elements", &
    u, results)

<Resonances: test declarations>+≡
  public :: resonances_7

<Resonances: tests>+≡
  subroutine resonances_7 (u)
    integer, intent(in) :: u
    type(resonance_info_t) :: res_info
    type(resonance_history_t) :: res_history

```

```

type(resonance_tree_t) :: res_tree
type(resonance_history_set_t) :: res_set
type(model_data_t), target :: model
type(flavor_t) :: flv

write (u, "(A)")  "* Test output: resonances_7"
write (u, "(A)")  "* Purpose: test tree format"
write (u, "(A)")

write (u, "(A)")  "* Read model file"

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* Initialize, fill and freeze resonance history set"
write (u, "(A)")

call res_set%init (initial_size = 2)

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_history%clear ()

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (7, 23, model, 5)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_info%init (3, -24, model, 5)
call res_history%add_resonance (res_info)
call res_info%init (7, 25, model, 5)
call res_history%add_resonance (res_info)
call res_set%enter (res_history)
call res_history%clear ()

call res_set%freeze ()

call res_set%write (u, show_trees = .true.)

write (u, "(A)")
write (u, "(A)")  "* Extract tree #1"
write (u, "(A)")

```

```

call res_set%get_tree (1, res_tree)
call res_tree%write (u)

write (u, *)
write (u, "(1x,A,1x,I0)") "n_resonances =", res_tree%get_n_resonances ()

write (u, *)
write (u, "(1x,A,1x)", advance="no") "flv(r1) ="
flv = res_tree%get_flv (1)
call flv%write (u)
write (u, *)
write (u, "(1x,A,1x)", advance="no") "flv(r2) ="
flv = res_tree%get_flv (2)
call flv%write (u)
write (u, *)

write (u, *)
write (u, "(1x,A)") "[offset = 2, 4]"
write (u, "(1x,A,9(1x,I0))") "children(r1) =", &
    res_tree%get_children(1, 2, 4)
write (u, "(1x,A,9(1x,I0))") "children(r2) =", &
    res_tree%get_children(2, 2, 4)

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call model%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: resonances_7"

end subroutine resonances_7

```

19.6 Mappings

Mappings are objects that encode the transformation of the interval $(0,1)$ to a physical variable m^2 or $\cos\theta$ (and back), as it is used in the phase space parameterization. The mapping objects contain fixed parameters, the associated methods implement the mapping and inverse mapping operations, including the computation of the Jacobian (phase space factor).

```
<mappings.f90>≡  
  <File header>  
  
  module mappings  
  
    <Use kinds>  
    use kinds, only: TC  
    <Use strings>  
    use io_units  
    use constants, only: pi  
    use format_defs, only: FMT_19  
    use diagnostics  
    use md5  
    use model_data  
    use flavors  
  
    <Standard module head>  
  
    <Mappings: public>  
  
    <Mappings: parameters>  
  
    <Mappings: types>  
  
    <Mappings: interfaces>  
  
    contains  
  
    <Mappings: procedures>  
  
  end module mappings
```

19.6.1 Default parameters

This type holds the default parameters, needed for setting the scale in cases where no mass parameter is available. The contents are public.

```
<Mappings: public>≡  
  public :: mapping_defaults_t  
  
<Mappings: types>≡  
  type :: mapping_defaults_t  
    real(default) :: energy_scale = 10  
    real(default) :: invariant_mass_scale = 10  
    real(default) :: momentum_transfer_scale = 10  
    logical :: step_mapping = .true.  
    logical :: step_mapping_exp = .true.
```

```

        logical :: enable_s_mapping = .false.
contains
  <Mappings: mapping defaults: TBP>
end type mapping_defaults_t

```

Output.

```

<Mappings: mapping defaults: TBP>≡
  procedure :: write => mapping_defaults_write

<Mappings: procedures>≡
  subroutine mapping_defaults_write (object, unit)
    class(mapping_defaults_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A," // FMT_19 // ")") "energy scale = ", &
      object%energy_scale
    write (u, "(3x,A," // FMT_19 // ")") "mass scale = ", &
      object%invariant_mass_scale
    write (u, "(3x,A," // FMT_19 // ")") "q scale = ", &
      object%momentum_transfer_scale
    write (u, "(3x,A,L1)") "step mapping = ", &
      object%step_mapping
    write (u, "(3x,A,L1)") "step exp. mode = ", &
      object%step_mapping_exp
    write (u, "(3x,A,L1)") "allow s mapping = ", &
      object%enable_s_mapping
  end subroutine mapping_defaults_write

<Mappings: public>+≡
  public :: mapping_defaults_md5sum

<Mappings: procedures>+≡
  function mapping_defaults_md5sum (mapping_defaults) result (md5sum_map)
    character(32) :: md5sum_map
    type(mapping_defaults_t), intent(in) :: mapping_defaults
    integer :: u
    u = free_unit ()
    open (u, status = "scratch")
    write (u, *) mapping_defaults%energy_scale
    write (u, *) mapping_defaults%invariant_mass_scale
    write (u, *) mapping_defaults%momentum_transfer_scale
    write (u, *) mapping_defaults%step_mapping
    write (u, *) mapping_defaults%step_mapping_exp
    write (u, *) mapping_defaults%enable_s_mapping
    rewind (u)
    md5sum_map = md5sum (u)
    close (u)
  end function mapping_defaults_md5sum

```


19.6.2 The Mapping type

Each mapping has a type (e.g., s-channel, infrared), a binary code (redundant, but useful for debugging), and a reference particle. The flavor code of this particle is stored for bookkeeping reasons, what matters are the mass and width of this particle. Furthermore, depending on the type, various mapping parameters can be set and used.

The parameters **a1** to **a3** (for m^2 mappings) and **b1** to **b3** (for $\cos\theta$ mappings) are values that are stored once to speed up the calculation, if **variable_limits** is false. The exact meaning of these parameters depends on the mapping type. The limits are fixed if there is a fixed c.m. energy.

```

⟨Mappings: public⟩+≡
    public :: mapping_t

⟨Mappings: types⟩+≡
    type :: mapping_t
    private
        integer :: type = NO_MAPPING
        integer(TC) :: bincode
        type(flavor_t) :: flv
        real(default) :: mass = 0
        real(default) :: width = 0
        logical :: a_unknown = .true.
        real(default) :: a1 = 0
        real(default) :: a2 = 0
        real(default) :: a3 = 0
        logical :: b_unknown = .true.
        real(default) :: b1 = 0
        real(default) :: b2 = 0
        real(default) :: b3 = 0
        logical :: variable_limits = .true.
    contains
        ⟨Mappings: mapping: TBP⟩
    end type mapping_t

```

The valid mapping types. The extra type **STEP_MAPPING** is used only internally.

```

⟨Mappings: parameters⟩≡
    ⟨Mapping modes⟩

```

19.6.3 Screen output

Do not write empty mappings.

```

⟨Mappings: public⟩+≡
    public :: mapping_write

⟨Mappings: procedures⟩+≡
    subroutine mapping_write (map, unit, verbose)
        type(mapping_t), intent(in) :: map
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u
        character(len=9) :: str
        u = given_output_unit (unit); if (u < 0) return
    end subroutine mapping_write

```

```

select case(map%type)
case(S_CHANNEL); str = "s_channel"
case(COLLINEAR); str = "collinear"
case(INFRARED); str = "infrared "
case(RADIATION); str = "radiation"
case(T_CHANNEL); str = "t_channel"
case(U_CHANNEL); str = "u_channel"
case(STEP_MAPPING_E); str = "step_exp"
case(STEP_MAPPING_H); str = "step_hyp"
case(ON_SHELL); str = "on_shell"
case default; str = "??????"
end select
if (map%type /= NO_MAPPING) then
write (u, '(1x,A,I4,A)') &
"Branch #", map%bincode, ": " // &
"Mapping (" // str // ") for particle " // &
',' // char (map%flv%get_name ()) // ','
if (present (verbose)) then
if (verbose) then
select case (map%type)
case (S_CHANNEL, RADIATION, STEP_MAPPING_E, STEP_MAPPING_H)
write (u, "(1x,A,3(" // FMT_19 // "))" ) &
" m/w = ", map%mass, map%width
case default
write (u, "(1x,A,3(" // FMT_19 // "))" ) &
" m = ", map%mass
end select
select case (map%type)
case (S_CHANNEL, T_CHANNEL, U_CHANNEL, &
STEP_MAPPING_E, STEP_MAPPING_H, &
COLLINEAR, INFRARED, RADIATION)
write (u, "(1x,A,3(" // FMT_19 // "))" ) &
" a1/2/3 = ", map%a1, map%a2, map%a3
end select
select case (map%type)
case (T_CHANNEL, U_CHANNEL, COLLINEAR)
write (u, "(1x,A,3(" // FMT_19 // "))" ) &
" b1/2/3 = ", map%b1, map%b2, map%b3
end select
end if
end if
end if
end subroutine mapping_write

```

19.6.4 Define a mapping

The initialization routine sets the mapping type and the particle (binary code and flavor code) for which the mapping applies (e.g., a Z resonance in branch #3).

```

<Mappings: public>+≡
public :: mapping_init

```

```

<Mappings: procedures>+≡
subroutine mapping_init (mapping, brcode, type, f, model)
  type(mapping_t), intent(inout) :: mapping
  integer(TC), intent(in) :: brcode
  type(string_t), intent(in) :: type
  integer, intent(in), optional :: f
  class(model_data_t), intent(in), optional, target :: model
  mapping%brcode = brcode
  select case (char (type))
    case ("s_channel"); mapping%type = S_CHANNEL
    case ("collinear"); mapping%type = COLLINEAR
    case ("infrared"); mapping%type = INFRARED
    case ("radiation"); mapping%type = RADIATION
    case ("t_channel"); mapping%type = T_CHANNEL
    case ("u_channel"); mapping%type = U_CHANNEL
    case ("step_exp"); mapping%type = STEP_MAPPING_E
    case ("step_hyp"); mapping%type = STEP_MAPPING_H
    case ("on_shell"); mapping%type = ON_SHELL
    case default
      call msg_bug ("Mappings: encountered undefined mapping key '" &
        // char (type) // "'")
  end select
  if (present (f) .and. present (model)) call mapping%flv%init (f, model)
end subroutine mapping_init

```

This sets the actual mass and width, using a parameter set. Since the auxiliary parameters will only be determined when the mapping is first called, they are marked as unknown.

```

<Mappings: public>+≡
public :: mapping_set_parameters

<Mappings: procedures>+≡
subroutine mapping_set_parameters (map, mapping_defaults, variable_limits)
  type(mapping_t), intent(inout) :: map
  type(mapping_defaults_t), intent(in) :: mapping_defaults
  logical, intent(in) :: variable_limits
  if (map%type /= NO_MAPPING) then
    map%mass = map%flv%get_mass ()
    map%width = map%flv%get_width ()
    map%variable_limits = variable_limits
    map%a_unknown = .true.
    map%b_unknown = .true.
    select case (map%type)
      case (S_CHANNEL)
        if (map%mass <= 0) then
          call mapping_write (map)
          call msg_fatal &
            & (" S-channel resonance must have positive mass")
        else if (map%width <= 0) then
          call mapping_write (map)
          call msg_fatal &
            & (" S-channel resonance must have positive width")
        end if
      case (RADIATION)
    end select
  end if
end subroutine mapping_set_parameters

```

```

        map%width = max (map%width, mapping_defaults%energy_scale)
    case (INFRARED, COLLINEAR)
        map%mass = max (map%mass, mapping_defaults%invariant_mass_scale)
    case (T_CHANNEL, U_CHANNEL)
        map%mass = max (map%mass, mapping_defaults%momentum_transfer_scale)
    end select
end if
end subroutine mapping_set_parameters

```

For a step mapping the mass and width are set directly, instead of being determined from the flavor parameter (which is meaningless here). They correspond to the effective upper bound of phase space due to a resonance, as opposed to the absolute upper bound.

```

<Mappings: public>+≡
    public :: mapping_set_step_mapping_parameters

<Mappings: procedures>+≡
    subroutine mapping_set_step_mapping_parameters (map, &
        mass, width, variable_limits)
        type(mapping_t), intent(inout) :: map
        real(default), intent(in) :: mass, width
        logical, intent(in) :: variable_limits
        select case (map%type)
        case (STEP_MAPPING_E, STEP_MAPPING_H)
            map%variable_limits = variable_limits
            map%a_unknown = .true.
            map%b_unknown = .true.
            map%mass = mass
            map%width = width
        end select
    end subroutine mapping_set_step_mapping_parameters

```

19.6.5 Retrieve contents

Return true if there is any / an s-channel mapping.

```

<Mappings: public>+≡
    public :: mapping_is_set
    public :: mapping_is_s_channel
    public :: mapping_is_on_shell

<Mappings: mapping: TBP>≡
    procedure :: is_set => mapping_is_set
    procedure :: is_s_channel => mapping_is_s_channel
    procedure :: is_on_shell => mapping_is_on_shell

<Mappings: procedures>+≡
    function mapping_is_set (mapping) result (flag)
        class(mapping_t), intent(in) :: mapping
        logical :: flag
        flag = mapping%type /= NO_MAPPING
    end function mapping_is_set

    function mapping_is_s_channel (mapping) result (flag)

```

```

class(mapping_t), intent(in) :: mapping
logical :: flag
flag = mapping%type == S_CHANNEL
end function mapping_is_s_channel

function mapping_is_on_shell (mapping) result (flag)
class(mapping_t), intent(in) :: mapping
logical :: flag
flag = mapping%type == ON_SHELL
end function mapping_is_on_shell

```

Return the binary code for the mapped particle.

```

⟨Mappings: mapping: TBP⟩+≡
  procedure :: get_bincode => mapping_get_bincode

⟨Mappings: procedures⟩+≡
  function mapping_get_bincode (mapping) result (bincode)
class(mapping_t), intent(in) :: mapping
integer(TC) :: bincode
bincode = mapping%bincode
end function mapping_get_bincode

```

Return the flavor object for the mapped particle.

```

⟨Mappings: mapping: TBP⟩+≡
  procedure :: get_flv => mapping_get_flv

⟨Mappings: procedures⟩+≡
  function mapping_get_flv (mapping) result (flv)
class(mapping_t), intent(in) :: mapping
type(flavor_t) :: flv
flv = mapping%flv
end function mapping_get_flv

```

Return stored mass and width, respectively.

```

⟨Mappings: public⟩+≡
  public :: mapping_get_mass
  public :: mapping_get_width

⟨Mappings: procedures⟩+≡
  function mapping_get_mass (mapping) result (mass)
real(default) :: mass
type(mapping_t), intent(in) :: mapping
mass = mapping%mass
end function mapping_get_mass

function mapping_get_width (mapping) result (width)
real(default) :: width
type(mapping_t), intent(in) :: mapping
width = mapping%width
end function mapping_get_width

```

19.6.6 Compare mappings

Equality for single mappings and arrays

```

<Mappings: public>+≡
    public :: operator(==)

<Mappings: interfaces>≡
    interface operator(==)
        module procedure mapping_equal
    end interface

<Mappings: procedures>+≡
    function mapping_equal (m1, m2) result (equal)
        type(mapping_t), intent(in) :: m1, m2
        logical :: equal
        if (m1%type == m2%type) then
            select case (m1%type)
            case (NO_MAPPING)
                equal = .true.
            case (S_CHANNEL, RADIATION, STEP_MAPPING_E, STEP_MAPPING_H)
                equal = (m1%mass == m2%mass) .and. (m1%width == m2%width)
            case default
                equal = (m1%mass == m2%mass)
            end select
        else
            equal = .false.
        end if
    end function mapping_equal

```

19.6.7 Mappings of the invariant mass

Inserting an x value between 0 and 1, we want to compute the corresponding invariant mass $m^2(x)$ and the jacobian, aka phase space factor $f(x)$. We also need the reverse operation.

In general, the phase space factor f is defined by

$$\frac{1}{s} \int_{m_{\min}^2}^{m_{\max}^2} dm^2 g(m^2) = \int_0^1 dx \frac{1}{s} \frac{dm^2}{dx} g(m^2(x)) = \int_0^1 dx f(x) g(x), \quad (19.8)$$

where thus

$$f(x) = \frac{1}{s} \frac{dm^2}{dx}. \quad (19.9)$$

With this mapping, a function of the form

$$g(m^2) = c \frac{dx(m^2)}{dm^2} \quad (19.10)$$

is mapped to a constant:

$$\frac{1}{s} \int_{m_{\min}^2}^{m_{\max}^2} dm^2 g(m^2) = \int_0^1 dx f(x) g(m^2(x)) = \int_0^1 dx \frac{c}{s}. \quad (19.11)$$

Here is the mapping routine. Input are the available energy squared s , the limits for m^2 , and the x value. Output are the m^2 value and the phase space factor f .

```

<Mappings: public>+≡
  public :: mapping_compute_msq_from_x

<Mappings: procedures>+≡
  subroutine mapping_compute_msq_from_x (map, s, msq_min, msq_max, msq, f, x)
    type(mapping_t), intent(inout) :: map
    real(default), intent(in) :: s, msq_min, msq_max
    real(default), intent(out) :: msq, f
    real(default), intent(in) :: x
    real(default) :: z, msq0, msq1, tmp
    integer :: type
    type = map%type
    if (s == 0) &
      call msg_fatal (" Applying msq mapping for zero energy")
    <Modify mapping type if necessary>
    select case(type)
    case (NO_MAPPING)
      <Constants for trivial msq mapping>
      <Apply trivial msq mapping>
    case (S_CHANNEL)
      <Constants for s-channel resonance mapping>
      <Apply s-channel resonance mapping>
    case (COLLINEAR, INFRARED, RADIATION)
      <Constants for s-channel pole mapping>
      <Apply s-channel pole mapping>
    case (T_CHANNEL, U_CHANNEL)
      <Constants for t-channel pole mapping>
      <Apply t-channel pole mapping>
    case (STEP_MAPPING_E)
      <Constants for exponential step mapping>
      <Apply exponential step mapping>
    case (STEP_MAPPING_H)
      <Constants for hyperbolic step mapping>
      <Apply hyperbolic step mapping>
    case default
      call msg_fatal ( " Attempt to apply undefined msq mapping")
    end select
  end subroutine mapping_compute_msq_from_x

```

The inverse mapping

```

<Mappings: public>+≡
  public :: mapping_compute_x_from_msq

<Mappings: procedures>+≡
  subroutine mapping_compute_x_from_msq (map, s, msq_min, msq_max, msq, f, x)
    type(mapping_t), intent(inout) :: map
    real(default), intent(in) :: s, msq_min, msq_max
    real(default), intent(in) :: msq
    real(default), intent(out) :: f, x
    real(default) :: msq0, msq1, tmp, z
    integer :: type

```

```

type = map%type
if (s == 0) &
    call msg_fatal (" Applying inverse msq mapping for zero energy")
<Modify mapping type if necessary>
select case (type)
case (NO_MAPPING)
    <Constants for trivial msq mapping>
    <Apply inverse trivial msq mapping>
case (S_CHANNEL)
    <Constants for s-channel resonance mapping>
    <Apply inverse s-channel resonance mapping>
case (COLLINEAR, INFRARED, RADIATION)
    <Constants for s-channel pole mapping>
    <Apply inverse s-channel pole mapping>
case (T_CHANNEL, U_CHANNEL)
    <Constants for t-channel pole mapping>
    <Apply inverse t-channel pole mapping>
case (STEP_MAPPING_E)
    <Constants for exponential step mapping>
    <Apply inverse exponential step mapping>
case (STEP_MAPPING_H)
    <Constants for hyperbolic step mapping>
    <Apply inverse hyperbolic step mapping>
case default
    call msg_fatal ( " Attempt to apply undefined msq mapping")
end select
end subroutine mapping_compute_x_from_msq

```

Trivial mapping

We simply map the boundaries of the interval (m_{\min}, m_{\max}) to $(0, 1)$:

$$m^2 = (1 - x)m_{\min}^2 + xm_{\max}^2; \quad (19.12)$$

the inverse is

$$x = \frac{m^2 - m_{\min}^2}{m_{\max}^2 - m_{\min}^2}. \quad (19.13)$$

Hence

$$f(x) = \frac{m_{\max}^2 - m_{\min}^2}{s}, \quad (19.14)$$

and we have, as required,

$$f(x) \frac{dx}{dm^2} = \frac{1}{s}. \quad (19.15)$$

We store the constant parameters the first time the mapping is called – or, if limits vary, recompute them each time.

```

<Constants for trivial msq mapping>≡
if (map%variable_limits .or. map%a_unknown) then
    map%a1 = 0
    map%a2 = msq_max - msq_min
    map%a3 = map%a2 / s
    map%a_unknown = .false.
end if

```



```

⟨Apply trivial msq mapping⟩≡
  msq = (1-x) * msq_min + x * msq_max
  f = map%a3
⟨Apply inverse trivial msq mapping⟩≡
  if (map%a2 /= 0) then
    x = (msq - msq_min) / map%a2
  else
    x = 0
  end if
  f = map%a3

```

Resonance or step mapping does not make much sense if the resonance mass is outside the kinematical bounds. If this is the case, revert to `NO_MAPPING`. This is possible even if the kinematical bounds vary from event to event.

```

⟨Modify mapping type if necessary⟩≡
  select case (type)
  case (S_CHANNEL, STEP_MAPPING_E, STEP_MAPPING_H)
    msq0 = map%mass**2
    if (msq0 < msq_min .or. msq0 > msq_max) type = NO_MAPPING
  end select

```

Breit-Wigner mapping

A Breit-Wigner resonance with mass M and width Γ is flattened by the following mapping:

This mapping does not make much sense if the resonance mass is too low. If this is the case, revert to `NO_MAPPING`. There is a tricky point with this if the mass is too high: `msq_max` is not a constant if structure functions are around. However, switching the type depending on the overall energy does not change the integral, it is just another branching point.

$$m^2 = M(M + t\Gamma), \quad (19.16)$$

where

$$t = \tan \left[(1-x) \arctan \frac{m_{\min}^2 - M^2}{M\Gamma} + x \arctan \frac{m_{\max}^2 - M^2}{M\Gamma} \right]. \quad (19.17)$$

The inverse:

$$x = \frac{\arctan \frac{m^2 - M^2}{M\Gamma} - \arctan \frac{m_{\min}^2 - M^2}{M\Gamma}}{\arctan \frac{m_{\max}^2 - M^2}{M\Gamma} - \arctan \frac{m_{\min}^2 - M^2}{M\Gamma}} \quad (19.18)$$

The phase-space factor of this transformation is

$$f(x) = \frac{M\Gamma}{s} \left(\arctan \frac{m_{\max}^2 - M^2}{M\Gamma} - \arctan \frac{m_{\min}^2 - M^2}{M\Gamma} \right) (1 + t^2). \quad (19.19)$$

This maps any function proportional to

$$g(m^2) = \frac{M\Gamma}{(m^2 - M^2)^2 + M^2\Gamma^2} \quad (19.20)$$

to a constant times $1/s$.

```

⟨Constants for s-channel resonance mapping⟩≡

```

```

if (map%variable_limits .or. map%a_unknown) then
  msq0 = map%mass ** 2
  map%a1 = atan ((msq_min - msq0) / (map%mass * map%width))
  map%a2 = atan ((msq_max - msq0) / (map%mass * map%width))
  map%a3 = (map%a2 - map%a1) * (map%mass * map%width) / s
  map%a_unknown = .false.
end if

⟨Apply s-channel resonance mapping⟩≡
z = (1-x) * map%a1 + x * map%a2
if (-pi/2 < z .and. z < pi/2) then
  tmp = tan (z)
  msq = map%mass * (map%mass + map%width * tmp)
  f = map%a3 * (1 + tmp**2)
else
  msq = 0
  f = 0
end if

⟨Apply inverse s-channel resonance mapping⟩≡
tmp = (msq - msq0) / (map%mass * map%width)
x = (atan (tmp) - map%a1) / (map%a2 - map%a1)
f = map%a3 * (1 + tmp**2)

```

Mapping for massless splittings

This mapping accounts for approximately scale-invariant behavior where $\ln M^2$ is evenly distributed.

$$m^2 = m_{\min}^2 + M^2 (\exp(xL) - 1) \quad (19.21)$$

where

$$L = \ln \left(\frac{m_{\max}^2 - m_{\min}^2}{M^2} + 1 \right). \quad (19.22)$$

The inverse:

$$x = \frac{1}{L} \ln \left(\frac{m^2 - m_{\min}^2}{M^2} + 1 \right) \quad (19.23)$$

The constant M is a characteristic scale. Above this scale ($m^2 - m_{\min}^2 \gg M^2$), this mapping behaves like $x \propto \ln m^2$, while below the scale it reverts to a linear mapping.

The phase-space factor is

$$f(x) = \frac{M^2}{s} \exp(xL) L. \quad (19.24)$$

A function proportional to

$$g(m^2) = \frac{1}{(m^2 - m_{\min}^2) + M^2} \quad (19.25)$$

is mapped to a constant, i.e., a simple pole near m_{\min} with a regulator mass M .

This type of mapping is useful for massless collinear and infrared singularities, where the scale is stored as the mass parameter. In the radiation case

(IR radiation off massive particle), the heavy particle width is the characteristic scale.

```

⟨Constants for s-channel pole mapping⟩≡
  if (map%variable_limits .or. map%a_unknown) then
    if (type == RADIATION) then
      msq0 = map%width**2
    else
      msq0 = map%mass**2
    end if
    map%a1 = msq0
    map%a2 = log ((msq_max - msq_min) / msq0 + 1)
    map%a3 = map%a2 / s
    map%a_unknown = .false.
  end if

⟨Apply s-channel pole mapping⟩≡
  msq1 = map%a1 * exp (x * map%a2)
  msq = msq1 - map%a1 + msq_min
  f = map%a3 * msq1

⟨Apply inverse s-channel pole mapping⟩≡
  msq1 = msq - msq_min + map%a1
  x = log (msq1 / map%a1) / map%a2
  f = map%a3 * msq1

```

Mapping for t-channel poles

This is also approximately scale-invariant, and we use the same type of mapping as before. However, we map $1/x$ singularities at both ends of the interval; again, the mapping becomes linear when the distance is less than M^2 :

$$m^2 = \begin{cases} m_{\min}^2 + M^2 (\exp(xL) - 1) & \text{for } 0 < x < \frac{1}{2} \\ m_{\max}^2 - M^2 (\exp((1-x)L) - 1) & \text{for } \frac{1}{2} \leq x < 1 \end{cases} \quad (19.26)$$

where

$$L = 2 \ln \left(\frac{m_{\max}^2 - m_{\min}^2}{2M^2} + 1 \right). \quad (19.27)$$

The inverse:

$$x = \begin{cases} \frac{1}{L} \ln \left(\frac{m^2 - m_{\min}^2}{M^2} + 1 \right) & \text{for } m^2 < (m_{\max}^2 - m_{\min}^2)/2 \\ 1 - \frac{1}{L} \ln \left(\frac{m_{\max}^2 - m^2}{M^2} + 1 \right) & \text{for } m^2 \geq (m_{\max}^2 - m_{\min}^2)/2 \end{cases} \quad (19.28)$$

The phase-space factor is

$$f(x) = \begin{cases} \frac{M^2}{s} \exp(xL) L. & \text{for } 0 < x < \frac{1}{2} \\ \frac{M^2}{s} \exp((1-x)L) L. & \text{for } \frac{1}{2} \leq x < 1 \end{cases} \quad (19.29)$$

A (continuous) function proportional to

$$g(m^2) = \begin{cases} 1/(m^2 - m_{\min}^2) + M^2 & \text{for } m^2 < (m_{\max}^2 - m_{\min}^2)/2 \\ 1/((m_{\max}^2 - m^2) + M^2) & \text{for } m^2 \geq (m_{\max}^2 - m_{\min}^2)/2 \end{cases} \quad (19.30)$$

is mapped to a constant by this mapping, i.e., poles near both ends of the interval.

```

⟨Constants for t-channel pole mapping⟩≡
  if (map%variable_limits .or. map%a_unknown) then
    msq0 = map%mass**2
    map%a1 = msq0
    map%a2 = 2 * log ((msq_max - msq_min)/(2*msq0) + 1)
    map%a3 = map%a2 / s
    map%a_unknown = .false.
  end if

⟨Apply t-channel pole mapping⟩≡
  if (x < .5_default) then
    msq1 = map%a1 * exp (x * map%a2)
    msq = msq1 - map%a1 + msq_min
  else
    msq1 = map%a1 * exp ((1-x) * map%a2)
    msq = -(msq1 - map%a1) + msq_max
  end if
  f = map%a3 * msq1

⟨Apply inverse t-channel pole mapping⟩≡
  if (msq < (msq_max + msq_min)/2) then
    msq1 = msq - msq_min + map%a1
    x = log (msq1/map%a1) / map%a2
  else
    msq1 = msq_max - msq + map%a1
    x = 1 - log (msq1/map%a1) / map%a2
  end if
  f = map%a3 * msq1

```

19.6.8 Step mapping

Step mapping is useful when the allowed range for a squared-mass variable is large, but only a fraction at the lower end is populated because the particle in question is an (off-shell) decay product of a narrow resonance. I.e., if the resonance was forced to be on-shell, the upper end of the range would be the resonance mass, minus the effective (real or resonance) mass of the particle(s) in the sibling branch of the decay.

The edge of this phase space section has a width which is determined by the width of the parent, plus the width of the sibling branch. (The widths might be added in quadrature, but this precision is probably not important.)

Fermi function

A possible mapping is derived from the Fermi function which has precisely this behavior. The Fermi function is given by

$$f(x) = \frac{1}{1 + \exp \frac{x-\mu}{\gamma}} \quad (19.31)$$

where x is taken as the invariant mass squared, μ is the invariant mass squared of the edge, and γ is the effective width which is given by the widths of the

parent and the sibling branch. (Widths might be added in quadrature, but we do not require this level of precision.)

$$x = \frac{m^2 - m_{\min}^2}{\Delta m^2} \quad (19.32)$$

$$\mu = \frac{m_{\max, \text{eff}}^2 - m_{\min}^2}{\Delta m^2} \quad (19.33)$$

$$\gamma = \frac{2m_{\max, \text{eff}}\Gamma}{\Delta m^2} \quad (19.34)$$

with

$$\Delta m^2 = m_{\max}^2 - m_{\min}^2 \quad (19.35)$$

m^2 is thus given by

$$m^2(x) = xm_{\max}^2 + (1-x)m_{\min}^2 \quad (19.36)$$

For the mapping, we compute the integral $g(x)$ of the Fermi function, normalized such that $g(0) = 0$ and $g(1) = 1$. We introduce the abbreviations

$$\alpha = 1 - \gamma \ln \frac{1 + \beta e^{1/\gamma}}{1 + \beta} \quad (19.37)$$

$$\beta = e^{-\mu/\gamma} \quad (19.38)$$

and obtain

$$g(x) = \frac{1}{\alpha} \left(x - \gamma \ln \frac{1 + \beta e^{x/\gamma}}{1 + \beta} \right) \quad (19.39)$$

The actual mapping is the inverse function $h(y) = g^{-1}(y)$,

$$h(y) = -\gamma \ln \left(e^{-\alpha y/\gamma} (1 + \beta) - \beta \right) \quad (19.40)$$

The Jacobian is

$$\frac{dh}{dy} = \alpha \left(1 - e^{\alpha y/\gamma} \frac{\beta}{1 + \beta} \right)^{-1} \quad (19.41)$$

which is equal to $1/(dg/dx)$, namely

$$\frac{dg}{dx} = \frac{1}{\alpha} \frac{1}{1 + \beta e^{x/\gamma}} \quad (19.42)$$

The final result is

$$\int_{m_{\min}^2}^{m_{\max}^2} dm^2 F(m^2) = \Delta m^2 \int_0^1 dx F(m^2(x)) \quad (19.43)$$

$$= \Delta m^2 \int_0^1 dy F(m^2(h(y))) \frac{dh}{dy} \quad (19.44)$$

Here is the implementation. We fill **a1**, **a2**, **a3** with α, β, γ , respectively.

```

⟨Constants for exponential step mapping⟩≡
  if (map%variable_limits .or. map%a_unknown) then
    map%a3 = max (2 * map%mass * map%width / (msq_max - msq_min), 0.01_default)
    map%a2 = exp (- (map%mass**2 - msq_min) / (msq_max - msq_min) &
                  / map%a3)
    map%a1 = 1 - map%a3 * log ((1 + map%a2 * exp (1 / map%a3)) / (1 + map%a2))
  end if

```

```

⟨Apply exponential step mapping⟩≡
  tmp = exp (- x * map%a1 / map%a3) * (1 + map%a2)
  z = - map%a3 * log (tmp - map%a2)
  msq = z * msq_max + (1 - z) * msq_min
  f = map%a1 / (1 - map%a2 / tmp) * (msq_max - msq_min) / s

⟨Apply inverse exponential step mapping⟩≡
  z = (msq - msq_min) / (msq_max - msq_min)
  tmp = 1 + map%a2 * exp (z / map%a3)
  x = (z - map%a3 * log (tmp / (1 + map%a2))) &
    / map%a1
  f = map%a1 * tmp * (msq_max - msq_min) / s

```

Hyperbolic mapping

The Fermi function has the drawback that it decreases exponentially. It might be preferable to take a function with a power-law decrease, such that the high-mass region is not completely depopulated.

Here, we start with the actual mapping which we take as

$$h(y) = \frac{b}{a-y} - \frac{b}{a} + \mu y \quad (19.45)$$

with the abbreviation

$$a = \frac{1}{2} \left(1 + \sqrt{1 + \frac{4b}{1-\mu}} \right) \quad (19.46)$$

This is a hyperbola in the xy plane. The derivative is

$$\frac{dh}{dy} = \frac{b}{(a-y)^2} + \mu \quad (19.47)$$

The constants correspond to

$$\mu = \frac{m_{\text{max,eff}}^2 - m_{\text{min}}^2}{\Delta m^2} \quad (19.48)$$

$$b = \frac{1}{\mu} \left(\frac{2m_{\text{max,eff}}\Gamma}{\Delta m^2} \right)^2 \quad (19.49)$$

The inverse function is the solution of a quadratic equation,

$$g(x) = \frac{1}{2} \left[\left(a + \frac{x}{\mu} + \frac{b}{a\mu} \right) - \sqrt{\left(a - \frac{x}{\mu} \right)^2 + 2\frac{b}{a\mu} \left(a + \frac{x}{\mu} \right) + \left(\frac{b}{a\mu} \right)^2} \right] \quad (19.50)$$

The constants $a_{1,2,3}$ are identified with a, b, μ .

```

⟨Constants for hyperbolic step mapping⟩≡
  if (map%variable_limits .or. map%a_unknown) then
    map%a3 = (map%mass**2 - msq_min) / (msq_max - msq_min)
    map%a2 = max ((2 * map%mass * map%width / (msq_max - msq_min))**2 &
      / map%a3, 1e-6_default)
    map%a1 = (1 + sqrt (1 + 4 * map%a2 / (1 - map%a3))) / 2
  end if

```

```

⟨Apply hyperbolic step mapping⟩≡
  z = map%a2 / (map%a1 - x) - map%a2 / map%a1 + map%a3 * x
  msq = z * msq_max + (1 - z) * msq_min
  f = (map%a2 / (map%a1 - x)**2 + map%a3) * (msq_max - msq_min) / s

⟨Apply inverse hyperbolic step mapping⟩≡
  z = (msq - msq_min) / (msq_max - msq_min)
  tmp = map%a2 / (map%a1 * map%a3)
  x = ((map%a1 + z / map%a3 + tmp) &
        - sqrt((map%a1 - z / map%a3)**2 + 2 * tmp * (map%a1 + z / map%a3) &
              + tmp**2)) / 2
  f = (map%a2 / (map%a1 - x)**2 + map%a3) * (msq_max - msq_min) / s

```

19.6.9 Mappings of the polar angle

The other type of singularity, a simple pole just outside the integration region, can occur in the integration over $\cos\theta$. This applies to exchange of massless (or light) particles.

Double poles (Coulomb scattering) are also possible, but only in certain cases. These are also handled by the single-pole mapping.

The mapping is analogous to the previous m^2 pole mapping, but with a different normalization and notation of variables:

$$\frac{1}{2} \int_{-1}^1 d\cos\theta g(\theta) = \int_0^1 dx \frac{d\cos\theta}{dx} g(\theta(x)) = \int_0^1 dx f(x) g(x), \quad (19.51)$$

where thus

$$f(x) = \frac{1}{2} \frac{d\cos\theta}{dx}. \quad (19.52)$$

With this mapping, a function of the form

$$g(\theta) = c \frac{dx(\cos\theta)}{d\cos\theta} \quad (19.53)$$

is mapped to a constant:

$$\int_{-1}^1 d\cos\theta g(\theta) = \int_0^1 dx f(x) g(\theta(x)) = \int_0^1 dx c. \quad (19.54)$$

```

⟨Mappings: public⟩+≡
  public :: mapping_compute_ct_from_x

⟨Mappings: procedures⟩+≡
  subroutine mapping_compute_ct_from_x (map, s, ct, st, f, x)
    type(mapping_t), intent(inout) :: map
    real(default), intent(in) :: s
    real(default), intent(out) :: ct, st, f
    real(default), intent(in) :: x
    real(default) :: tmp, ct1
    select case (map%type)
    case (NO_MAPPING, S_CHANNEL, INFRARED, RADIATION, &
          STEP_MAPPING_E, STEP_MAPPING_H)
      ⟨Apply trivial ct mapping⟩
    case (T_CHANNEL, U_CHANNEL, COLLINEAR)

```

```

    <Constants for ct pole mapping>
    <Apply ct pole mapping>
    case default
        call msg_fatal (" Attempt to apply undefined ct mapping")
    end select
end subroutine mapping_compute_ct_from_x

<Mappings: public>+≡
    public :: mapping_compute_x_from_ct

<Mappings: procedures>+≡
    subroutine mapping_compute_x_from_ct (map, s, ct, f, x)
        type(mapping_t), intent(inout) :: map
        real(default), intent(in) :: s
        real(default), intent(in) :: ct
        real(default), intent(out) :: f, x
        real(default) :: ct1
        select case (map%type)
            case (NO_MAPPING, S_CHANNEL, INFRARED, RADIATION, &
                STEP_MAPPING_E, STEP_MAPPING_H)
                <Apply inverse trivial ct mapping>
            case (T_CHANNEL, U_CHANNEL, COLLINEAR)
                <Constants for ct pole mapping>
                <Apply inverse ct pole mapping>
            case default
                call msg_fatal (" Attempt to apply undefined inverse ct mapping")
            end select
        end select
    end subroutine mapping_compute_x_from_ct

```

Trivial mapping

This is just the mapping of the interval $(-1, 1)$ to $(0, 1)$:

$$\cos \theta = -1 + 2x \quad (19.55)$$

and

$$f(x) = 1 \quad (19.56)$$

with the inverse

$$x = \frac{1 + \cos \theta}{2} \quad (19.57)$$

```

<Apply trivial ct mapping>≡
    tmp = 2 * (1-x)
    ct = 1 - tmp
    st = sqrt (tmp * (2-tmp))
    f = 1

<Apply inverse trivial ct mapping>≡
    x = (ct + 1) / 2
    f = 1

```


Pole mapping

As above for m^2 , we simultaneously map poles at both ends of the $\cos \theta$ interval. The formulae are completely analogous:

$$\cos \theta = \begin{cases} \frac{M^2}{s} [\exp(xL) - 1] - 1 & \text{for } x < \frac{1}{2} \\ -\frac{M^2}{s} [\exp((1-x)L) - 1] + 1 & \text{for } x \geq \frac{1}{2} \end{cases} \quad (19.58)$$

where

$$L = 2 \ln \frac{M^2 + s}{M^2}. \quad (19.59)$$

Inverse:

$$x = \begin{cases} \frac{1}{2L} \ln \frac{1 + \cos \theta + M^2/s}{M^2/s} & \text{for } \cos \theta < 0 \\ 1 - \frac{1}{2L} \ln \frac{1 - \cos \theta + M^2/s}{M^2/s} & \text{for } \cos \theta \geq 0 \end{cases} \quad (19.60)$$

The phase-space factor:

$$f(x) = \begin{cases} \frac{M^2}{s} \exp(xL) L & \text{for } x < \frac{1}{2} \\ \frac{M^2}{s} \exp((1-x)L) L & \text{for } x \geq \frac{1}{2} \end{cases} \quad (19.61)$$

```

⟨Constants for ct pole mapping⟩≡
  if (map%variable_limits .or. map%b_unknown) then
    map%b1 = map%mass**2 / s
    map%b2 = log ((map%b1 + 1) / map%b1)
    map%b3 = 0
    map%b_unknown = .false.
  end if

⟨Apply ct pole mapping⟩≡
  if (x < .5_default) then
    ct1 = map%b1 * exp (2 * x * map%b2)
    ct = ct1 - map%b1 - 1
  else
    ct1 = map%b1 * exp (2 * (1-x) * map%b2)
    ct = -(ct1 - map%b1) + 1
  end if
  if (ct >= -1 .and. ct <= 1) then
    st = sqrt (1 - ct**2)
    f = ct1 * map%b2
  else
    ct = 1; st = 0; f = 0
  end if

⟨Apply inverse ct pole mapping⟩≡
  if (ct < 0) then
    ct1 = ct + map%b1 + 1
    x = log (ct1 / map%b1) / (2 * map%b2)
  else
    ct1 = -ct + map%b1 + 1
    x = 1 - log (ct1 / map%b1) / (2 * map%b2)
  end if
  f = ct1 * map%b2

```

19.7 Phase-space trees

The phase space evaluation is organized in terms of trees, where each branch corresponds to three integrations: m^2 , $\cos\theta$, and ϕ . The complete tree thus makes up a specific parameterization of the multidimensional phase-space integral. For the multi-channel integration, the phase-space tree is a single channel.

The trees imply mappings of formal Feynman tree graphs into arrays of integer numbers: Each branch, corresponding to a particular line in the graph, is assigned an integer code c (with kind value $\text{TC} = \text{tree code}$).

In this integer, each bit determines whether a particular external momentum flows through the line. The external branches therefore have codes 1, 2, 4, 8, ... An internal branch has those bits ORed corresponding to the momenta flowing through it. For example, a branch with momentum $p_1 + p_4$ has code $2^0 + 2^3 = 1 + 8 = 9$.

There is a two-fold ambiguity: Momentum conservation implies that the branch with code

$$c_0 = \sum_{i=1}^{n(\text{ext})} 2^{i-1} \quad (19.62)$$

i.e. the branch with momentum $p_1 + p_2 + \dots p_n$ has momentum zero, which is equivalent to tree code 0 by definition. Correspondingly,

$$c \quad \text{and} \quad c_0 - c = c \text{ XOR } c_0 \quad (19.63)$$

are equivalent. E.g., if there are five externals with codes $c = 1, 2, 4, 8, 16$, then $c = 9$ and $\bar{c} = 31 - 9 = 22$ are equivalent.

This ambiguity may be used to assign a direction to the line: If all momenta are understood as outgoing, $c = 9$ in the example above means $p_1 + p_4$, but $c = 22$ means $p_2 + p_3 + p_5 = -(p_1 + p_4)$.

Here we make use of the ambiguity in a slightly different way. First, the initial particles are singled out as those externals with the highest bits, the IN-bits. (Here: 8 and 16 for a $2 \rightarrow 3$ scattering process, 16 only for a $1 \rightarrow 4$ decay.) Then we invert those codes where all IN-bits are set. For a decay process this maps each tree of an equivalence class onto a unique representative (that one with the smallest integer codes). For a scattering process we proceed further:

The ambiguity remains in all branches where only one IN-bit is set, including the initial particles. If there are only externals with this property, we have an s -channel graph which we leave as it is. In all other cases, an internal with only one IN-bit is a t -channel line, which for phase space integration should be associated with one of the initial momenta as a reference axis. We take that one whose bit is set in the current tree code. (E.g., for branch $c = 9$ we use the initial particle $c = 8$ as reference axis, whereas for the same branch we would take $c = 16$ if it had been assigned $\bar{c} = 31 - 9 = 22$ as tree code.) Thus, different ways of coding the same t -channel graph imply different phase space parameterizations.

s -channel graphs have a unique parameterization. The same sets of parameterizations are used for t -channel graphs, except for the reference frames of their angular parts. We map each t -channel graph onto an s -channel graph as follows:

Working in ascending order, for each t -channel line (whose code has exactly one IN-bit set) the attached initial line is flipped upstream, while the outgoing

line is flipped downstream. (This works only if t -channel graphs are always parameterized beginning at their outer vertices, which we require as a restriction.) After all possible flips have been applied, we have an s -channel graph. We only have to remember the initial particle a vertex was originally attached to.

```

<phs_trees.f90>≡
  <File header>

  module phs_trees

    <Use kinds>
      use kinds, only: TC
    <Use strings>
      use io_units
      use constants, only: twopi, twopi2, twopi5
      use format_defs, only: FMT_19
      use numeric_utils, only: vanishes
      use diagnostics
      use lorentz
      use permutations, only: permutation_t, permutation_size
      use permutations, only: permutation_init, permutation_find
      use permutations, only: tc_decay_level, tc_permute
      use model_data
      use flavors
      use resonances, only: resonance_history_t, resonance_info_t
      use mappings

    <Standard module head>

    <PHS trees: public>

    <PHS trees: types>

    contains

    <PHS trees: procedures>

  end module phs_trees

```

19.7.1 Particles

We define a particle type which contains only four-momentum and invariant mass squared, and a flag that tells whether the momentum is filled or not.

```

<PHS trees: public>≡
  public :: phs_prt_t

<PHS trees: types>≡
  type :: phs_prt_t
    private
    logical :: defined = .false.
    type(vector4_t) :: p
    real(default) :: p2
  end type phs_prt_t

```

Set contents:

```
<PHS trees: public>+≡
  public :: phs_prt_set_defined
  public :: phs_prt_set_undefined
  public :: phs_prt_set_momentum
  public :: phs_prt_set_msq

<PHS trees: procedures>≡
  elemental subroutine phs_prt_set_defined (prt)
    type(phs_prt_t), intent(inout) :: prt
    prt%defined = .true.
  end subroutine phs_prt_set_defined

  elemental subroutine phs_prt_set_undefined (prt)
    type(phs_prt_t), intent(inout) :: prt
    prt%defined = .false.
  end subroutine phs_prt_set_undefined

  elemental subroutine phs_prt_set_momentum (prt, p)
    type(phs_prt_t), intent(inout) :: prt
    type(vector4_t), intent(in) :: p
    prt%p = p
  end subroutine phs_prt_set_momentum

  elemental subroutine phs_prt_set_msq (prt, p2)
    type(phs_prt_t), intent(inout) :: prt
    real(default), intent(in) :: p2
    prt%p2 = p2
  end subroutine phs_prt_set_msq
```

Access methods:

```
<PHS trees: public>+≡
  public :: phs_prt_is_defined
  public :: phs_prt_get_momentum
  public :: phs_prt_get_msq

<PHS trees: procedures>+≡
  elemental function phs_prt_is_defined (prt) result (defined)
    logical :: defined
    type(phs_prt_t), intent(in) :: prt
    defined = prt%defined
  end function phs_prt_is_defined

  elemental function phs_prt_get_momentum (prt) result (p)
    type(vector4_t) :: p
    type(phs_prt_t), intent(in) :: prt
    p = prt%p
  end function phs_prt_get_momentum

  elemental function phs_prt_get_msq (prt) result (p2)
    real(default) :: p2
    type(phs_prt_t), intent(in) :: prt
    p2 = prt%p2
  end function phs_prt_get_msq
```

Addition of momenta (invariant mass square is computed).

```

<PHS trees: public>+≡
    public :: phs_prt_combine

<PHS trees: procedures>+≡
    elemental subroutine phs_prt_combine (prt, prt1, prt2)
        type(phs_prt_t), intent(inout) :: prt
        type(phs_prt_t), intent(in) :: prt1, prt2
        prt%defined = .true.
        prt%p = prt1%p + prt2%p
        prt%p2 = prt%p ** 2
        call phs_prt_check (prt)
    end subroutine phs_prt_combine

```

Output

```

<PHS trees: public>+≡
    public :: phs_prt_write

<PHS trees: procedures>+≡
    subroutine phs_prt_write (prt, unit)
        type(phs_prt_t), intent(in) :: prt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        if (prt%defined) then
            call vector4_write (prt%p, u)
            write (u, "(1x,A,1x," // FMT_19 // ")") "T = ", prt%p2
        else
            write (u, "(3x,A)") "[undefined]"
        end if
    end subroutine phs_prt_write

<PHS trees: public>+≡
    public :: phs_prt_check

<PHS trees: procedures>+≡
    elemental subroutine phs_prt_check (prt)
        type(phs_prt_t), intent(inout) :: prt
        if (prt%p2 < 0._default) then
            prt%p2 = 0._default
        end if
    end subroutine phs_prt_check

```

19.7.2 The phase-space tree type

Definition

In the concrete implementation, each branch c may have two *daughters* c_1 and c_2 such that $c_1 + c_2 = c$, a *sibling* c_s and a *mother* c_m such that $c + c_s = c_m$, and a *friend* which is kept during flips, such that it can indicate a fixed reference frame. Absent entries are set $c = 0$.

First, declare the branch type. There is some need to have this public. Give initializations for all components, so no `init` routine is necessary. The branch has some information about the associated coordinates and about connections.

```

(PHS trees: types)+≡
  type :: phs_branch_t
  private
    logical :: set = .false.
    logical :: inverted_decay = .false.
    logical :: inverted_axis = .false.
    integer(TC) :: mother = 0
    integer(TC) :: sibling = 0
    integer(TC) :: friend = 0
    integer(TC) :: origin = 0
    integer(TC), dimension(2) :: daughter = 0
    integer :: firstborn = 0
    logical :: has_children = .false.
    logical :: has_friend = .false.
    logical :: is_real = .false.
  end type phs_branch_t

```

The tree type: No initialization, this is done by `phs_tree_init`. In addition to the branch array which

The branches are collected in an array which holds all possible branches, of which only a few are set. After flips have been applied, the branch $c_M = \sum_{i=1}^{n(\text{fin})} 2^{i-1}$ must be there, indicating the mother of all decay products. In addition, we should check for consistency at the beginning.

`n_branches` is the number of those actually set. `n externals` defines the number of significant bit, and `mask` is a code where all bits are set. Analogous: `n_in` and `mask_in` for the incoming particles.

The `mapping` array contains the mappings associated to the branches (corresponding indices). The array `mass_sum` contains the sum of the real masses of the external final-state particles associated to the branch. During phase-space evaluation, this determines the boundaries.

```

(PHS trees: public)+≡
  public :: phs_tree_t
(PHS trees: types)+≡
  type :: phs_tree_t
  private
    integer :: n_branches, n externals, n_in, n_msq, n_angles
    integer(TC) :: n_branches_tot, n_branches_out
    integer(TC) :: mask, mask_in, mask_out
    type(phs_branch_t), dimension(:), allocatable :: branch
    type(mapping_t), dimension(:), allocatable :: mapping
    real(default), dimension(:), allocatable :: mass_sum
    real(default), dimension(:), allocatable :: effective_mass
    real(default), dimension(:), allocatable :: effective_width
    logical :: real_phsp = .false.
    integer, dimension(:), allocatable :: momentum_link
  contains
    (PHS trees: phs tree: TBP)
  end type phs_tree_t

```

The maximum number of external particles that can be represented is related to the bit size of the integer that stores binary codes. With the default integer of 32 bit on common machines, this is more than enough space. If TC is actually the default integer kind, there is no need to keep it separate, but doing so marks this as a special type of integer. So, just state that the maximum number is 32:

```
<Limits: public parameters>≡
    integer, parameter, public :: MAX_EXTERNAL = 32
```

Constructor and destructor

Allocate memory for a phase-space tree with given number of externals and incoming. The number of allocated branches can easily become large, but appears manageable for realistic cases, e.g., for `n_in=2` and `n_out=8` we get $2^{10}-1 = 1023$.

```
<PHS trees: public>+≡
    public :: phs_tree_init
    public :: phs_tree_final
```

Here we set the masks for incoming and for all externals.

```
<PHS trees: phs tree: TBP>≡
    procedure :: init => phs_tree_init
    procedure :: final => phs_tree_final
```

```
<PHS trees: procedures>+≡
    elemental subroutine phs_tree_init (tree, n_in, n_out, n_masses, n_angles)
        class(phs_tree_t), intent(inout) :: tree
        integer, intent(in) :: n_in, n_out, n_masses, n_angles
        integer(TC) :: i
        tree%n_externals = n_in + n_out
        tree%n_branches_tot = 2**(n_in+n_out) - 1
        tree%n_branches_out = 2**n_out - 1
        tree%mask = 0
        do i = 0, n_in + n_out - 1
            tree%mask = ibset (tree%mask, i)
        end do
        tree%n_in = n_in
        tree%mask_in = 0
        do i = n_out, n_in + n_out - 1
            tree%mask_in = ibset (tree%mask_in, i)
        end do
        tree%mask_out = ieor (tree%mask, tree%mask_in)
        tree%n_msq = n_masses
        tree%n_angles = n_angles
        allocate (tree%branch (tree%n_branches_tot))
        tree%n_branches = 0
        allocate (tree%mapping (tree%n_branches_out))
        allocate (tree%mass_sum (tree%n_branches_out))
        allocate (tree%effective_mass (tree%n_branches_out))
        allocate (tree%effective_width (tree%n_branches_out))
    end subroutine phs_tree_init

    elemental subroutine phs_tree_final (tree)
        class(phs_tree_t), intent(inout) :: tree
        deallocate (tree%branch)
        deallocate (tree%mapping)
```

```

        deallocate (tree%mass_sum)
        deallocate (tree%effective_mass)
        deallocate (tree%effective_width)
    end subroutine phs_tree_final

```

Screen output

Write only the branches that are set:

```

<PHS trees: public>+≡
    public :: phs_tree_write

<PHS trees: phs tree: TBP>+≡
    procedure :: write => phs_tree_write

<PHS trees: procedures>+≡
    subroutine phs_tree_write (tree, unit)
        class(phs_tree_t), intent(in) :: tree
        integer, intent(in), optional :: unit
        integer :: u
        integer(TC) :: k
        u = given_output_unit (unit); if (u < 0) return
        write (u, '(3X,A,1x,I0,5X,A,I3)') &
            'External:', tree%n_externals, 'Mask:', tree%mask
        write (u, '(3X,A,1x,I0,5X,A,I3)') &
            'Incoming:', tree%n_in, 'Mask:', tree%mask_in
        write (u, '(3X,A,1x,I0,5X,A,I3)') &
            'Branches:', tree%n_branches
        do k = size (tree%branch), 1, -1
            if (tree%branch(k)%set) &
                call phs_branch_write (tree%branch(k), unit=unit, kval=k)
        end do
        do k = 1, size (tree%mapping)
            call mapping_write (tree%mapping (k), unit, verbose=.true.)
        end do
        write (u, "(3x,A)") "Arrays: mass_sum, effective_mass, effective_width"
        do k = 1, size (tree%mass_sum)
            if (tree%branch(k)%set) then
                write (u, "(5x,I0,3(2x," // FMT_19 // ")") k, tree%mass_sum(k), &
                    tree%effective_mass(k), tree%effective_width(k)
            end if
        end do
    end subroutine phs_tree_write

    subroutine phs_branch_write (b, unit, kval)
        type(phs_branch_t), intent(in) :: b
        integer, intent(in), optional :: unit
        integer(TC), intent(in), optional :: kval
        integer :: u
        integer(TC) :: k
        character(len=6) :: tmp
        character(len=1) :: firstborn(2), sign_decay, sign_axis
        integer :: i
        u = given_output_unit (unit); if (u < 0) return
        k = 0; if (present (kval)) k = kval

```



```

if (b%origin /= 0) then
  write(tmp, '(A,I4,A)') '(', b%origin, ')'
else
  tmp = ' '
end if
do i=1, 2
  if (b%firstborn == i) then
    firstborn(i) = "*"
  else
    firstborn(i) = " "
  end if
end do
if (b%inverted_decay) then
  sign_decay = "-"
else
  sign_decay = "+"
end if
if (b%inverted_axis) then
  sign_axis = "-"
else
  sign_axis = "+"
end if
if (b%has_children) then
  if (b%has_friend) then
    write(u, '(4X,A1,I0,3x,A,1X,A,I0,A1,1x,I0,A1,1X,A1,1X,A,1x,I0)') &
      & ' ', k, tmp, &
      & 'Daughters: ', &
      & b%daughter(1), firstborn(1), &
      & b%daughter(2), firstborn(2), sign_decay, &
      & 'Friend: ', b%friend
  else
    write(u, '(4X,A1,I0,3x,A,1X,A,I0,A1,1x,I0,A1,1X,A1,1X,A)') &
      & ' ', k, tmp, &
      & 'Daughters: ', &
      & b%daughter(1), firstborn(1), &
      & b%daughter(2), firstborn(2), sign_decay, &
      & '(axis '//sign_axis//')'
  end if
else
  write(u, '(5X,I0)') k
end if
end subroutine phs_branch_write

```

19.7.3 PHS tree setup

Transformation into an array of branch codes and back

Assume that the tree/array has been created before with the appropriate length and is empty.

```

<PHS trees: public>+≡
public :: phs_tree_from_array

```

```

<PHS trees: phs tree: TBP>+≡
  procedure :: from_array => phs_tree_from_array

<PHS trees: procedures>+≡
  subroutine phs_tree_from_array (tree, a)
    class(phs_tree_t), intent(inout) :: tree
    integer(TC), dimension(:), intent(in) :: a
    integer :: i
    integer(TC) :: k
    <Set branches from array a>
    <Set external branches if necessary>
    <Check number of branches>
    <Determine the connections>
    contains
    <Subroutine: set relatives>
    end subroutine phs_tree_from_array

```

First, set all branches specified by the user. If all IN-bits are set, we invert the branch code.

```

<Set branches from array a>≡
  do i=1, size(a)
    k = a(i)
    if (iand(k, tree%mask_in) == tree%mask_in) k = ieor(tree%mask, k)
    tree%branch(k)%set = .true.
    tree%n_branches = tree%n_branches+1
  end do

```

The external branches are understood, so set them now if not yet done. In all cases ensure that the representative with one bit set is used, except for decays where the in-particle is represented by all OUT-bits set instead.

```

<Set external branches if necessary>≡
  do i=0, tree%n externals-1
    k = ibset(0,i)
    if (iand(k, tree%mask_in) == tree%mask_in) k = ieor(tree%mask, k)
    if (tree%branch(ieor(tree%mask, k))%set) then
      tree%branch(ieor(tree%mask, k))%set = .false.
      tree%branch(k)%set = .true.
    else if (.not.tree%branch(k)%set) then
      tree%branch(k)%set = .true.
      tree%n_branches = tree%n_branches+1
    end if
  end do

```

Now the number of branches set can be checked. Here we assume that the tree is binary. For three externals there are three branches in total, and for each additional external branches we get another internal one.

```

<Check number of branches>≡
  if (tree%n_branches /= tree%n externals*2-3) then
    call phs_tree_write (tree)
    call msg_bug &
      & (" Wrong number of branches set in phase space tree")
  end if

```

For all branches that are set, except for the externals, we try to find the daughter branches:

(Determine the connections)≡

```
do k=1, size (tree%branch)
  if (tree%branch(k)%set .and. tc_decay_level (k) /= 1) then
    call branch_set_relatives(k)
  end if
end do
```

To this end, we scan all codes less than the current code, whether we can find two branches which are set and which together give the current code. After that, the tree may still not be connected, but at least we know if a branch does not have daughters: This indicates some inconsistency.

The algorithm ensures that, at this stage, the first daughter has a smaller code value than the second one.

(Subroutine: set relatives)≡

```
subroutine branch_set_relatives (k)
  integer(TC), intent(in) :: k
  integer(TC) :: m,n
  do m=1, k-1
    if (iand(k,m)==m) then
      n = ieor(k,m)
      if ( tree%branch(m)%set .and. tree%branch(n)%set ) then
        tree%branch(k)%daughter(1) = m; tree%branch(k)%daughter(2) = n
        tree%branch(m)%mother      = k; tree%branch(n)%mother      = k
        tree%branch(m)%sibling      = n; tree%branch(n)%sibling      = m
        tree%branch(k)%has_children = .true.
        return
      end if
    end if
  end do
  call phs_tree_write (tree)
  call msg_bug &
    & (" Missing daughter branch(es) in phase space tree")
end subroutine branch_set_relatives
```

The inverse: this is trivial, fortunately.

Flip t -channel into s -channel

Flipping the tree is done upwards, beginning from the decay products. First we select a t -channel branch k : one which is set, which does have an IN-bit, and which is not an external particle.

Next, we determine the adjacent in-particle (called the 'friend' f here, since it will provide the reference axis for the angular integration). In addition, we look for the 'mother' and 'sibling' of this particle. If the latter field is empty, we select the (unique) other out-particle which has no mother, calling the internal subroutine `find_orphan`.

The flip is done as follows: We assume that the first daughter d is an s -channel line, which is true if the daughters are sorted. This will stay the first daughter. The second one is a t -channel line; it is exchanged with the 'sibling'

s. The new line which replaces the branch k is just the sum of s and d. In addition, we have to rearrange the relatives of s and d, as well of f.

Finally, we flip 'sibling' and 'friend' and set the new s-channel branch n which replaces the t-channel branch k. After this is complete, we are ready to execute another flip.

[Although the friend is not needed for the final flip, since it would be an initial particle anyway, we need to know whether we have t- or u-channel.]

```

<PHS trees: public>+≡
    public :: phs_tree_flip_t_to_s_channel

<PHS trees: procedures>+≡
    subroutine phs_tree_flip_t_to_s_channel (tree)
        type(phs_tree_t), intent(inout) :: tree
        integer(TC) :: k, f, m, n, d, s
        if (tree%n_in == 2) then
            FLIP: do k=3, tree%mask-1
                if (.not. tree%branch(k)%set) cycle FLIP
                f = iand(k,tree%mask_in)
                if (f==0 .or. f==k) cycle FLIP
                m = tree%branch(k)%mother
                s = tree%branch(k)%sibling
                if (s==0) call find_orphan(s)
                d = tree%branch(k)%daughter(1)
                n = ior(d,s)
                tree%branch(k)%set = .false.
                tree%branch(n)%set = .true.
                tree%branch(n)%origin = k
                tree%branch(n)%daughter(1) = d; tree%branch(d)%mother = n
                tree%branch(n)%daughter(2) = s; tree%branch(s)%mother = n
                tree%branch(n)%has_children = .true.
                tree%branch(d)%sibling = s; tree%branch(s)%sibling = d
                tree%branch(n)%sibling = f; tree%branch(f)%sibling = n
                tree%branch(n)%mother = m
                tree%branch(f)%mother = m
                if (m/=0) then
                    tree%branch(m)%daughter(1) = n
                    tree%branch(m)%daughter(2) = f
                end if
                tree%branch(n)%friend = f
                tree%branch(n)%has_friend = .true.
                tree%branch(n)%firstborn = 2
            end do FLIP
        end if
    contains
        subroutine find_orphan(s)
            integer(TC) :: s
            do s=1, tree%mask_out
                if (tree%branch(s)%set .and. tree%branch(s)%mother==0) return
            end do
            call phs_tree_write (tree)
            call msg_bug (" Can't flip phase space tree to channel")
        end subroutine find_orphan
    end subroutine phs_tree_flip_t_to_s_channel

```

After the tree has been flipped, one may need to determine what has become of a particular t -channel branch. This function gives the bincode of the flipped tree. If the original bincode does not contain IN-bits, we leave it as it is.

```

<PHS trees: procedures>+≡
function tc_flipped (tree, kt) result (ks)
  type(phs_tree_t), intent(in) :: tree
  integer(TC), intent(in) :: kt
  integer(TC) :: ks
  if (iand (kt, tree%mask_in) == 0) then
    ks = kt
  else
    ks = tree%branch(iand (kt, tree%mask_out))%mother
  end if
end function tc_flipped

```

Scan a tree and make sure that the first daughter has always a smaller code than the second one. Furthermore, delete any **friend** entry in the root branch – this branching has the incoming particle direction as axis anyway. Keep track of reordering by updating **inverted_axis**, **inverted_decay** and **firstborn**.

```

<PHS trees: public>+≡
public :: phs_tree_canonicalize

<PHS trees: procedures>+≡
subroutine phs_tree_canonicalize (tree)
  type(phs_tree_t), intent(inout) :: tree
  integer :: n_out
  integer(TC) :: k_out
  call branch_canonicalize (tree%branch(tree%mask_out))
  n_out = tree%n_externals - tree%n_in
  k_out = tree%mask_out
  if (tree%branch(k_out)%has_friend &
    & .and. tree%branch(k_out)%friend == ibset (0, n_out)) then
    tree%branch(k_out)%inverted_axis = .not.tree%branch(k_out)%inverted_axis
  end if
  tree%branch(k_out)%has_friend = .false.
  tree%branch(k_out)%friend = 0
contains
recursive subroutine branch_canonicalize (b)
  type(phs_branch_t), intent(inout) :: b
  integer(TC) :: d1, d2
  if (b%has_children) then
    d1 = b%daughter(1)
    d2 = b%daughter(2)
    if (d1 > d2) then
      b%daughter(1) = d2
      b%daughter(2) = d1
      b%inverted_decay = .not.b%inverted_decay
      if (b%firstborn /= 0) b%firstborn = 3 - b%firstborn
    end if
    call branch_canonicalize (tree%branch(b%daughter(1)))
    call branch_canonicalize (tree%branch(b%daughter(2)))
  end if
end subroutine branch_canonicalize

```

```
end subroutine phs_tree_canonicalize
```

Mappings

Initialize a mapping for the current tree. This is done while reading from file, so the mapping parameters are read, but applied to the flipped tree. Thus, the size of the array of mappings is given by the number of outgoing particles only.

```
<PHS trees: public>+≡
  public :: phs_tree_init_mapping

<PHS trees: phs tree: TBP>+≡
  procedure :: init_mapping => phs_tree_init_mapping

<PHS trees: procedures>+≡
  subroutine phs_tree_init_mapping (tree, k, type, pdg, model)
    class(phs_tree_t), intent(inout) :: tree
    integer(TC), intent(in) :: k
    type(string_t), intent(in) :: type
    integer, intent(in) :: pdg
    class(model_data_t), intent(in), target :: model
    integer(TC) :: kk
    kk = tc_flipped (tree, k)
    call mapping_init (tree%mapping(kk), kk, type, pdg, model)
  end subroutine phs_tree_init_mapping
```

Set the physical parameters for the mapping, using a specific parameter set. Also set the mass sum array.

```
<PHS trees: public>+≡
  public :: phs_tree_set_mapping_parameters

<PHS trees: phs tree: TBP>+≡
  procedure :: set_mapping_parameters => phs_tree_set_mapping_parameters

<PHS trees: procedures>+≡
  subroutine phs_tree_set_mapping_parameters &
    (tree, mapping_defaults, variable_limits)
    class(phs_tree_t), intent(inout) :: tree
    type(mapping_defaults_t), intent(in) :: mapping_defaults
    logical, intent(in) :: variable_limits
    integer(TC) :: k
    do k = 1, tree%n_branches_out
      call mapping_set_parameters &
        (tree%mapping(k), mapping_defaults, variable_limits)
    end do
  end subroutine phs_tree_set_mapping_parameters
```

Return the mapping for the sum of all outgoing particles. This should either be no mapping or a global s-channel mapping.

```
<PHS trees: public>+≡
  public :: phs_tree_assign_s_mapping
```

```

<PHS trees: procedures>+≡
  subroutine phs_tree_assign_s_mapping (tree, mapping)
    type(phs_tree_t), intent(in) :: tree
    type(mapping_t), intent(out) :: mapping
    mapping = tree%mapping(tree%mask_out)
  end subroutine phs_tree_assign_s_mapping

```

Kinematics

Fill the mass sum array, starting from the external particles and working down to the tree root. For each bincode k we scan the bits in k ; if only one is set, we take the physical mass of the corresponding external particle; if more than one is set, we sum up the two masses (which we know have already been set).

```

<PHS trees: public>+≡
  public :: phs_tree_set_mass_sum

<PHS trees: phs tree: TBP>+≡
  procedure :: set_mass_sum => phs_tree_set_mass_sum

<PHS trees: procedures>+≡
  subroutine phs_tree_set_mass_sum (tree, flv)
    class(phs_tree_t), intent(inout) :: tree
    type(flavor_t), dimension(:), intent(in) :: flv
    integer(TC) :: k
    integer :: i
    tree%mass_sum = 0
    do k = 1, tree%n_branches_out
      do i = 0, size(flav) - 1
        if (btest(k,i)) then
          if (ibclr(k,i) == 0) then
            tree%mass_sum(k) = flv(i+1)%get_mass ()
          else
            tree%mass_sum(k) = &
              tree%mass_sum(ibclr(k,i)) + tree%mass_sum(ibset(0,i))
          end if
        end if
      end do
    end do
  end subroutine phs_tree_set_mass_sum

```

Set the effective masses and widths. For each non-resonant branch in a tree, the effective mass is equal to the sum of the effective masses of the children (and analogous for the width). External particles have their real mass and width zero. For resonant branches, we insert mass and width from the corresponding mapping.

This routine has `phs_tree_set_mass_sum` and `phs_tree_set_mapping_parameters` as prerequisites.

```

<PHS trees: public>+≡
  public :: phs_tree_set_effective_masses

<PHS trees: phs tree: TBP>+≡
  procedure :: set_effective_masses => phs_tree_set_effective_masses

```

```

<PHS trees: procedures>+≡
  subroutine phs_tree_set_effective_masses (tree)
    class(phs_tree_t), intent(inout) :: tree
    tree%effective_mass = 0
    tree%effective_width = 0
    call set_masses_x (tree%mask_out)
  contains
    recursive subroutine set_masses_x (k)
      integer(TC), intent(in) :: k
      integer(TC) :: k1, k2
      if (tree%branch(k)%has_children) then
        k1 = tree%branch(k)%daughter(1)
        k2 = tree%branch(k)%daughter(2)
        call set_masses_x (k1)
        call set_masses_x (k2)
        if (mapping_is_s_channel (tree%mapping(k))) then
          tree%effective_mass(k) = mapping_get_mass (tree%mapping(k))
          tree%effective_width(k) = mapping_get_width (tree%mapping(k))
        else
          tree%effective_mass(k) = &
            tree%effective_mass(k1) + tree%effective_mass(k2)
          tree%effective_width(k) = &
            tree%effective_width(k1) + tree%effective_width(k2)
        end if
      else
        tree%effective_mass(k) = tree%mass_sum(k)
      end if
    end subroutine set_masses_x
  end subroutine phs_tree_set_effective_masses

```

Define step mappings, recursively, for the decay products of all intermediate resonances. Step mappings account for the fact that a branch may originate from a resonance, which almost replaces the upper limit on the possible invariant mass. The step mapping implements a smooth cutoff that interpolates between the resonance and the real kinematic limit. The mapping width determines the sharpness of the cutoff.

Step mappings are inserted only for branches that are not mapped otherwise.

At each branch, we record the mass that is effectively available for phase space, by taking the previous limit and subtracting the effective mass of the sibling branch. Widths are added, not subtracted.

If we encounter a resonance decay, we discard the previous limit and replace it by the mass and width of the resonance, also subtracting the sibling branch.

Initially, the limit is zero, so it becomes negative at any branch. Only if there is a resonance, the limit becomes positive. Whenever the limit is positive, and the current branch decays, we activate a step mapping for the current branch.

As a result, step mappings are implemented for all internal lines that originate from an intermediate resonance decay.

The flag `variable_limits` applies to the ultimate limit from the available energy, not to the intermediate resonances whose masses are always fixed.

This routine requires `phs_tree_set_effective_masses`

```

<PHS trees: public>+≡
  public :: phs_tree_set_step_mappings

```


(PHS trees: procedures)+≡

```

subroutine phs_tree_set_step_mappings (tree, exp_type, variable_limits)
  type(phs_tree_t), intent(inout) :: tree
  logical, intent(in) :: exp_type
  logical, intent(in) :: variable_limits
  type(string_t) :: map_str
  integer(TC) :: k
  if (exp_type) then
    map_str = "step_exp"
  else
    map_str = "step_hyp"
  end if
  k = tree%mask_out
  call set_step_mappings_x (k, 0._default, 0._default)
contains
  recursive subroutine set_step_mappings_x (k, m_limit, w_limit)
    integer(TC), intent(in) :: k
    real(default), intent(in) :: m_limit, w_limit
    integer(TC), dimension(2) :: kk
    real(default), dimension(2) :: m, w
    if (tree%branch(k)%has_children) then
      if (m_limit > 0) then
        if (.not. mapping_is_set (tree%mapping(k))) then
          call mapping_init (tree%mapping(k), k, map_str)
          call mapping_set_step_mapping_parameters (tree%mapping(k), &
            m_limit, w_limit, &
            variable_limits)
        end if
      end if
      kk = tree%branch(k)%daughter
      m = tree%effective_mass(kk)
      w = tree%effective_width(kk)
      if (mapping_is_s_channel (tree%mapping(k))) then
        call set_step_mappings_x (kk(1), &
          mapping_get_mass (tree%mapping(k)) - m(2), &
          mapping_get_width (tree%mapping(k)) + w(2))
        call set_step_mappings_x (kk(2), &
          mapping_get_mass (tree%mapping(k)) - m(1), &
          mapping_get_width (tree%mapping(k)) + w(1))
      else if (m_limit > 0) then
        call set_step_mappings_x (kk(1), &
          m_limit - m(2), &
          w_limit + w(2))
        call set_step_mappings_x (kk(2), &
          m_limit - m(1), &
          w_limit + w(1))
      else
        call set_step_mappings_x (kk(1), &
          - m(2), &
          + w(2))
        call set_step_mappings_x (kk(2), &
          - m(1), &
          + w(1))
      end if
    end if
  end if
end if

```

```

        end if
    end subroutine set_step_mappings_x
end subroutine phs_tree_set_step_mappings

```

Resonance structure

We identify the resonances within a tree as the set of s-channel mappings. The `resonance_history_t` type serves as the result container.

```

<PHS trees: phs tree: TBP>+≡
    procedure :: extract_resonance_history => phs_tree_extract_resonance_history

<PHS trees: procedures>+≡
    subroutine phs_tree_extract_resonance_history (tree, res_history)
        class(phs_tree_t), intent(in) :: tree
        type(resonance_history_t), intent(out) :: res_history
        type(resonance_info_t) :: res_info
        integer :: i
        if (allocated (tree%mapping)) then
            do i = 1, size (tree%mapping)
                associate (mapping => tree%mapping(i))
                    if (mapping%is_s_channel ()) then
                        call res_info%init (mapping%get_bincode (), mapping%get_flv (), &
                            n_out = tree%n externals - tree%n_in)
                        call res_history%add_resonance (res_info)
                    end if
                end associate
            end do
        end if
    end subroutine phs_tree_extract_resonance_history

```

Structural comparison

This function allows to check whether one tree is the permutation of another one. The permutation is applied to the second tree in the argument list. We do not make up a temporary permuted tree, but compare the two trees directly. The branches are scanned recursively, where for each daughter we check the friend and the mapping as well. Once a discrepancy is found, the recursion is exited immediately.

```

<PHS trees: public>+≡
    public :: phs_tree_equivalent

<PHS trees: procedures>+≡
    function phs_tree_equivalent (t1, t2, perm) result (is_equal)
        type(phs_tree_t), intent(in) :: t1, t2
        type(permutation_t), intent(in) :: perm
        logical :: equal, is_equal
        integer(TC) :: k1, k2, mask_in
        k1 = t1%mask_out
        k2 = t2%mask_out
        mask_in = t1%mask_in
        equal = .true.
    end function phs_tree_equivalent

```

```

call check (t1%branch(k1), t2%branch(k2), k1, k2)
is_equal = equal
contains
recursive subroutine check (b1, b2, k1, k2)
  type(phs_branch_t), intent(in) :: b1, b2
  integer(TC), intent(in) :: k1, k2
  integer(TC), dimension(2) :: d1, d2, pd2
  integer :: i
  if (.not.b1%has_friend .and. .not.b2%has_friend) then
    equal = .true.
  else if (b1%has_friend .and. b2%has_friend) then
    equal = (b1%friend == tc_permute (b2%friend, perm, mask_in))
  end if
  if (equal) then
    if (b1%has_children .and. b2%has_children) then
      d1 = b1%daughter
      d2 = b2%daughter
      do i=1, 2
        pd2(i) = tc_permute (d2(i), perm, mask_in)
      end do
      if (d1(1)==pd2(1) .and. d1(2)==pd2(2)) then
        equal = (b1%firstborn == b2%firstborn)
        if (equal) call check &
          & (t1%branch(d1(1)), t2%branch(d2(1)), d1(1), d2(1))
        if (equal) call check &
          & (t1%branch(d1(2)), t2%branch(d2(2)), d1(2), d2(2))
      else if (d1(1)==pd2(2) .and. d1(2)==pd2(1)) then
        equal = ( (b1%firstborn == 0 .and. b2%firstborn == 0) &
          & .or. (b1%firstborn == 3 - b2%firstborn) )
        if (equal) call check &
          & (t1%branch(d1(1)), t2%branch(d2(2)), d1(1), d2(2))
        if (equal) call check &
          & (t1%branch(d1(2)), t2%branch(d2(1)), d1(2), d2(1))
      else
        equal = .false.
      end if
    end if
  end if
  if (equal) then
    equal = (t1%mapping(k1) == t2%mapping(k2))
  end if
end subroutine check
end function phs_tree_equivalent

```

Scan two decay trees and determine the correspondence of mass variables, i.e., the permutation that transfers the ordered list of mass variables belonging to the second tree into the first one. Mass variables are assigned beginning from branches and ending at the root.

```

<PHS trees: public>+≡
  public :: phs_tree_find_msq_permutation

<PHS trees: procedures>+≡
  subroutine phs_tree_find_msq_permutation (tree1, tree2, perm2, msq_perm)
    type(phs_tree_t), intent(in) :: tree1, tree2

```

```

type(permutation_t), intent(in) :: perm2
type(permutation_t), intent(out) :: msq_perm
type(permutation_t) :: perm1
integer(TC) :: mask_in, root
integer(TC), dimension(:), allocatable :: index1, index2
integer :: i
allocate (index1 (tree1%n_msq), index2 (tree2%n_msq))
call permutation_init (perm1, permutation_size (perm2))
mask_in = tree1%mask_in
root = tree1%mask_out
i = 0
call tree_scan (tree1, root, perm1, index1)
i = 0
call tree_scan (tree2, root, perm2, index2)
call permutation_find (msq_perm, index1, index2)
contains
recursive subroutine tree_scan (tree, k, perm, index)
  type(phas_tree_t), intent(in) :: tree
  integer(TC), intent(in) :: k
  type(permutation_t), intent(in) :: perm
  integer, dimension(:), intent(inout) :: index
  if (tree%branch(k)%has_children) then
    call tree_scan (tree, tree%branch(k)%daughter(1), perm, index)
    call tree_scan (tree, tree%branch(k)%daughter(2), perm, index)
    i = i + 1
    if (i <= size (index)) index(i) = tc_permute (k, perm, mask_in)
  end if
end subroutine tree_scan
end subroutine phs_tree_find_msq_permutation

```

<PHS trees: public>+≡

```
public :: phs_tree_find_angle_permutation
```

<PHS trees: procedures>+≡

```

subroutine phs_tree_find_angle_permutation &
  (tree1, tree2, perm2, angle_perm, sig2)
  type(phas_tree_t), intent(in) :: tree1, tree2
  type(permutation_t), intent(in) :: perm2
  type(permutation_t), intent(out) :: angle_perm
  logical, dimension(:), allocatable, intent(out) :: sig2
  type(permutation_t) :: perm1
  integer(TC) :: mask_in, root
  integer(TC), dimension(:), allocatable :: index1, index2
  logical, dimension(:), allocatable :: sig1
  integer :: i
  allocate (index1 (tree1%n_angles), index2 (tree2%n_angles))
  allocate (sig1 (tree1%n_angles), sig2 (tree2%n_angles))
  call permutation_init (perm1, permutation_size (perm2))
  mask_in = tree1%mask_in
  root = tree1%mask_out
  i = 0
  call tree_scan (tree1, root, perm1, index1, sig1)
  i = 0
  call tree_scan (tree2, root, perm2, index2, sig2)

```

```

    call permutation_find (angle_perm, index1, index2)
contains
  recursive subroutine tree_scan (tree, k, perm, index, sig)
    type(phs_tree_t), intent(in) :: tree
    integer(TC), intent(in) :: k
    type(permutation_t), intent(in) :: perm
    integer, dimension(:), intent(inout) :: index
    logical, dimension(:), intent(inout) :: sig
    integer(TC) :: k1, k2, kp
    logical :: s
    if (tree%branch(k)%has_children) then
      k1 = tree%branch(k)%daughter(1)
      k2 = tree%branch(k)%daughter(2)
      s = (tc_permute(k1, perm, mask_in) < tc_permute(k2, perm, mask_in))
      kp = tc_permute (k, perm, mask_in)
      i = i + 1
      index(i) = kp
      sig(i) = s
      i = i + 1
      index(i) = - kp
      sig(i) = s
      call tree_scan (tree, k1, perm, index, sig)
      call tree_scan (tree, k2, perm, index, sig)
    end if
  end subroutine tree_scan
end subroutine phs_tree_find_angle_permutation

```

19.7.4 Phase-space evaluation

Phase-space volume

We compute the phase-space volume recursively, following the same path as for computing other kinematical variables. However, the volume depends just on $\sqrt{\hat{s}}$, not on the momentum configuration.

Note: counting branches, we may replace this by a simple formula.

```

<PHS trees: public>+≡
  public :: phs_tree_compute_volume

<PHS trees: procedures>+≡
  subroutine phs_tree_compute_volume (tree, sqrts, volume)
    type(phs_tree_t), intent(in) :: tree
    real(default), intent(in) :: sqrts
    real(default), intent(out) :: volume
    integer(TC) :: k
    k = tree%mask_out
    if (tree%branch(k)%has_children) then
      call compute_volume_x (tree%branch(k), k, volume, .true.)
    else
      volume = 1
    end if
  end subroutine
contains
  recursive subroutine compute_volume_x (b, k, volume, initial)
    type(phs_branch_t), intent(in) :: b

```

```

integer(TC), intent(in) :: k
real(default), intent(out) :: volume
logical, intent(in) :: initial
integer(TC) :: k1, k2
real(default) :: v1, v2
k1 = b%daughter(1); k2 = b%daughter(2)
if (tree%branch(k1)%has_children) then
  call compute_volume_x (tree%branch(k1), k1, v1, .false.)
else
  v1 = 1
end if
if (tree%branch(k2)%has_children) then
  call compute_volume_x (tree%branch(k2), k2, v2, .false.)
else
  v2 = 1
end if
if (initial) then
  volume = v1 * v2 / (4 * twopi5)
else
  volume = v1 * v2 * sqrts**2 / (4 * twopi2)
end if
end subroutine compute_volume_x
end subroutine phs_tree_compute_volume

```

Determine momenta

This is done in two steps: First the masses are determined. This step may fail, in which case `ok` is set to false. If successful, we generate angles and the actual momenta. The array `decay_p` serves for transferring the individual three-momenta of the daughter particles in their mother rest frame from the mass generation to the momentum generation step.

```

<PHS trees: public>+≡
  public :: phs_tree_compute_momenta_from_x

<PHS trees: procedures>+≡
  subroutine phs_tree_compute_momenta_from_x &
    (tree, prt, factor, volume, sqrts, x, ok)
    type(phs_tree_t), intent(inout) :: tree
    type(phs_prt_t), dimension(:), intent(inout) :: prt
    real(default), intent(out) :: factor, volume
    real(default), intent(in) :: sqrts
    real(default), dimension(:), intent(in) :: x
    logical, intent(out) :: ok
    real(default), dimension(tree%mask_out) :: decay_p
    integer :: n1, n2
    integer :: n_out
    if (tree%real_phsp) then
      n_out = tree%n_externals - tree%n_in - 1
      n1 = max (n_out-2, 0)
      n2 = n1 + max (2*n_out, 0)
    else
      n1 = tree%n_msq
      n2 = n1 + tree%n_angles
    end if
  end subroutine

```

```

end if
call phs_tree_set_msq &
    (tree, prt, factor, volume, decay_p, sqrts, x(1:n1), ok)
if (ok) call phs_tree_set_angles &
    (tree, prt, factor, decay_p, sqrts, x(n1+1:n2))
end subroutine phs_tree_compute_momenta_from_x

```

Mass generation is done recursively. The ok flag causes the filled tree to be discarded if set to `.false.` This happens if a three-momentum turns out to be imaginary, indicating impossible kinematics. The index ix tells us how far we have used up the input array x.

(PHS trees: procedures)+≡

```

subroutine phs_tree_set_msq &
    (tree, prt, factor, volume, decay_p, sqrts, x, ok)
type(phs_tree_t), intent(inout) :: tree
type(phs_prt_t), dimension(:), intent(inout) :: prt
real(default), intent(out) :: factor, volume
real(default), dimension(:), intent(out) :: decay_p
real(default), intent(in) :: sqrts
real(default), dimension(:), intent(in) :: x
logical, intent(out) :: ok
integer :: ix
integer(TC) :: k
real(default) :: m_tot
ok = .true.
ix = 1
k = tree%mask_out
m_tot = tree%mass_sum(k)
decay_p(k) = 0.
if (m_tot < sqrts .or. k == 1) then
    if (tree%branch(k)%has_children) then
        call set_msq_x (tree%branch(k), k, factor, volume, .true.)
    else
        factor = 1
        volume = 1
    end if
else
    ok = .false.
end if
contains
recursive subroutine set_msq_x (b, k, factor, volume, initial)
    type(phs_branch_t), intent(in) :: b
    integer(TC), intent(in) :: k
    real(default), intent(out) :: factor, volume
    logical, intent(in) :: initial
    real(default) :: msq, m, m_min, m_max, m1, m2, msq1, msq2, lda, rlda
    integer(TC) :: k1, k2
    real(default) :: f1, f2, v1, v2
    k1 = b%daughter(1); k2 = b%daughter(2)
    if (tree%branch(k1)%has_children) then
        call set_msq_x (tree%branch(k1), k1, f1, v1, .false.)
        if (.not.ok) return
    else

```

```

        f1 = 1;  v1 = 1
    end if
    if (tree%branch(k2)%has_children) then
        call set_msq_x (tree%branch(k2), k2, f2, v2, .false.)
        if (.not.ok) return
    else
        f2 = 1;  v2 = 1
    end if
    m_min = tree%mass_sum(k)
    if (initial) then
        msq = sqrts**2
        m = sqrts
        m_max = sqrts
        factor = f1 * f2
        volume = v1 * v2 / (4 * twopi5)
    else
        m_max = sqrts - m_tot + m_min
        call mapping_compute_msq_from_x &
            (tree%mapping(k), sqrts**2, m_min**2, m_max**2, msq, factor, &
             x(ix)); ix = ix + 1
        if (msq >= 0) then
            m = sqrt (msq)
            factor = f1 * f2 * factor
            volume = v1 * v2 * sqrts**2 / (4 * twopi2)
            call phs_prt_set_msq (prt(k), msq)
            call phs_prt_set_defined (prt(k))
        else
            ok = .false.
        end if
    end if
    if (ok) then
        msq1 = phs_prt_get_msq (prt(k1)); m1 = sqrt (msq1)
        msq2 = phs_prt_get_msq (prt(k2)); m2 = sqrt (msq2)
        lda = lambda (msq, msq1, msq2)
        if (lda > 0 .and. m > m1 + m2 .and. m <= m_max) then
            rlda = sqrt (lda)
            decay_p(k1) = rlda / (2*m)
            decay_p(k2) = - decay_p(k1)
            factor = rlda / msq * factor
        else
            ok = .false.
        end if
    end if
end subroutine set_msq_x

end subroutine phs_tree_set_msq

```

The heart of phase space generation: Now we have the invariant masses, let us generate angles. At each branch, we take a Lorentz transformation and augment it by a boost to the current particle rest frame, and by rotations ϕ and θ around the z and y axis, respectively. This transformation is passed down to the daughter particles, if present.

(PHS trees: procedures)+≡


```

subroutine phs_tree_set_angles (tree, prt, factor, decay_p, sqrts, x)
  type(phs_tree_t), intent(inout) :: tree
  type(phs_prt_t), dimension(:), intent(inout) :: prt
  real(default), intent(inout) :: factor
  real(default), dimension(:), intent(in) :: decay_p
  real(default), intent(in) :: sqrts
  real(default), dimension(:), intent(in) :: x
  integer :: ix
  integer(TC) :: k
  ix = 1
  k = tree%mask_out
  call set_angles_x (tree%branch(k), k)
contains
  recursive subroutine set_angles_x (b, k, L0)
    type(phs_branch_t), intent(in) :: b
    integer(TC), intent(in) :: k
    type(lorentz_transformation_t), intent(in), optional :: L0
    real(default) :: m, msq, ct, st, phi, f, E, p, bg
    type(lorentz_transformation_t) :: L, LL
    integer(TC) :: k1, k2
    type(vector3_t) :: axis
    p = decay_p(k)
    msq = phs_prt_get_msq (prt(k)); m = sqrt (msq)
    E = sqrt (msq + p**2)
    if (present (L0)) then
      call phs_prt_set_momentum (prt(k), L0 * vector4_moving (E,p,3))
    else
      call phs_prt_set_momentum (prt(k), vector4_moving (E,p,3))
    end if
    call phs_prt_set_defined (prt(k))
    if (b%has_children) then
      k1 = b%daughter(1)
      k2 = b%daughter(2)
      if (m > 0) then
        bg = p / m
      else
        bg = 0
      end if
      phi = x(ix) * twopi; ix = ix + 1
      call mapping_compute_ct_from_x &
        (tree%mapping(k), sqrts**2, ct, st, f, x(ix)); ix = ix + 1
      factor = factor * f
      if (.not. b%has_friend) then
        L = LT_compose_r2_r3_b3 (ct, st, cos(phi), sin(phi), bg)
        !!! The function above is equivalent to:
        ! L = boost (bg,3) * rotation (phi,3) * rotation (ct,st,2)
      else
        LL = boost (-bg,3); if (present (L0)) LL = LL * inverse(L0)
        axis = space_part ( &
          LL * phs_prt_get_momentum (prt(tree%branch(k)%friend)) )
        L = boost(bg,3) * rotation_to_2nd (vector3_canonical(3), axis) &
          * LT_compose_r2_r3_b3 (ct, st, cos(phi), sin(phi), 0._default)
      end if
      if (present (L0)) L = L0 * L
    end if
  end subroutine set_angles_x
end subroutine phs_tree_set_angles

```

```

        call set_angles_x (tree%branch(k1), k1, L)
        call set_angles_x (tree%branch(k2), k2, L)
    end if
end subroutine set_angles_x

end subroutine phs_tree_set_angles

```

Recover random numbers

For the other channels we want to compute the random numbers that would have generated the momenta that we already know.

```

<PHS trees: public>+≡
    public :: phs_tree_compute_x_from_momenta

<PHS trees: procedures>+≡
    subroutine phs_tree_compute_x_from_momenta (tree, prt, factor, sqrts, x)
        type(phs_tree_t), intent(inout) :: tree
        type(phs_prt_t), dimension(:), intent(in) :: prt
        real(default), intent(out) :: factor
        real(default), intent(in) :: sqrts
        real(default), dimension(:), intent(inout) :: x
        real(default), dimension(tree%mask_out) :: decay_p
        integer :: n1, n2
        n1 = tree%n_msq
        n2 = n1 + tree%n_angles
        call phs_tree_get_msq &
            (tree, prt, factor, decay_p, sqrts, x(1:n1))
        call phs_tree_get_angles &
            (tree, prt, factor, decay_p, sqrts, x(n1+1:n2))
    end subroutine phs_tree_compute_x_from_momenta

```

The inverse operation follows exactly the same steps. The tree is `inout` because it contains mappings whose parameters can be reset when the mapping is applied.

```

<PHS trees: procedures>+≡
    subroutine phs_tree_get_msq (tree, prt, factor, decay_p, sqrts, x)
        type(phs_tree_t), intent(inout) :: tree
        type(phs_prt_t), dimension(:), intent(in) :: prt
        real(default), intent(out) :: factor
        real(default), dimension(:), intent(out) :: decay_p
        real(default), intent(in) :: sqrts
        real(default), dimension(:), intent(inout) :: x
        integer :: ix
        integer(TC) :: k
        real(default) :: m_tot
        ix = 1
        k = tree%mask_out
        m_tot = tree%mass_sum(k)
        decay_p(k) = 0.
        if (tree%branch(k)%has_children) then
            call get_msq_x (tree%branch(k), k, factor, .true.)
        else

```

```

        factor = 1
    end if
contains
    recursive subroutine get_msq_x (b, k, factor, initial)
        type(phs_branch_t), intent(in) :: b
        integer(TC), intent(in) :: k
        real(default), intent(out) :: factor
        logical, intent(in) :: initial
        real(default) :: msq, m, m_min, m_max, msq1, msq2, lda, rlda
        integer(TC) :: k1, k2
        real(default) :: f1, f2
        k1 = b%daughter(1); k2 = b%daughter(2)
        if (tree%branch(k1)%has_children) then
            call get_msq_x (tree%branch(k1), k1, f1, .false.)
        else
            f1 = 1
        end if
        if (tree%branch(k2)%has_children) then
            call get_msq_x (tree%branch(k2), k2, f2, .false.)
        else
            f2 = 1
        end if
        m_min = tree%mass_sum(k)
        m_max = sqrts - m_tot + m_min
        msq = phs_prt_get_msq (prt(k)); m = sqrt (msq)
        if (initial) then
            factor = f1 * f2
        else
            call mapping_compute_x_from_msq &
                (tree%mapping(k), sqrts**2, m_min**2, m_max**2, msq, factor, &
                 x(ix)); ix = ix + 1
            factor = f1 * f2 * factor
        end if
        msq1 = phs_prt_get_msq (prt(k1))
        msq2 = phs_prt_get_msq (prt(k2))
        lda = lambda (msq, msq1, msq2)
        if (lda > 0) then
            rlda = sqrt (lda)
            decay_p(k1) = rlda / (2 * m)
            decay_p(k2) = - decay_p(k1)
            factor = rlda / msq * factor
        else
            decay_p(k1) = 0
            decay_p(k2) = 0
            factor = 0
        end if
    end subroutine get_msq_x

end subroutine phs_tree_get_msq

```

This subroutine is the most time-critical part of the whole program. Therefore, we do not exactly parallel the angle generation routine above but make sure that things get evaluated only if they are really needed, at the expense of

readability. Particularly important is to have as few multiplications of Lorentz transformations as possible.

(PHS trees: procedures)+≡

```

subroutine phs_tree_get_angles (tree, prt, factor, decay_p, sqrts, x)
  type(phs_tree_t), intent(inout) :: tree
  type(phs_prt_t), dimension(:), intent(in) :: prt
  real(default), intent(inout) :: factor
  real(default), dimension(:), intent(in) :: decay_p
  real(default), intent(in) :: sqrts
  real(default), dimension(:), intent(out) :: x
  integer :: ix
  integer(TC) :: k
  ix = 1
  k = tree%mask_out
  if (tree%branch(k)%has_children) then
    call get_angles_x (tree%branch(k), k)
  end if
contains
  recursive subroutine get_angles_x (b, k, ct0, st0, phi0, L0)
    type(phs_branch_t), intent(in) :: b
    integer(TC), intent(in) :: k
    real(default), intent(in), optional :: ct0, st0, phi0
    type(lorentz_transformation_t), intent(in), optional :: L0
    real(default) :: cp0, sp0, m, msq, ct, st, phi, bg, f
    type(lorentz_transformation_t) :: L, LL
    type(vector4_t) :: p1, pf
    type(vector3_t) :: n, axis
    integer(TC) :: k1, k2, kf
    logical :: has_friend, need_L
    k1 = b%daughter(1)
    k2 = b%daughter(2)
    kf = b%friend
    has_friend = b%has_friend
    if (present(L0)) then
      p1 = L0 * phs_prt_get_momentum (prt(k1))
      if (has_friend) pf = L0 * phs_prt_get_momentum (prt(kf))
    else
      p1 = phs_prt_get_momentum (prt(k1))
      if (has_friend) pf = phs_prt_get_momentum (prt(kf))
    end if
    if (present(phi0)) then
      cp0 = cos (phi0)
      sp0 = sin (phi0)
    end if
    msq = phs_prt_get_msq (prt(k)); m = sqrt (msq)
    if (m > 0) then
      bg = decay_p(k) / m
    else
      bg = 0
    end if
    if (has_friend) then
      if (present (phi0)) then
        axis = axis_from_p_r3_r2_b3 (pf, cp0, -sp0, ct0, -st0, -bg)
        LL = rotation_to_2nd (axis, vector3_canonical (3)) &

```

```

        * LT_compose_r3_r2_b3 (cp0, -sp0, ct0, -st0, -bg)
    else
        axis = axis_from_p_b3 (pf, -bg)
        LL = rotation_to_2nd (axis, vector3_canonical(3))
        if (.not. vanishes (bg)) LL = LL * boost(-bg, 3)
    end if
    n = space_part (LL * p1)
else if (present (phi0)) then
    n = axis_from_p_r3_r2_b3 (p1, cp0, -sp0, ct0, -st0, -bg)
else
    n = axis_from_p_b3 (p1, -bg)
end if
phi = azimuthal_angle (n)
x(ix) = phi / twopi; ix = ix + 1
ct = polar_angle_ct (n)
st = sqrt (1 - ct**2)
call mapping_compute_x_from_ct (tree%mapping(k), sqrts**2, ct, f, &
    x(ix)); ix = ix + 1
factor = factor * f
if (tree%branch(k1)%has_children .or. tree%branch(k2)%has_children) then
    need_L = .true.
    if (has_friend) then
        if (present (L0)) then
            L = LL * L0
        else
            L = LL
        end if
    else if (present (L0)) then
        L = LT_compose_r3_r2_b3 (cp0, -sp0, ct0, -st0, -bg) * L0
    else if (present (phi0)) then
        L = LT_compose_r3_r2_b3 (cp0, -sp0, ct0, -st0, -bg)
    else if (bg /= 0) then
        L = boost(-bg, 3)
    else
        need_L = .false.
    end if
    if (need_L) then
        if (tree%branch(k1)%has_children) &
            call get_angles_x (tree%branch(k1), k1, ct, st, phi, L)
        if (tree%branch(k2)%has_children) &
            call get_angles_x (tree%branch(k2), k2, ct, st, phi, L)
    else
        if (tree%branch(k1)%has_children) &
            call get_angles_x (tree%branch(k1), k1, ct, st, phi)
        if (tree%branch(k2)%has_children) &
            call get_angles_x (tree%branch(k2), k2, ct, st, phi)
    end if
end if
end subroutine get_angles_x
end subroutine phs_tree_get_angles

```

Auxiliary stuff

This calculates all momenta that are not yet known by summing up daughter particle momenta. The external particles must be known. Only composite particles not yet known are calculated.

```
(PHS trees: public)+≡
    public :: phs_tree_combine_particles

(PHS trees: procedures)+≡
    subroutine phs_tree_combine_particles (tree, prt)
        type(phs_tree_t), intent(in) :: tree
        type(phs_prt_t), dimension(:), intent(inout) :: prt
        call combine_particles_x (tree%mask_out)
    contains
        recursive subroutine combine_particles_x (k)
            integer(TC), intent(in) :: k
            integer :: k1, k2
            if (tree%branch(k)%has_children) then
                k1 = tree%branch(k)%daughter(1); k2 = tree%branch(k)%daughter(2)
                call combine_particles_x (k1)
                call combine_particles_x (k2)
                if (.not. prt(k)%defined) then
                    call phs_prt_combine (prt(k), prt(k1), prt(k2))
                end if
            end if
        end subroutine combine_particles_x
    end subroutine phs_tree_combine_particles
```

The previous routine is to be evaluated at runtime. Instead of scanning trees, we can as well set up a multiplication table. This is generated here. Note that the table is `intent(out)`.

```
(PHS trees: public)+≡
    public :: phs_tree_setup_prt_combinations

(PHS trees: procedures)+≡
    subroutine phs_tree_setup_prt_combinations (tree, comb)
        type(phs_tree_t), intent(in) :: tree
        integer, dimension(:,:), intent(out) :: comb
        comb = 0
        call setup_prt_combinations_x (tree%mask_out)
    contains
        recursive subroutine setup_prt_combinations_x (k)
            integer(TC), intent(in) :: k
            integer, dimension(2) :: kk
            if (tree%branch(k)%has_children) then
                kk = tree%branch(k)%daughter
                call setup_prt_combinations_x (kk(1))
                call setup_prt_combinations_x (kk(2))
                comb(:,k) = kk
            end if
        end subroutine setup_prt_combinations_x
    end subroutine phs_tree_setup_prt_combinations
```

```

<PHS trees: public>+≡
    public :: phs_tree_reshuffle_mappings

<PHS trees: procedures>+≡
    subroutine phs_tree_reshuffle_mappings (tree)
        type(phs_tree_t), intent(inout) :: tree
        integer(TC) :: k0, k_old, k_new, k2
        integer :: i
        type(mapping_t) :: mapping_tmp
        real(default) :: mass_tmp
        do i = 1, size (tree%momentum_link)
            if (i /= tree%momentum_link (i)) then
                k_old = 2**(i-tree%n_in-1)
                k_new = 2**(tree%momentum_link(i)-tree%n_in-1)
                k0 = tree%branch(k_old)%mother
                k2 = k_new + tree%branch(k_old)%sibling
                mapping_tmp = tree%mapping(k0)
                mass_tmp = tree%mass_sum(k0)
                tree%mapping(k0) = tree%mapping(k2)
                tree%mapping(k2) = mapping_tmp
                tree%mass_sum(k0) = tree%mass_sum(k2)
                tree%mass_sum(k2) = mass_tmp
            end if
        end do
    end subroutine phs_tree_reshuffle_mappings

```

```

<PHS trees: public>+≡
    public :: phs_tree_set_momentum_links

<PHS trees: procedures>+≡
    subroutine phs_tree_set_momentum_links (tree, list)
        type(phs_tree_t), intent(inout) :: tree
        integer, dimension(:), allocatable :: list
        tree%momentum_link = list
    end subroutine phs_tree_set_momentum_links

```

19.7.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<phs_trees_ut.f90>≡
    <File header>

    module phs_trees_ut
        use unit_tests
        use phs_trees_uti

    <Standard module head>

    <PHS trees: public test>

    contains

    <PHS trees: test driver>

```

```

end module phs_trees_ut

<phs_trees_uti.f90>≡
<File header>

module phs_trees_uti

  !!!<Use kinds>
  use kinds, only: TC
  <Use strings>
  use flavors, only: flavor_t
  use model_data, only: model_data_t

  use resonances, only: resonance_history_t
  use mappings, only: mapping_defaults_t

  use phs_trees

  <Standard module head>

  <PHS trees: test declarations>

  contains

  <PHS trees: tests>

end module phs_trees_uti
API: driver for the unit tests below.
<PHS trees: public test>≡
  public :: phs_trees_test
<PHS trees: test driver>≡
  subroutine phs_trees_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <PHS trees: execute tests>
  end subroutine phs_trees_test

Create a simple  $2 \rightarrow 3$  PHS tree and display it.
<PHS trees: execute tests>≡
  call test (phs_tree_1, "phs_tree_1", &
    "check phs tree setup", &
    u, results)
<PHS trees: test declarations>≡
  public :: phs_tree_1
<PHS trees: tests>≡
  subroutine phs_tree_1 (u)
    integer, intent(in) :: u
    type(phs_tree_t) :: tree
    type(model_data_t), target :: model
    type(flavor_t), dimension(5) :: flv
    integer :: i

```



```

write (u, "(A)")  "* Test output: phs_tree_1"
write (u, "(A)")  "* Purpose: test PHS tree routines"
write (u, "(A)")

write (u, "(A)")  "* Read model file"

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* Set up flavors"
write (u, "(A)")

call flv%init ([1, -2, 24, 5, -5], model)
do i = 1, 5
    write (u, "(1x)", advance="no")
    call flv(i)%write (u)
end do
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Create tree"
write (u, "(A)")

call tree%init (2, 3, 0, 0)
call tree%from_array ([integer(TC) :: 1, 2, 3, 4, 7, 8, 16])
call tree%set_mass_sum (flv)
call tree%set_effective_masses ()

call tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call tree%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_tree_1"

end subroutine phs_tree_1

```

The analogous tree with resonance (s-channel) mappings.

```

<PHS trees: execute tests>+≡
    call test (phs_tree_2, "phs_tree_2", &
        "check phs tree with resonances", &
        u, results)

<PHS trees: test declarations>+≡
    public :: phs_tree_2

<PHS trees: tests>+≡
    subroutine phs_tree_2 (u)
        integer, intent(in) :: u
        type(phs_tree_t) :: tree

```

```

type(model_data_t), target :: model
type(mapping_defaults_t) :: mapping_defaults
type(flavor_t), dimension(5) :: flv
type(resonance_history_t) :: res_history
integer :: i

write (u, "(A)")  "* Test output: phs_tree_2"
write (u, "(A)")  "* Purpose: test PHS tree with resonances"
write (u, "(A)")

write (u, "(A)")  "* Read model file"

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* Set up flavors"
write (u, "(A)")

call flv%init ([1, -2, 24, 5, -5], model)
do i = 1, 5
    write (u, "(1x)", advance="no")
    call flv(i)%write (u)
end do
write (u, *)

write (u, "(A)")
write (u, "(A)")  "* Create tree with mappings"
write (u, "(A)")

call tree%init (2, 3, 0, 0)
call tree%from_array ([integer(TC) :: 1, 2, 3, 4, 7, 8, 16])
call tree%set_mass_sum (flv)

call tree%init_mapping (3_TC, var_str ("s_channel"), -24, model)
call tree%init_mapping (7_TC, var_str ("s_channel"), 23, model)

call tree%set_mapping_parameters (mapping_defaults, variable_limits=.false.)
call tree%set_effective_masses ()

call tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract resonances from mappings"
write (u, "(A)")

call tree%extract_resonance_history (res_history)
call res_history%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call tree%final ()
call model%final ()

```

```
write (u, "(A)")  
write (u, "(A)")  "* Test output end: phs_tree_2"  
  
end subroutine phs_tree_2
```

19.8 The phase-space forest

Simply stated, a phase-space forest is a collection of phase-space trees. More precisely, a `phs_forest` object contains all parameterizations of phase space that `WHIZARD` will use for a single hard process, prepared in the form of `phs_tree` objects. This is suitable for evaluation by the `VAMP` integration package: each parameterization (tree) is a valid channel in the multi-channel adaptive integration, and each variable in a tree corresponds to an integration dimension, defined by an appropriate mapping of the $(0, 1)$ interval to the allowed range of the integration variable.

The trees are grouped in groves. The trees (integration channels) within a grove share a common weight, assuming that they are related by some approximate symmetry.

Trees/channels that are related by an exact symmetry are connected by an array of equivalences; each equivalence object holds the data that relate one channel to another.

The phase-space setup, i.e., the detailed structure of trees and forest, are read from a file. Therefore, this module also contains the syntax definition and the parser needed for interpreting this file.

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

```
  module phs_forests
```

```
    <Use kinds>
```

```
      use kinds, only: TC
```

```
    <Use strings>
```

```
      use io_units
```

```
      use format_defs, only: FMT_19
```

```
      use diagnostics
```

```
      use lorentz
```

```
      use numeric_utils
```

```
      use permutations
```

```
      use ifiles
```

```
      use syntax_rules
```

```
      use lexers
```

```
      use parser
```

```
      use model_data
```

```
      use model_data
```

```
      use flavors
```

```
      use interactions
```

```
      use phs_base
```

```
      use resonances, only: resonance_history_t
```

```
      use resonances, only: resonance_history_set_t
```

```
      use mappings
```

```
      use phs_trees
```

```
    <Standard module head>
```

```
    <PHS forests: public>
```

```

<PHS forests: types>

<PHS forests: interfaces>

<PHS forests: variables>

contains

<PHS forests: procedures>

end module phs_forests

```

19.8.1 Phase-space setup parameters

This transparent container holds the parameters that the algorithm needs for phase-space setup, with reasonable defaults.

The threshold mass (for considering a particle as effectively massless) is specified separately for s- and t-channel. The default is to treat W and Z bosons as massive in the s-channel, but as massless in the t-channel. The b -quark is treated always massless, the t -quark always massive.

```

<PHS forests: public>≡
  public :: phs_parameters_t

<PHS forests: types>≡
  type :: phs_parameters_t
    real(default) :: sqrts = 0
    real(default) :: m_threshold_s = 50._default
    real(default) :: m_threshold_t = 100._default
    integer :: off_shell = 1
    integer :: t_channel = 2
    logical :: keep_nonresonant = .true.
  contains
    <PHS forests: phs parameters: TBP>
  end type phs_parameters_t

```

Write phase-space parameters to file.

```

<PHS forests: phs parameters: TBP>≡
  procedure :: write => phs_parameters_write

<PHS forests: procedures>≡
  subroutine phs_parameters_write (phs_par, unit)
    class(phs_parameters_t), intent(in) :: phs_par
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A," // FMT_19 // ")") "sqrts          = ", phs_par%sqrts
    write (u, "(3x,A," // FMT_19 // ")") "m_threshold_s = ", phs_par%m_threshold_s
    write (u, "(3x,A," // FMT_19 // ")") "m_threshold_t = ", phs_par%m_threshold_t
    write (u, "(3x,A,I0)") "off_shell = ", phs_par%off_shell
    write (u, "(3x,A,I0)") "t_channel = ", phs_par%t_channel
    write (u, "(3x,A,L1)") "keep_nonresonant = ", phs_par%keep_nonresonant
  end subroutine phs_parameters_write

```

Read phase-space parameters from file.

```
(PHS forests: public)+≡
  public :: phs_parameters_read

(PHS forests: procedures)+≡
  subroutine phs_parameters_read (phs_par, unit)
    type(phs_parameters_t), intent(out) :: phs_par
    integer, intent(in) :: unit
    character(20) :: dummy
    character :: equals
    read (unit, *) dummy, equals, phs_par%sqrts
    read (unit, *) dummy, equals, phs_par%m_threshold_s
    read (unit, *) dummy, equals, phs_par%m_threshold_t
    read (unit, *) dummy, equals, phs_par%off_shell
    read (unit, *) dummy, equals, phs_par%t_channel
    read (unit, *) dummy, equals, phs_par%keep_nonresonant
  end subroutine phs_parameters_read
```

Comparison.

```
(PHS forests: interfaces)≡
  interface operator(==)
    module procedure phs_parameters_eq
  end interface
  interface operator(/=)
    module procedure phs_parameters_ne
  end interface

(PHS forests: procedures)+≡
  function phs_parameters_eq (phs_par1, phs_par2) result (equal)
    logical :: equal
    type(phs_parameters_t), intent(in) :: phs_par1, phs_par2
    equal = phs_par1%sqrts == phs_par2%sqrts &
      .and. phs_par1%m_threshold_s == phs_par2%m_threshold_s &
      .and. phs_par1%m_threshold_t == phs_par2%m_threshold_t &
      .and. phs_par1%off_shell == phs_par2%off_shell &
      .and. phs_par1%t_channel == phs_par2%t_channel &
      .and.(phs_par1%keep_nonresonant .eqv. phs_par2%keep_nonresonant)
  end function phs_parameters_eq

  function phs_parameters_ne (phs_par1, phs_par2) result (ne)
    logical :: ne
    type(phs_parameters_t), intent(in) :: phs_par1, phs_par2
    ne = phs_par1%sqrts /= phs_par2%sqrts &
      .or. phs_par1%m_threshold_s /= phs_par2%m_threshold_s &
      .or. phs_par1%m_threshold_t /= phs_par2%m_threshold_t &
      .or. phs_par1%off_shell /= phs_par2%off_shell &
      .or. phs_par1%t_channel /= phs_par2%t_channel &
      .or.(phs_par1%keep_nonresonant .neqv. phs_par2%keep_nonresonant)
  end function phs_parameters_ne
```

19.8.2 Equivalences

This type holds information about equivalences between phase-space trees. We make a linked list, where each node contains the two trees which are equivalent and the corresponding permutation of external particles. Two more arrays are to be filled: The permutation of mass variables and the permutation of angular variables, where the signature indicates a necessary exchange of daughter branches.

```
(PHS forests: types)+≡
  type :: equivalence_t
  private
  integer :: left, right
  type(permutation_t) :: perm
  type(permutation_t) :: msq_perm, angle_perm
  logical, dimension(:), allocatable :: angle_sig
  type(equivalence_t), pointer :: next => null ()
end type equivalence_t
```

```
(PHS forests: types)+≡
  type :: equivalence_list_t
  private
  integer :: length = 0
  type(equivalence_t), pointer :: first => null ()
  type(equivalence_t), pointer :: last => null ()
end type equivalence_list_t
```

Append an equivalence to the list

```
(PHS forests: procedures)+≡
  subroutine equivalence_list_add (eql, left, right, perm)
  type(equivalence_list_t), intent(inout) :: eql
  integer, intent(in) :: left, right
  type(permutation_t), intent(in) :: perm
  type(equivalence_t), pointer :: eq
  allocate (eq)
  eq%left = left
  eq%right = right
  eq%perm = perm
  if (associated (eql%last)) then
    eql%last%next => eq
  else
    eql%first => eq
  end if
  eql%last => eq
  eql%length = eql%length + 1
end subroutine equivalence_list_add
```

Delete the list contents. Has to be pure because it is called from an elemental subroutine.

```
(PHS forests: procedures)+≡
  pure subroutine equivalence_list_final (eql)
  type(equivalence_list_t), intent(inout) :: eql
  type(equivalence_t), pointer :: eq
```

```

do while (associated (eql%first))
  eq => eql%first
  eql%first => eql%first%next
  deallocate (eq)
end do
eql%last => null ()
eql%length = 0
end subroutine equivalence_list_final

```

Make a deep copy of the equivalence list. This allows for deep copies of groves and forests.

```

(PHS forests: interfaces)+≡
interface assignment(=)
  module procedure equivalence_list_assign
end interface

(PHS forests: procedures)+≡
subroutine equivalence_list_assign (eql_out, eql_in)
  type(equivalence_list_t), intent(out) :: eql_out
  type(equivalence_list_t), intent(in) :: eql_in
  type(equivalence_t), pointer :: eq, eq_copy
  eq => eql_in%first
  do while (associated (eq))
    allocate (eq_copy)
    eq_copy = eq
    eq_copy%next => null ()
    if (associated (eql_out%first)) then
      eql_out%last%next => eq_copy
    else
      eql_out%first => eq_copy
    end if
    eql_out%last => eq_copy
    eq => eq%next
  end do
end subroutine equivalence_list_assign

```

The number of list entries

```

(PHS forests: procedures)+≡
elemental function equivalence_list_length (eql) result (length)
  integer :: length
  type(equivalence_list_t), intent(in) :: eql
  length = eql%length
end function equivalence_list_length

```

Recursively write the equivalences list

```

(PHS forests: procedures)+≡
subroutine equivalence_list_write (eql, unit)
  type(equivalence_list_t), intent(in) :: eql
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  if (associated (eql%first)) then

```



```

        call equivalence_write_rec (eql%first, u)
    else
        write (u, *) " [empty]"
    end if
contains
recursive subroutine equivalence_write_rec (eq, u)
    type(equivalence_t), intent(in) :: eq
    integer, intent(in) :: u
    integer :: i
    write (u, "(3x,A,1x,I0,1x,I0,2x,A)", advance="no") &
        "Equivalence:", eq%left, eq%right, "Final state permutation:"
    call permutation_write (eq%perm, u)
    write (u, "(1x,12x,1x,A,1x)", advance="no") &
        "      msq permutation:  "
    call permutation_write (eq%msq_perm, u)
    write (u, "(1x,12x,1x,A,1x)", advance="no") &
        "      angle permutation:"
    call permutation_write (eq%angle_perm, u)
    write (u, "(1x,12x,1x,26x)", advance="no")
    do i = 1, size (eq%angle_sig)
        if (eq%angle_sig(i)) then
            write (u, "(1x,A)", advance="no") "+"
        else
            write (u, "(1x,A)", advance="no") "-"
        end if
    end do
    write (u, *)
    if (associated (eq%next)) call equivalence_write_rec (eq%next, u)
end subroutine equivalence_write_rec
end subroutine equivalence_list_write

```

19.8.3 Groves

A grove is a group of trees (phase-space channels) that share a common weight in the integration. Within a grove, channels can be declared equivalent, so they also share their integration grids (up to symmetries). The grove contains a list of equivalences. The `tree_count_offset` is the total number of trees of the preceding groves; when the trees are counted per forest (integration channels), the offset has to be added to all tree indices.

```

<PHS forests: types>+≡
    type :: phs_grove_t
    private
    integer :: tree_count_offset
    type(phs_tree_t), dimension(:), allocatable :: tree
    type(equivalence_list_t) :: equivalence_list
end type phs_grove_t

```

Call `phs_tree_init` which is also elemental:

```

<PHS forests: procedures>+≡
    elemental subroutine phs_grove_init &
        (grove, n_trees, n_in, n_out, n_masses, n_angles)

```

```

    type(phs_grove_t), intent(inout) :: grove
    integer, intent(in) :: n_trees, n_in, n_out, n_masses, n_angles
    grove%tree_count_offset = 0
    allocate (grove%tree (n_trees))
    call phs_tree_init (grove%tree, n_in, n_out, n_masses, n_angles)
end subroutine phs_grove_init

```

The trees do not have pointer components, thus no call to `phs_tree_final`:

```

<PHS forests: procedures>+≡
    elemental subroutine phs_grove_final (grove)
        type(phs_grove_t), intent(inout) :: grove
        deallocate (grove%tree)
        call equivalence_list_final (grove%equivalence_list)
    end subroutine phs_grove_final

```

Deep copy.

```

<PHS forests: interfaces>+≡
    interface assignment(=)
        module procedure phs_grove_assign0
        module procedure phs_grove_assign1
    end interface

<PHS forests: procedures>+≡
    subroutine phs_grove_assign0 (grove_out, grove_in)
        type(phs_grove_t), intent(out) :: grove_out
        type(phs_grove_t), intent(in) :: grove_in
        grove_out%tree_count_offset = grove_in%tree_count_offset
        if (allocated (grove_in%tree)) then
            allocate (grove_out%tree (size (grove_in%tree)))
            grove_out%tree = grove_in%tree
        end if
        grove_out%equivalence_list = grove_in%equivalence_list
    end subroutine phs_grove_assign0

    subroutine phs_grove_assign1 (grove_out, grove_in)
        type(phs_grove_t), dimension(:), intent(out) :: grove_out
        type(phs_grove_t), dimension(:), intent(in) :: grove_in
        integer :: i
        do i = 1, size (grove_in)
            call phs_grove_assign0 (grove_out(i), grove_in(i))
        end do
    end subroutine phs_grove_assign1

```

Get the global (s-channel) mappings. Implemented as a subroutine which returns an array (slice).

```

<PHS forests: procedures>+≡
    subroutine phs_grove_assign_s_mappings (grove, mapping)
        type(phs_grove_t), intent(in) :: grove
        type(mapping_t), dimension(:), intent(out) :: mapping
        integer :: i
        if (size (mapping) == size (grove%tree)) then
            do i = 1, size (mapping)

```

```

        call phs_tree_assign_s_mapping (grove%tree(i), mapping(i))
    end do
else
    call msg_bug ("phs_grove_assign_s_mappings: array size mismatch")
end if
end subroutine phs_grove_assign_s_mappings

```

19.8.4 The forest type

This is a collection of trees and associated particles. In a given tree, each branch code corresponds to a particle in the `prt` array. Furthermore, we have an array of mass sums which is independent of the decay tree and of the particular event. The mappings directly correspond to the decay trees, and the decay groves collect the trees in classes. The permutation list consists of all permutations of outgoing particles that map the decay forest onto itself.

The particle codes `flv` (one for each external particle) are needed for determining masses and such. The trees and associated information are collected in the `grove` array, together with a lookup table that associates tree indices to groves. Finally, the `prt` array serves as workspace for phase-space evaluation.

The `prt_combination` is a list of index pairs, namely the particle momenta pairs that need to be combined in order to provide all momentum combinations that the phase-space trees need to know.

```

(PHS forests: public)+≡
    public :: phs_forest_t

(PHS forests: types)+≡
    type :: phs_forest_t
    private
        integer :: n_in, n_out, n_tot
        integer :: n_masses, n_angles, n_dimensions
        integer :: n_trees, n_equivalences
        type(flavor_t), dimension(:), allocatable :: flv
        type(phs_grove_t), dimension(:), allocatable :: grove
        integer, dimension(:), allocatable :: grove_lookup
        type(phs_prt_t), dimension(:), allocatable :: prt_in
        type(phs_prt_t), dimension(:), allocatable :: prt_out
        type(phs_prt_t), dimension(:), allocatable :: prt
        integer(TC), dimension(:,:), allocatable :: prt_combination
        type(mapping_t), dimension(:), allocatable :: s_mapping
    contains
        (PHS forests: phs_forest: TBP)
    end type phs_forest_t

```

The initialization merely allocates memory. We have to know how many trees there are in each grove, so we can initialize everything. The number of groves is the size of the `n_tree` array.

In the `grove_lookup` table we store the grove index that belongs to each absolute tree index. The difference between the absolute index and the relative (to the grove) index is stored, for each grove, as `tree_count_offset`.

The particle array is allocated according to the total number of branches each tree has, but not filled.

```

(PHS forests: public)+≡
    public :: phs_forest_init

(PHS forests: procedures)+≡
    subroutine phs_forest_init (forest, n_tree, n_in, n_out)
        type(phs_forest_t), intent(inout) :: forest
        integer, dimension(:), intent(in) :: n_tree
        integer, intent(in) :: n_in, n_out
        integer :: g, count, k_root
        forest%n_in = n_in
        forest%n_out = n_out
        forest%n_tot = n_in + n_out
        forest%n_masses = max (n_out - 2, 0)
        forest%n_angles = max (2*n_out - 2, 0)
        forest%n_dimensions = forest%n_masses + forest%n_angles
        forest%n_trees = sum (n_tree)
        forest%n_equivalences = 0
        allocate (forest%grove (size (n_tree)))
        call phs_grove_init &
            (forest%grove, n_tree, n_in, n_out, forest%n_masses, &
             forest%n_angles)
        allocate (forest%grove_lookup (forest%n_trees))
        count = 0
        do g = 1, size (forest%grove)
            forest%grove(g)%tree_count_offset = count
            forest%grove_lookup (count+1:count+n_tree(g)) = g
            count = count + n_tree(g)
        end do
        allocate (forest%prt_in (n_in))
        allocate (forest%prt_out (forest%n_out))
        k_root = 2**forest%n_tot - 1
        allocate (forest%prt (k_root))
        allocate (forest%prt_combination (2, k_root))
        allocate (forest%s_mapping (forest%n_trees))
    end subroutine phs_forest_init

```

Assign the global (s-channel) mappings.

```

(PHS forests: public)+≡
    public :: phs_forest_set_s_mappings

(PHS forests: procedures)+≡
    subroutine phs_forest_set_s_mappings (forest)
        type(phs_forest_t), intent(inout) :: forest
        integer :: g, i0, i1, n
        do g = 1, size (forest%grove)
            call phs_forest_get_grove_bounds (forest, g, i0, i1, n)
            call phs_grove_assign_s_mappings &
                (forest%grove(g), forest%s_mapping(i0:i1))
        end do
    end subroutine phs_forest_set_s_mappings

```

The grove finalizer is called because it contains the equivalence list:

```

<PHS forests: public>+=
    public :: phs_forest_final

<PHS forests: procedures>+=
    subroutine phs_forest_final (forest)
        type(phs_forest_t), intent(inout) :: forest
        if (allocated (forest%grove)) then
            call phs_grove_final (forest%grove)
            deallocate (forest%grove)
        end if
        if (allocated (forest%grove_lookup)) deallocate (forest%grove_lookup)
        if (allocated (forest%prt)) deallocate (forest%prt)
        if (allocated (forest%s_mapping)) deallocate (forest%s_mapping)
    end subroutine phs_forest_final

```

19.8.5 Screen output

Write the particles that are non-null, then the trees which point to them:

```

<PHS forests: public>+=
    public :: phs_forest_write

<PHS forests: phs forest: TBP>=
    procedure :: write => phs_forest_write

<PHS forests: procedures>+=
    subroutine phs_forest_write (forest, unit)
        class(phs_forest_t), intent(in) :: forest
        integer, intent(in), optional :: unit
        integer :: u
        integer :: i, g, k
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1x,A)") "Phase space forest:"
        write (u, "(3x,A,I0)") "n_in = ", forest%n_in
        write (u, "(3x,A,I0)") "n_out = ", forest%n_out
        write (u, "(3x,A,I0)") "n_tot = ", forest%n_tot
        write (u, "(3x,A,I0)") "n_masses = ", forest%n_masses
        write (u, "(3x,A,I0)") "n_angles = ", forest%n_angles
        write (u, "(3x,A,I0)") "n_dim = ", forest%n_dimensions
        write (u, "(3x,A,I0)") "n_trees = ", forest%n_trees
        write (u, "(3x,A,I0)") "n_equiv = ", forest%n_equivalences
        write (u, "(3x,A)", advance="no") "flavors ="
        if (allocated (forest%flv)) then
            do i = 1, size (forest%flv)
                write (u, "(1x,I0)", advance="no") forest%flv(i)%get_pdg ()
            end do
            write (u, "(A)")
        else
            write (u, "(1x,A)") "[empty]"
        end if
        write (u, "(1x,A)") "Particle combinations:"
        if (allocated (forest%prt_combination)) then
            do k = 1, size (forest%prt_combination, 2)
                if (forest%prt_combination(1, k) /= 0) then

```

```

        write (u, "(3x,I0,1x,'<=',1x,I0,1x,'+',1x,I0)") &
            k, forest%prt_combination(:,k)
    end if
end do
else
    write (u, "(3x,A)") " [empty]"
end if
write (u, "(1x,A)") "Groves and trees:"
if (allocated (forest%grove)) then
    do g = 1, size (forest%grove)
        write (u, "(3x,A,1x,I0)") "Grove    ", g
        call phs_grove_write (forest%grove(g), unit)
    end do
else
    write (u, "(3x,A)") " [empty]"
end if
write (u, "(1x,A,I0)") "Total number of equivalences: ", &
    forest%n_equivalences
write (u, "(A)")
write (u, "(1x,A)") "Global s-channel mappings:"
if (allocated (forest%s_mapping)) then
    do i = 1, size (forest%s_mapping)
        associate (mapping => forest%s_mapping(i))
            if (mapping_is_s_channel (mapping) &
                .or. mapping_is_on_shell (mapping)) then
                write (u, "(1x,I0,':',1x)", advance="no") i
                call mapping_write (forest%s_mapping(i), unit)
            end if
        end associate
    end do
else
    write (u, "(3x,A)") " [empty]"
end if
write (u, "(A)")
write (u, "(1x,A)") "Incoming particles:"
if (allocated (forest%prt_in)) then
    if (any (phs_prt_is_defined (forest%prt_in))) then
        do i = 1, size (forest%prt_in)
            if (phs_prt_is_defined (forest%prt_in(i))) then
                write (u, "(1x,A,1x,I0)") "Particle", i
                call phs_prt_write (forest%prt_in(i), u)
            end if
        end do
    else
        write (u, "(3x,A)") "[all undefined]"
    end if
else
    write (u, "(3x,A)") " [empty]"
end if
write (u, "(A)")
write (u, "(1x,A)") "Outgoing particles:"
if (allocated (forest%prt_out)) then
    if (any (phs_prt_is_defined (forest%prt_out))) then
        do i = 1, size (forest%prt_out)

```

```

        if (phs_prt_is_defined (forest%prt_out(i))) then
            write (u, "(1x,A,1x,I0)" "Particle", i
                call phs_prt_write (forest%prt_out(i), u)
            end if
        end do
    else
        write (u, "(3x,A)" "[all undefined]"
    end if
else
    write (u, "(1x,A)" " [empty]"
end if
write (u, "(A)")
write (u, "(1x,A)" "Tree particles:"
if (allocated (forest%prt)) then
    if (any (phs_prt_is_defined (forest%prt))) then
        do i = 1, size (forest%prt)
            if (phs_prt_is_defined (forest%prt(i))) then
                write (u, "(1x,A,1x,I0)" "Particle", i
                    call phs_prt_write (forest%prt(i), u)
                end if
            end do
        else
            write (u, "(3x,A)" "[all undefined]"
        end if
    else
        write (u, "(3x,A)" " [empty]"
    end if
end subroutine phs_forest_write

subroutine phs_grove_write (grove, unit)
    type(phs_grove_t), intent(in) :: grove
    integer, intent(in), optional :: unit
    integer :: u
    integer :: t
    u = given_output_unit (unit); if (u < 0) return
    do t = 1, size (grove%tree)
        write (u, "(3x,A,I0)" "Tree      ", t
            call phs_tree_write (grove%tree(t), unit)
        end do
    write (u, "(1x,A)" "Equivalence list:"
        call equivalence_list_write (grove%equivalence_list, unit)
    end subroutine phs_grove_write

```

Deep copy.

```

<PHS forests: public>+≡
    public :: assignment(=)

<PHS forests: interfaces>+≡
    interface assignment(=)
        module procedure phs_forest_assign
    end interface

<PHS forests: procedures>+≡
    subroutine phs_forest_assign (forest_out, forest_in)

```

```

type(phs_forest_t), intent(out) :: forest_out
type(phs_forest_t), intent(in) :: forest_in
forest_out%n_in = forest_in%n_in
forest_out%n_out = forest_in%n_out
forest_out%n_tot = forest_in%n_tot
forest_out%n_masses = forest_in%n_masses
forest_out%n_angles = forest_in%n_angles
forest_out%n_dimensions = forest_in%n_dimensions
forest_out%n_trees = forest_in%n_trees
forest_out%n_equivalences = forest_in%n_equivalences
if (allocated (forest_in%flv)) then
    allocate (forest_out%flv (size (forest_in%flv)))
    forest_out%flv = forest_in%flv
end if
if (allocated (forest_in%grove)) then
    allocate (forest_out%grove (size (forest_in%grove)))
    forest_out%grove = forest_in%grove
end if
if (allocated (forest_in%grove_lookup)) then
    allocate (forest_out%grove_lookup (size (forest_in%grove_lookup)))
    forest_out%grove_lookup = forest_in%grove_lookup
end if
if (allocated (forest_in%prt_in)) then
    allocate (forest_out%prt_in (size (forest_in%prt_in)))
    forest_out%prt_in = forest_in%prt_in
end if
if (allocated (forest_in%prt_out)) then
    allocate (forest_out%prt_out (size (forest_in%prt_out)))
    forest_out%prt_out = forest_in%prt_out
end if
if (allocated (forest_in%prt)) then
    allocate (forest_out%prt (size (forest_in%prt)))
    forest_out%prt = forest_in%prt
end if
if (allocated (forest_in%s_mapping)) then
    allocate (forest_out%s_mapping (size (forest_in%s_mapping)))
    forest_out%s_mapping = forest_in%s_mapping
end if
if (allocated (forest_in%prt_combination)) then
    allocate (forest_out%prt_combination &
              (2, size (forest_in%prt_combination, 2)))
    forest_out%prt_combination = forest_in%prt_combination
end if
end subroutine phs_forest_assign

```

19.8.6 Accessing contents

Get the number of integration parameters

(PHS forests: public)+≡

```
public :: phs_forest_get_n_parameters
```

(PHS forests: procedures)+≡

```
function phs_forest_get_n_parameters (forest) result (n)
```



```

integer :: n
type(phs_forest_t), intent(in) :: forest
n = forest%n_dimensions
end function phs_forest_get_n_parameters

```

Get the number of integration channels

```

<PHS forests: public>+≡
public :: phs_forest_get_n_channels

<PHS forests: procedures>+≡
function phs_forest_get_n_channels (forest) result (n)
integer :: n
type(phs_forest_t), intent(in) :: forest
n = forest%n_trees
end function phs_forest_get_n_channels

```

Get the number of groves

```

<PHS forests: public>+≡
public :: phs_forest_get_n_groves

<PHS forests: procedures>+≡
function phs_forest_get_n_groves (forest) result (n)
integer :: n
type(phs_forest_t), intent(in) :: forest
n = size (forest%grove)
end function phs_forest_get_n_groves

```

Get the index bounds for a specific grove.

```

<PHS forests: public>+≡
public :: phs_forest_get_grove_bounds

<PHS forests: procedures>+≡
subroutine phs_forest_get_grove_bounds (forest, g, i0, i1, n)
type(phs_forest_t), intent(in) :: forest
integer, intent(in) :: g
integer, intent(out) :: i0, i1, n
n = size (forest%grove(g)%tree)
i0 = forest%grove(g)%tree_count_offset + 1
i1 = forest%grove(g)%tree_count_offset + n
end subroutine phs_forest_get_grove_bounds

```

Get the number of equivalences

```

<PHS forests: public>+≡
public :: phs_forest_get_n_equivalences

<PHS forests: procedures>+≡
function phs_forest_get_n_equivalences (forest) result (n)
integer :: n
type(phs_forest_t), intent(in) :: forest
n = forest%n_equivalences
end function phs_forest_get_n_equivalences

```

Return true if a particular channel has a global (s-channel) mapping; also return the resonance mass and width for this mapping.

```

(PHS forests: public)+≡
  public :: phs_forest_get_s_mapping
  public :: phs_forest_get_on_shell

(PHS forests: procedures)+≡
  subroutine phs_forest_get_s_mapping (forest, channel, flag, mass, width)
    type(phs_forest_t), intent(in) :: forest
    integer, intent(in) :: channel
    logical, intent(out) :: flag
    real(default), intent(out) :: mass, width
    flag = mapping_is_s_channel (forest%s_mapping(channel))
    if (flag) then
      mass = mapping_get_mass (forest%s_mapping(channel))
      width = mapping_get_width (forest%s_mapping(channel))
    else
      mass = 0
      width = 0
    end if
  end subroutine phs_forest_get_s_mapping

  subroutine phs_forest_get_on_shell (forest, channel, flag, mass)
    type(phs_forest_t), intent(in) :: forest
    integer, intent(in) :: channel
    logical, intent(out) :: flag
    real(default), intent(out) :: mass
    flag = mapping_is_on_shell (forest%s_mapping(channel))
    if (flag) then
      mass = mapping_get_mass (forest%s_mapping(channel))
    else
      mass = 0
    end if
  end subroutine phs_forest_get_on_shell

```

Extract the set of unique resonance histories, in form of an array.

```

(PHS forests: phs_forest: TBP)+≡
  procedure :: extract_resonance_history_set &
    => phs_forest_extract_resonance_history_set

(PHS forests: procedures)+≡
  subroutine phs_forest_extract_resonance_history_set &
    (forest, res_set, include_trivial)
    class(phs_forest_t), intent(in) :: forest
    type(resonance_history_set_t), intent(out) :: res_set
    logical, intent(in), optional :: include_trivial
    type(resonance_history_t) :: rh
    integer :: g, t
    logical :: triv
    triv = .false.; if (present (include_trivial)) triv = include_trivial
    call res_set%init ()
    do g = 1, size (forest%grove)
      associate (grove => forest%grove(g))
        do t = 1, size (grove%tree)

```

```

        call grove%tree(t)%extract_resonance_history (rh)
        call res_set%enter (rh, include_trivial)
    end do
end associate
end do
call res_set%freeze ()
end subroutine phs_forest_extract_resonance_history_set

```

19.8.7 Read the phase space setup from file

The phase space setup is stored in a file. The file may be generated by the `cascades` module below, or by other means. This file has to be read and parsed to create the PHS forest as the internal phase-space representation.

Create lexer and syntax:

(*PHS forests: procedures*) +=

```

subroutine define_phs_forest_syntax (ifile)
    type(ifile_t) :: ifile
    call ifile_append (ifile, "SEQ phase_space_list = process_phase_space*")
    call ifile_append (ifile, "SEQ process_phase_space = " &
        // "process_def process_header phase_space")
    call ifile_append (ifile, "SEQ process_def = process process_list")
    call ifile_append (ifile, "KEY process")
    call ifile_append (ifile, "LIS process_list = process_tag*")
    call ifile_append (ifile, "IDE process_tag")
    call ifile_append (ifile, "SEQ process_header = " &
        // "md5sum_process = md5sum " &
        // "md5sum_model_par = md5sum " &
        // "md5sum_phs_config = md5sum " &
        // "sqrts = real " &
        // "m_threshold_s = real " &
        // "m_threshold_t = real " &
        // "off_shell = integer " &
        // "t_channel = integer " &
        // "keep_nonresonant = logical")
    call ifile_append (ifile, "KEY '='")
    call ifile_append (ifile, "KEY '-'")
    call ifile_append (ifile, "KEY md5sum_process")
    call ifile_append (ifile, "KEY md5sum_model_par")
    call ifile_append (ifile, "KEY md5sum_phs_config")
    call ifile_append (ifile, "KEY sqrts")
    call ifile_append (ifile, "KEY m_threshold_s")
    call ifile_append (ifile, "KEY m_threshold_t")
    call ifile_append (ifile, "KEY off_shell")
    call ifile_append (ifile, "KEY t_channel")
    call ifile_append (ifile, "KEY keep_nonresonant")
    call ifile_append (ifile, "QUO md5sum = '""' ... '""'")
    call ifile_append (ifile, "REA real")
    call ifile_append (ifile, "INT integer")
    call ifile_append (ifile, "IDE logical")
    call ifile_append (ifile, "SEQ phase_space = grove_def+")
    call ifile_append (ifile, "SEQ grove_def = grove tree_def+")
    call ifile_append (ifile, "KEY grove")
end subroutine

```

```

call ifile_append (ifile, "SEQ tree_def = tree bincodes mapping*")
call ifile_append (ifile, "KEY tree")
call ifile_append (ifile, "SEQ bincodes = bincodes*")
call ifile_append (ifile, "INT bincodes")
call ifile_append (ifile, "SEQ mapping = map bincodes channel signed_pdg")
call ifile_append (ifile, "KEY map")
call ifile_append (ifile, "ALT channel = &
    &s_channel | t_channel | u_channel | &
    &collinear | infrared | radiation | on_shell")
call ifile_append (ifile, "KEY s_channel")
! call ifile_append (ifile, "KEY t_channel")    !!! Key already exists
call ifile_append (ifile, "KEY u_channel")
call ifile_append (ifile, "KEY collinear")
call ifile_append (ifile, "KEY infrared")
call ifile_append (ifile, "KEY radiation")
call ifile_append (ifile, "KEY on_shell")
call ifile_append (ifile, "ALT signed_pdg = &
    &pdg | negative_pdg")
call ifile_append (ifile, "SEQ negative_pdg = '-' pdg")
call ifile_append (ifile, "INT pdg")
end subroutine define_phs_forest_syntax

```

The model-file syntax and lexer are fixed, therefore stored as module variables:

```

<PHS forests: variables>≡
    type(syntax_t), target, save :: syntax_phs_forest

<PHS forests: public>+≡
    public :: syntax_phs_forest_init

<PHS forests: procedures>+≡
    subroutine syntax_phs_forest_init ()
        type(ifile_t) :: ifile
        call define_phs_forest_syntax (ifile)
        call syntax_init (syntax_phs_forest, ifile)
        call ifile_final (ifile)
    end subroutine syntax_phs_forest_init

<PHS forests: procedures>+≡
    subroutine lexer_init_phs_forest (lexer)
        type(lexer_t), intent(out) :: lexer
        call lexer_init (lexer, &
            comment_chars = "#!", &
            quote_chars = "'", &
            quote_match = "'", &
            single_chars = "-", &
            special_class = ["="] , &
            keyword_list = syntax_get_keyword_list_ptr (syntax_phs_forest))
    end subroutine lexer_init_phs_forest

<PHS forests: public>+≡
    public :: syntax_phs_forest_final

<PHS forests: procedures>+≡

```

```

subroutine syntax_phs_forest_final ()
  call syntax_final (syntax_phs_forest)
end subroutine syntax_phs_forest_final

```

<PHS forests: public>+≡

```

public :: syntax_phs_forest_write

```

<PHS forests: procedures>+≡

```

subroutine syntax_phs_forest_write (unit)
  integer, intent(in), optional :: unit
  call syntax_write (syntax_phs_forest, unit)
end subroutine syntax_phs_forest_write

```

The concrete parser and interpreter. Generate an input stream for the external `unit`, read the parse tree (with given `syntax` and `lexer`) from this stream, and transfer the contents of the parse tree to the PHS forest.

We look for the matching `process` tag, count groves and trees for initializing the forest, and fill the trees.

If the optional parameters are set, compare the parameters stored in the file to those. Set `match` true if everything agrees.

<PHS forests: public>+≡

```

public :: phs_forest_read

```

<PHS forests: interfaces>+≡

```

interface phs_forest_read
  module procedure phs_forest_read_file
  module procedure phs_forest_read_unit
  module procedure phs_forest_read_parse_tree
end interface

```

<PHS forests: procedures>+≡

```

subroutine phs_forest_read_file &
  (forest, filename, process_id, n_in, n_out, model, found, &
   md5sum_process, md5sum_model_par, &
   md5sum_phs_config, phs_par, match)
  type(phs_forest_t), intent(out) :: forest
  type(string_t), intent(in) :: filename
  type(string_t), intent(in) :: process_id
  integer, intent(in) :: n_in, n_out
  class(model_data_t), intent(in), target :: model
  logical, intent(out) :: found
  character(32), intent(in), optional :: &
    md5sum_process, md5sum_model_par, md5sum_phs_config
  type(phs_parameters_t), intent(in), optional :: phs_par
  logical, intent(out), optional :: match
  type(parse_tree_t), target :: parse_tree
  type(stream_t), target :: stream
  type(lexer_t) :: lexer
  call lexer_init_phs_forest (lexer)
  call stream_init (stream, char (filename))
  call lexer_assign_stream (lexer, stream)
  call parse_tree_init (parse_tree, syntax_phs_forest, lexer)
  call phs_forest_read (forest, parse_tree, &

```

```

        process_id, n_in, n_out, model, found, &
        md5sum_process, md5sum_model_par, md5sum_phs_config, phs_par, match)
    call stream_final (stream)
    call lexer_final (lexer)
    call parse_tree_final (parse_tree)
end subroutine phs_forest_read_file

subroutine phs_forest_read_unit &
    (forest, unit, process_id, n_in, n_out, model, found, &
     md5sum_process, md5sum_model_par, md5sum_phs_config, &
     phs_par, match)
    type(phs_forest_t), intent(out) :: forest
    integer, intent(in) :: unit
    type(string_t), intent(in) :: process_id
    integer, intent(in) :: n_in, n_out
    class(model_data_t), intent(in), target :: model
    logical, intent(out) :: found
    character(32), intent(in), optional :: &
        md5sum_process, md5sum_model_par, md5sum_phs_config
    type(phs_parameters_t), intent(in), optional :: phs_par
    logical, intent(out), optional :: match
    type(parse_tree_t), target :: parse_tree
    type(stream_t), target :: stream
    type(lexer_t) :: lexer
    call lexer_init_phs_forest (lexer)
    call stream_init (stream, unit)
    call lexer_assign_stream (lexer, stream)
    call parse_tree_init (parse_tree, syntax_phs_forest, lexer)
    call phs_forest_read (forest, parse_tree, &
        process_id, n_in, n_out, model, found, &
        md5sum_process, md5sum_model_par, md5sum_phs_config, &
        phs_par, match)
    call stream_final (stream)
    call lexer_final (lexer)
    call parse_tree_final (parse_tree)
end subroutine phs_forest_read_unit

subroutine phs_forest_read_parse_tree &
    (forest, parse_tree, process_id, n_in, n_out, model, found, &
     md5sum_process, md5sum_model_par, md5sum_phs_config, &
     phs_par, match)
    type(phs_forest_t), intent(out) :: forest
    type(parse_tree_t), intent(in), target :: parse_tree
    type(string_t), intent(in) :: process_id
    integer, intent(in) :: n_in, n_out
    class(model_data_t), intent(in), target :: model
    logical, intent(out) :: found
    character(32), intent(in), optional :: &
        md5sum_process, md5sum_model_par, md5sum_phs_config
    type(phs_parameters_t), intent(in), optional :: phs_par
    logical, intent(out), optional :: match
    type(parse_node_t), pointer :: node_header, node_phs, node_grove
    integer :: n_grove, g
    integer, dimension(:), allocatable :: n_tree

```

```

integer :: t
node_header => parse_tree_get_process_ptr (parse_tree, process_id)
found = associated (node_header); if (.not. found) return
if (present (match)) then
    call phs_forest_check_input (node_header, &
        md5sum_process, md5sum_model_par, md5sum_phs_config, phs_par, match)
    if (.not. match) return
end if
node_phs => parse_node_get_next_ptr (node_header)
n_grove = parse_node_get_n_sub (node_phs)
allocate (n_tree (n_grove))
do g = 1, n_grove
    node_grove => parse_node_get_sub_ptr (node_phs, g)
    n_tree(g) = parse_node_get_n_sub (node_grove) - 1
end do
call phs_forest_init (forest, n_tree, n_in, n_out)
do g = 1, n_grove
    node_grove => parse_node_get_sub_ptr (node_phs, g)
    do t = 1, n_tree(g)
        call phs_tree_set (forest%grove(g)%tree(t), &
            parse_node_get_sub_ptr (node_grove, t+1), model)
    end do
end do
end subroutine phs_forest_read_parse_tree

```

Check the input for consistency. If any MD5 sum or phase-space parameter disagrees, the phase-space file cannot be used. The MD5 sum checks are skipped if the stored MD5 sum is empty.

(*PHS forests: procedures*) +=

```

subroutine phs_forest_check_input (pn_header, &
    md5sum_process, md5sum_model_par, md5sum_phs_config, phs_par, match)
type(parse_node_t), intent(in), target :: pn_header
character(32), intent(in) :: &
    md5sum_process, md5sum_model_par, md5sum_phs_config
type(phs_parameters_t), intent(in), optional :: phs_par
logical, intent(out) :: match
type(parse_node_t), pointer :: pn_md5sum, pn_rval, pn_ival, pn_lval
character(32) :: md5sum
type(phs_parameters_t) :: phs_par_old
character(1) :: lstr
pn_md5sum => parse_node_get_sub_ptr (pn_header, 3)
md5sum = parse_node_get_string (pn_md5sum)
if (md5sum /= "" .and. md5sum /= md5sum_process) then
    call msg_message ("Phase space: discarding old configuration &
        &(process changed)")
    match = .false.; return
end if
pn_md5sum => parse_node_get_next_ptr (pn_md5sum, 3)
md5sum = parse_node_get_string (pn_md5sum)
if (md5sum /= "" .and. md5sum /= md5sum_model_par) then
    call msg_message ("Phase space: discarding old configuration &
        &(model parameters changed)")
    match = .false.; return

```

```

end if
pn_md5sum => parse_node_get_next_ptr (pn_md5sum, 3)
md5sum = parse_node_get_string (pn_md5sum)
if (md5sum /= "" .and. md5sum /= md5sum_phs_config) then
    call msg_message ("Phase space: discarding old configuration &
        &(configuration parameters changed)")
    match = .false.; return
end if
if (present (phs_par)) then
    pn_rval => parse_node_get_next_ptr (pn_md5sum, 3)
    phs_par_old%sqrts = parse_node_get_real (pn_rval)
    pn_rval => parse_node_get_next_ptr (pn_rval, 3)
    phs_par_old%m_threshold_s = parse_node_get_real (pn_rval)
    pn_rval => parse_node_get_next_ptr (pn_rval, 3)
    phs_par_old%m_threshold_t = parse_node_get_real (pn_rval)
    pn_ival => parse_node_get_next_ptr (pn_rval, 3)
    phs_par_old%off_shell = parse_node_get_integer (pn_ival)
    pn_ival => parse_node_get_next_ptr (pn_ival, 3)
    phs_par_old%t_channel = parse_node_get_integer (pn_ival)
    pn_lval => parse_node_get_next_ptr (pn_ival, 3)
    lstr = parse_node_get_string (pn_lval)
    read (lstr, "(L1)") phs_par_old%keep_nonresonant
    if (phs_par_old /= phs_par) then
        call msg_message &
            ("Phase space: discarding old configuration &
                &(configuration parameters changed)")
        match = .false.; return
    end if
end if
match = .true.
end subroutine phs_forest_check_input

```

Initialize a specific tree in the forest, using the contents of the 'tree' node. First, count the bincodes, allocate an array and read them in, and make the tree. Each *t*-channel tree is flipped to *s*-channel. Then, find mappings and initialize them.

(*PHS forests: procedures*) +=

```

subroutine phs_tree_set (tree, node, model)
    type(phs_tree_t), intent(inout) :: tree
    type(parse_node_t), intent(in), target :: node
    class(model_data_t), intent(in), target :: model
    type(parse_node_t), pointer :: node_bincodes, node_mapping, pn_pdg
    integer :: n_bincodes, offset
    integer(TC), dimension(:), allocatable :: bincodes
    integer :: b, n_mappings, m
    integer(TC) :: k
    type(string_t) :: type
    integer :: pdg
    node_bincodes => parse_node_get_sub_ptr (node, 2)
    if (associated (node_bincodes)) then
        select case (char (parse_node_get_rule_key (node_bincodes)))
        case ("bincodes")
            n_bincodes = parse_node_get_n_sub (node_bincodes)
            offset = 2

```



```

        case default
            n_bincodes = 0
            offset = 1
        end select
    else
        n_bincodes = 0
        offset = 2
    end if
    allocate (bincode (n_bincodes))
    do b = 1, n_bincodes
        bincode(b) = parse_node_get_integer &
            (parse_node_get_sub_ptr (node_bincodes, b))
    end do
    call phs_tree_from_array (tree, bincode)
    call phs_tree_flip_t_to_s_channel (tree)
    call phs_tree_canonicalize (tree)
    n_mappings = parse_node_get_n_sub (node) - offset
    do m = 1, n_mappings
        node_mapping => parse_node_get_sub_ptr (node, m + offset)
        k = parse_node_get_integer &
            (parse_node_get_sub_ptr (node_mapping, 2))
        type = parse_node_get_key &
            (parse_node_get_sub_ptr (node_mapping, 3))
        pn_pdg => parse_node_get_sub_ptr (node_mapping, 4)
        select case (char (pn_pdg%get_rule_key ()))
            case ("pdg")
                pdg = pn_pdg%get_integer ()
            case ("negative_pdg")
                pdg = - parse_node_get_integer (pn_pdg%get_sub_ptr (2))
            end select
        call phs_tree_init_mapping (tree, k, type, pdg, model)
    end do
end subroutine phs_tree_set

```

19.8.8 Preparation

The trees that we read from file do not carry flavor information. This is set separately:

The flavor list must be unique for a unique set of masses; if a given particle can have different flavor, the mass must be degenerate, so we can choose one of the possible flavor combinations.

(PHS forests: public)+≡

```
public :: phs_forest_set_flavors
```

(PHS forests: procedures)+≡

```

subroutine phs_forest_set_flavors (forest, flv, reshuffle, flv_extra)
    type(phs_forest_t), intent(inout) :: forest
    type(flavor_t), dimension(:), intent(in) :: flv
    integer, intent(in), dimension(:), allocatable, optional :: reshuffle
    type(flavor_t), intent(in), optional :: flv_extra
    integer :: i, n_flv0
    if (present (reshuffle) .and. present (flv_extra)) then
        n_flv0 = size (flv)
    end if
end subroutine

```

```

do i = 1, n_flv0
  if (reshuffle(i) <= n_flv0) then
    forest%flv(i) = flv (reshuffle(i))
  else
    forest%flv(i) = flv_extra
  end if
end do
else
  allocate (forest%flv (size (flv)))
  forest%flv = flv
end if
end subroutine phs_forest_set_flavors

```

(PHS forests: public)+≡

```
public :: phs_forest_set_momentum_links
```

(PHS forests: procedures)+≡

```

subroutine phs_forest_set_momentum_links (forest, list)
  type(phs_forest_t), intent(inout) :: forest
  integer, intent(in), dimension(:), allocatable :: list
  integer :: g, t
  do g = 1, size (forest%grove)
    do t = 1, size (forest%grove(g)%tree)
      associate (tree => forest%grove(g)%tree(t))
        call phs_tree_set_momentum_links (tree, list)
      !!! call phs_tree_reshuffle_mappings (tree)
      end associate
    end do
  end do
end subroutine phs_forest_set_momentum_links

```

Once the parameter set is fixed, the masses and the widths of the particles are known and the `mass_sum` arrays as well as the mapping parameters can be computed. Note that order is important: we first compute the mass sums, then the ordinary mappings. The resonances obtained here determine the effective masses, which in turn are used to implement step mappings for resonance decay products that are not mapped otherwise.

(PHS forests: public)+≡

```
public :: phs_forest_set_parameters
```

(PHS forests: procedures)+≡

```

subroutine phs_forest_set_parameters &
  (forest, mapping_defaults, variable_limits)
  type(phs_forest_t), intent(inout) :: forest
  type(mapping_defaults_t), intent(in) :: mapping_defaults
  logical, intent(in) :: variable_limits
  integer :: g, t
  do g = 1, size (forest%grove)
    do t = 1, size (forest%grove(g)%tree)
      call phs_tree_set_mass_sum &
        (forest%grove(g)%tree(t), forest%flv(forest%n_in+1:))
      call phs_tree_set_mapping_parameters (forest%grove(g)%tree(t), &
        mapping_defaults, variable_limits)
    end do
  end do
end subroutine phs_forest_set_parameters

```

```

        call phs_tree_set_effective_masses (forest%grove(g)%tree(t))
        if (mapping_defaults%step_mapping) then
            call phs_tree_set_step_mappings (forest%grove(g)%tree(t), &
                mapping_defaults%step_mapping_exp, variable_limits)
        end if
    end do
end do
end subroutine phs_forest_set_parameters

```

Generate the particle combination table. Scan all trees and merge their individual combination tables. At the end, valid entries are non-zero, and they indicate the indices of a pair of particles to be combined to a new particle. If a particle is accessible by more than one tree (this is usual), only keep the first possibility.

```

<PHS forests: public>+≡
    public :: phs_forest_setup_prt_combinations

<PHS forests: procedures>+≡
    subroutine phs_forest_setup_prt_combinations (forest)
        type(phs_forest_t), intent(inout) :: forest
        integer :: g, t
        integer, dimension(:, :), allocatable :: tree_prt_combination
        forest%prt_combination = 0
        allocate (tree_prt_combination (2, size (forest%prt_combination, 2)))
        do g = 1, size (forest%grove)
            do t = 1, size (forest%grove(g)%tree)
                call phs_tree_setup_prt_combinations &
                    (forest%grove(g)%tree(t), tree_prt_combination)
                where (tree_prt_combination /= 0 .and. forest%prt_combination == 0)
                    forest%prt_combination = tree_prt_combination
                end where
            end do
        end do
    end subroutine phs_forest_setup_prt_combinations

```

19.8.9 Accessing the particle arrays

Set the incoming particles from the contents of an interaction.

```

<PHS forests: public>+≡
    public :: phs_forest_set_prt_in

<PHS forests: interfaces>+≡
    interface phs_forest_set_prt_in
        module procedure phs_forest_set_prt_in_int, phs_forest_set_prt_in_mom
    end interface phs_forest_set_prt_in

<PHS forests: procedures>+≡
    subroutine phs_forest_set_prt_in_int (forest, int, lt_cm_to_lab)
        type(phs_forest_t), intent(inout) :: forest
        type(interaction_t), intent(in) :: int
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
        if (present (lt_cm_to_lab)) then
            call phs_prt_set_momentum (forest%prt_in, &
                inverse (lt_cm_to_lab) * &

```

```

        int%get_momenta (outgoing=.false.))
    else
        call phs_prt_set_momentum (forest%prt_in, &
            int%get_momenta (outgoing=.false.))
    end if
    associate (m_in => forest%flv(:forest%n_in)%get_mass ())
        call phs_prt_set_msq (forest%prt_in, m_in ** 2)
    end associate
    call phs_prt_set_defined (forest%prt_in)
end subroutine phs_forest_set_prt_in_int

subroutine phs_forest_set_prt_in_mom (forest, mom, lt_cm_to_lab)
    type(phs_forest_t), intent(inout) :: forest
    type(vector4_t), dimension(size (forest%prt_in)), intent(in) :: mom
    type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
    if (present (lt_cm_to_lab)) then
        call phs_prt_set_momentum (forest%prt_in, &
            inverse (lt_cm_to_lab) * mom)
    else
        call phs_prt_set_momentum (forest%prt_in, mom)
    end if
    associate (m_in => forest%flv(:forest%n_in)%get_mass ())
        call phs_prt_set_msq (forest%prt_in, m_in ** 2)
    end associate
    call phs_prt_set_defined (forest%prt_in)
end subroutine phs_forest_set_prt_in_mom

```

Set the outgoing particles from the contents of an interaction.

```

<PHS forests: public>+≡
    public :: phs_forest_set_prt_out

<PHS forests: interfaces>+≡
    interface phs_forest_set_prt_out
        module procedure phs_forest_set_prt_out_int, phs_forest_set_prt_out_mom
    end interface phs_forest_set_prt_out

<PHS forests: procedures>+≡
    subroutine phs_forest_set_prt_out_int (forest, int, lt_cm_to_lab)
        type(phs_forest_t), intent(inout) :: forest
        type(interaction_t), intent(in) :: int
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
        if (present (lt_cm_to_lab)) then
            call phs_prt_set_momentum (forest%prt_out, &
                inverse (lt_cm_to_lab) * &
                int%get_momenta (outgoing=.true.))
        else
            call phs_prt_set_momentum (forest%prt_out, &
                int%get_momenta (outgoing=.true.))
        end if
        associate (m_out => forest%flv(forest%n_in+1:)%get_mass ())
            call phs_prt_set_msq (forest%prt_out, m_out ** 2)
        end associate
        call phs_prt_set_defined (forest%prt_out)
    end subroutine phs_forest_set_prt_out_int

```

```

subroutine phs_forest_set_prt_out_mom (forest, mom, lt_cm_to_lab)
  type(phs_forest_t), intent(inout) :: forest
  type(vector4_t), dimension(size (forest%prt_out)), intent(in) :: mom
  type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
  if (present (lt_cm_to_lab)) then
    call phs_prt_set_momentum (forest%prt_out, &
      inverse (lt_cm_to_lab) * mom)
  else
    call phs_prt_set_momentum (forest%prt_out, mom)
  end if
  associate (m_out => forest%flv(forest%n_in+1:)%get_mass ())
    call phs_prt_set_msq (forest%prt_out, m_out ** 2)
  end associate
  call phs_prt_set_defined (forest%prt_out)
end subroutine phs_forest_set_prt_out_mom

```

Combine particles as described by the particle combination table. Particle momentum sums will be calculated only if the resulting particle is contained in at least one of the trees in the current forest. The others are kept undefined.

```

<PHS forests: public>+≡
  public :: phs_forest_combine_particles

<PHS forests: procedures>+≡
  subroutine phs_forest_combine_particles (forest)
    type(phs_forest_t), intent(inout) :: forest
    integer :: k
    integer, dimension(2) :: kk
    do k = 1, size (forest%prt_combination, 2)
      kk = forest%prt_combination(:,k)
      if (kk(1) /= 0) then
        call phs_prt_combine (forest%prt(k), &
          forest%prt(kk(1)), forest%prt(kk(2)))
      end if
    end do
  end subroutine phs_forest_combine_particles

```

Extract the outgoing particles and insert into an interaction.

```

<PHS forests: public>+≡
  public :: phs_forest_get_prt_out

<PHS forests: procedures>+≡
  subroutine phs_forest_get_prt_out (forest, int, lt_cm_to_lab)
    type(phs_forest_t), intent(in) :: forest
    type(interaction_t), intent(inout) :: int
    type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
    if (present (lt_cm_to_lab)) then
      call int%set_momenta (lt_cm_to_lab * &
        phs_prt_get_momentum (forest%prt_out), outgoing=.true.)
    else
      call int%set_momenta (phs_prt_get_momentum (forest%prt_out), &
        outgoing=.true.)
    end if
  end subroutine phs_forest_get_prt_out

```

Extract the outgoing particle momenta

```

(PHS forests: public)+≡
    public :: phs_forest_get_momenta_out

(PHS forests: procedures)+≡
    function phs_forest_get_momenta_out (forest, lt_cm_to_lab) result (p)
        type(phs_forest_t), intent(in) :: forest
        type(lorentz_transformation_t), intent(in), optional :: lt_cm_to_lab
        type(vector4_t), dimension(size (forest%prt_out)) :: p
        p = phs_prt_get_momentum (forest%prt_out)
        if (present (lt_cm_to_lab)) p = p * lt_cm_to_lab
    end function phs_forest_get_momenta_out

```

19.8.10 Find equivalences among phase-space trees

Scan phase space for equivalences. We generate the complete set of unique permutations for the given list of outgoing particles, and use this for scanning equivalences within each grove. We scan all pairs of trees, using all permutations. This implies that trivial equivalences are included, and equivalences between different trees are recorded twice. This is intentional.

```

(PHS forests: procedures)+≡
    subroutine phs_grove_set_equivalences (grove, perm_array)
        type(phs_grove_t), intent(inout) :: grove
        type(permutation_t), dimension(:), intent(in) :: perm_array
        type(equivalence_t), pointer :: eq
        integer :: t1, t2, i
        do t1 = 1, size (grove%tree)
            do t2 = 1, size (grove%tree)
                SCAN_PERM: do i = 1, size (perm_array)
                    if (phs_tree_equivalent &
                        (grove%tree(t1), grove%tree(t2), perm_array(i))) then
                        call equivalence_list_add &
                            (grove%equivalence_list, t1, t2, perm_array(i))
                        eq => grove%equivalence_list%last
                        call phs_tree_find_msq_permutation &
                            (grove%tree(t1), grove%tree(t2), eq%perm, &
                                eq%msq_perm)
                        call phs_tree_find_angle_permutation &
                            (grove%tree(t1), grove%tree(t2), eq%perm, &
                                eq%angle_perm, eq%angle_sig)
                    end if
                end do SCAN_PERM
            end do
        end do
    end subroutine phs_grove_set_equivalences

(PHS forests: public)+≡
    public :: phs_forest_set_equivalences

(PHS forests: procedures)+≡
    subroutine phs_forest_set_equivalences (forest)
        type(phs_forest_t), intent(inout) :: forest

```

```

type(permutation_t), dimension(:), allocatable :: perm_array
integer :: i
call permutation_array_make &
    (perm_array, forest%flv(forest%n_in+1:)%get_pdg ())
do i = 1, size (forest%grove)
    call phs_grove_set_equivalences (forest%grove(i), perm_array)
end do
forest%n_equivalences = sum (forest%grove%equivalence_list%length)
end subroutine phs_forest_set_equivalences

```

19.8.11 Interface for channel equivalences

Here, we store the equivalence list in the appropriate containers that the `phs_base` module provides. There is one separate list for each channel.

```

<PHS forests: public>+≡
    public :: phs_forest_get_equivalences

<PHS forests: procedures>+≡
    subroutine phs_forest_get_equivalences (forest, channel, azimuthal_dependence)
        type(phs_forest_t), intent(in) :: forest
        type(phs_channel_t), dimension(:), intent(out) :: channel
        logical, intent(in) :: azimuthal_dependence
        integer :: n_masses, n_angles
        integer :: mode_azimuthal_angle
        integer, dimension(:), allocatable :: n_eq
        type(equivalence_t), pointer :: eq
        integer, dimension(:), allocatable :: perm, mode
        integer :: g, c, j, left, right
        n_masses = forest%n_masses
        n_angles = forest%n_angles
        allocate (n_eq (forest%n_trees), source = 0)
        allocate (perm (forest%n_dimensions))
        allocate (mode (forest%n_dimensions), source = EQ_IDENTITY)
        do g = 1, size (forest%grove)
            eq => forest%grove(g)%equivalence_list%first
            do while (associated (eq))
                left = eq%left + forest%grove(g)%tree_count_offset
                n_eq(left) = n_eq(left) + 1
                eq => eq%next
            end do
        end do
        do c = 1, size (channel)
            allocate (channel(c)%eq (n_eq(c)))
            do j = 1, n_eq(c)
                call channel(c)%eq(j)%init (forest%n_dimensions)
            end do
        end do
        n_eq = 0
        if (azimuthal_dependence) then
            mode_azimuthal_angle = EQ_IDENTITY
        else
            mode_azimuthal_angle = EQ_INVARIANT
        end if
    end if

```

```

do g = 1, size (forest%grove)
  eq => forest%grove(g)%equivalence_list%first
  do while (associated (eq))
    left = eq%left + forest%grove(g)%tree_count_offset
    right = eq%right + forest%grove(g)%tree_count_offset
    do j = 1, n_masses
      perm(j) = permute (j, eq%msq_perm)
      mode(j) = EQ_IDENTITY
    end do
    do j = 1, n_angles
      perm(n_masses+j) = n_masses + permute (j, eq%angle_perm)
      if (j == 1) then
        mode(n_masses+j) = mode_azimuthal_angle ! first az. angle
      else if (mod(j,2) == 1) then
        mode(n_masses+j) = EQ_SYMMETRIC ! other az. angles
      else if (eq%angle_sig(j)) then
        mode(n_masses+j) = EQ_IDENTITY ! polar angle +
      else
        mode(n_masses+j) = EQ_INVERT ! polar angle -
      end if
    end do
    n_eq(left) = n_eq(left) + 1
    associate (eq_cur => channel(left)%eq(n_eq(left)))
      eq_cur%c = right
      eq_cur%perm = perm
      eq_cur%mode = mode
    end associate
    eq => eq%next
  end do
end do
end subroutine phs_forest_get_equivalences

```

19.8.12 Phase-space evaluation

Given one row of the **x** parameter array and the corresponding channel index, compute first all relevant momenta and then recover the remainder of the **x** array, the Jacobians **phs_factor**, and the phase-space volume.

The output argument **ok** indicates whether this was successful.

(PHS forests: public)+≡

```
public :: phs_forest_evaluate_selected_channel
```

(PHS forests: procedures)+≡

```

subroutine phs_forest_evaluate_selected_channel &
  (forest, channel, active, sqrts, x, phs_factor, volume, ok)
  type(phs_forest_t), intent(inout) :: forest
  integer, intent(in) :: channel
  logical, dimension(:), intent(in) :: active
  real(default), intent(in) :: sqrts
  real(default), dimension(:,:), intent(inout) :: x
  real(default), dimension(:), intent(out) :: phs_factor
  real(default), intent(out) :: volume
  logical, intent(out) :: ok
  integer :: g, t

```



```

integer(TC) :: k, k_root, k_in

g = forest%grove_lookup (channel)
t = channel - forest%grove(g)%tree_count_offset
call phs_prt_set_undefined (forest%prt)
call phs_prt_set_undefined (forest%prt_out)
k_in = forest%n_tot

do k = 1, forest%n_in
    forest%prt(ibset(0,k_in-k)) = forest%prt_in(k)
end do

do k = 1, forest%n_out
    call phs_prt_set_msq (forest%prt(ibset(0,k-1)), &
        forest%flv(forest%n_in+k)%get_mass () ** 2)
end do

k_root = 2**forest%n_out - 1
select case (forest%n_in)
case (1)
    forest%prt(k_root) = forest%prt_in(1)
case (2)
    call phs_prt_combine &
        (forest%prt(k_root), forest%prt_in(1), forest%prt_in(2))
end select
call phs_tree_compute_momenta_from_x (forest%grove(g)%tree(t), &
    forest%prt, phs_factor(channel), volume, sqrts, x(:,channel), ok)
if (ok) then
    do k = 1, forest%n_out
        forest%prt_out(k) = forest%prt(ibset(0,k-1))
    end do
end if
end subroutine phs_forest_evaluate_selected_channel

```

The remainder: recover x values for all channels except for the current channel.

NOTE: OpenMP not used for the first loop. `combine_particles` is not a channel-local operation.

(PHS forests: public)+≡

```
public :: phs_forest_evaluate_other_channels
```

(PHS forests: procedures)+≡

```

subroutine phs_forest_evaluate_other_channels &
    (forest, channel, active, sqrts, x, phs_factor, combine)
type(phs_forest_t), intent(inout) :: forest
integer, intent(in) :: channel
logical, dimension(:), intent(in) :: active
real(default), intent(in) :: sqrts
real(default), dimension(:,:), intent(inout) :: x
real(default), dimension(:), intent(inout) :: phs_factor
logical, intent(in) :: combine
integer :: g, t, ch, n_channel

g = forest%grove_lookup (channel)

```

```

t = channel - forest%grove(g)%tree_count_offset

n_channel = forest%n_trees
if (combine) then
  do ch = 1, n_channel
    if (ch == channel) cycle
    if (active(ch)) then
      g = forest%grove_lookup(ch)
      t = ch - forest%grove(g)%tree_count_offset
      call phs_tree_combine_particles &
        (forest%grove(g)%tree(t), forest%prt)
    end if
  end do
end if

!OMP PARALLEL PRIVATE (g,t,ch) SHARED(active,forest,sqrts,x,channel)
!OMP DO SCHEDULE(STATIC)
do ch = 1, n_channel
  if (ch == channel) cycle
  if (active(ch)) then
    g = forest%grove_lookup(ch)
    t = ch - forest%grove(g)%tree_count_offset
    call phs_tree_compute_x_from_momenta &
      (forest%grove(g)%tree(t), &
       forest%prt, phs_factor(ch), sqrts, x(:,ch))
  end if
end do
!OMP END DO
!OMP END PARALLEL

end subroutine phs_forest_evaluate_other_channels

```

The complement: recover one row of the x array and the associated Jacobian entry, corresponding to `channel`, from incoming and outgoing momenta. Also compute the phase-space volume.

```

<PHS forests: public>+≡
  public :: phs_forest_recover_channel

<PHS forests: procedures>+≡
  subroutine phs_forest_recover_channel &
    (forest, channel, sqrts, x, phs_factor, volume)
    type(phs_forest_t), intent(inout) :: forest
    integer, intent(in) :: channel
    real(default), intent(in) :: sqrts
    real(default), dimension(:,,:), intent(inout) :: x
    real(default), dimension(:), intent(inout) :: phs_factor
    real(default), intent(out) :: volume
    integer :: g, t
    integer(TC) :: k, k_in
    g = forest%grove_lookup (channel)
    t = channel - forest%grove(g)%tree_count_offset
    call phs_prt_set_undefined (forest%prt)
    k_in = forest%n_tot
    forall (k = 1:forest%n_in)

```

```

        forest%prt(ibset(0,k_in-k)) = forest%prt_in(k)
    end forall
    forall (k = 1:forest%n_out)
        forest%prt(ibset(0,k-1)) = forest%prt_out(k)
    end forall
    call phs_forest_combine_particles (forest)
    call phs_tree_compute_volume &
        (forest%grove(g)%tree(t), sqrts, volume)
    call phs_tree_compute_x_from_momenta &
        (forest%grove(g)%tree(t), &
        forest%prt, phs_factor(channel), sqrts, x(:,channel))
    end subroutine phs_forest_recover_channel

```

19.8.13 Unit tests

Test module, followed by the corresponding implementation module.

`<phs_forests_ut.f90>`≡

<File header>

```

module phs_forests_ut
    use unit_tests
    use phs_forests_uti

```

<Standard module head>

<PHS forests: public test>

contains

<PHS forests: test driver>

```

end module phs_forests_ut

```

`<phs_forests_uti.f90>`≡

<File header>

```

module phs_forests_uti

```

<Use kinds>

<Use strings>

```

    use io_units
    use format_defs, only: FMT_12
    use lorentz
    use flavors
    use interactions
    use model_data
    use mappings
    use phs_base
    use resonances, only: resonance_history_set_t

```

```

    use phs_forests

```

<Standard module head>

```

    <PHS forests: test declarations>

contains

    <PHS forests: tests>

    end module phs_forests_util

API: driver for the unit tests below.
<PHS forests: public test>≡
    public :: phs_forests_test

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

```

Basic universal test

Write a possible phase-space file for a $2 \rightarrow 3$ process and make the corresponding forest, print the forest. Choose some in-particle momenta and a random-number array and evaluate out-particles and phase-space factors.

```

<PHS forests: execute tests>≡
    call test (phs_forest_1, "phs_forest_1", &
        "check phs forest setup", &
        u, results)

<PHS forests: test declarations>≡
    public :: phs_forest_1

<PHS forests: tests>≡
    subroutine phs_forest_1 (u)
        use os_interface
        integer, intent(in) :: u
        type(phs_forest_t) :: forest
        type(phs_channel_t), dimension(:), allocatable :: channel
        type(model_data_t), target :: model
        type(string_t) :: process_id
        type(flavor_t), dimension(5) :: flv
        type(string_t) :: filename
        type(interaction_t) :: int
        integer :: unit_fix
        type(mapping_defaults_t) :: mapping_defaults
        logical :: found_process, ok
        integer :: n_channel, ch, i
        logical, dimension(4) :: active = .true.
        real(default) :: sqrts = 1000
        real(default), dimension(5,4) :: x
        real(default), dimension(4) :: factor
        real(default) :: volume
    end subroutine phs_forest_1

```

```

write (u, "(A)")  "* Test output: PHS forest"
write (u, "(A)")  "* Purpose: test PHS forest routines"
write (u, "(A)")

write (u, "(A)")  "* Reading model file"

call model%init_sm_test ()

write (u, "(A)")
write (u, "(A)")  "* Create phase-space file 'phs_forest_test.phs'"
write (u, "(A)")

call flv%init ([11, -11, 11, -11, 22], model)
unit_fix = free_unit ()
open (file="phs_forest_test.phs", unit=unit_fix, action="write")
write (unit_fix, *) "process foo"
write (unit_fix, *) 'md5sum_process      = "6ABA33BC2927925D0F073B1C1170780A"'
write (unit_fix, *) 'md5sum_model_par   = "1A0B151EE6E2DEB92D880320355A3EAB"'
write (unit_fix, *) 'md5sum_phs_config = "B6A8877058809A8BDD54753CDAB83ACE"'
write (unit_fix, *) "sqrts              = 100.00000000000000"
write (unit_fix, *) "m_threshold_s     = 50.00000000000000"
write (unit_fix, *) "m_threshold_t     = 100.00000000000000"
write (unit_fix, *) "off_shell        = 2"
write (unit_fix, *) "t_channel        = 6"
write (unit_fix, *) "keep_nonresonant = F"
write (unit_fix, *) ""
write (unit_fix, *) "  grove"
write (unit_fix, *) "    tree 3 7"
write (unit_fix, *) "      map 3 s_channel 23"
write (unit_fix, *) "    tree 5 7"
write (unit_fix, *) "    tree 6 7"
write (unit_fix, *) "  grove"
write (unit_fix, *) "    tree 9 11"
write (unit_fix, *) "      map 9 t_channel 22"
close (unit_fix)

write (u, "(A)")
write (u, "(A)")  "* Read phase-space file 'phs_forest_test.phs'"

call syntax_phs_forest_init ()
process_id = "foo"
filename = "phs_forest_test.phs"
call phs_forest_read &
  (forest, filename, process_id, 2, 3, model, found_process)

write (u, "(A)")
write (u, "(A)")  "* Set parameters, flavors, equiv, momenta"
write (u, "(A)")

call phs_forest_set_flavors (forest, flv)
call phs_forest_set_parameters (forest, mapping_defaults, .false.)
call phs_forest_setup_prt_combinations (forest)
call phs_forest_set_equivalences (forest)

```

```

call int%basic_init (2, 0, 3)
call int%set_momentum &
    (vector4_moving (500._default, 500._default, 3), 1)
call int%set_momentum &
    (vector4_moving (500._default,-500._default, 3), 2)
call phs_forest_set_prt_in (forest, int)
n_channel = 2
x = 0
x(:,n_channel) = [0.3, 0.4, 0.1, 0.9, 0.6]
write (u, "(A)") "    Input values:"
write (u, "(3x,5(1x," // FMT_12 // "))") x(:,n_channel)

write (u, "(A)")
write (u, "(A)") " * Evaluating phase space"

call phs_forest_evaluate_selected_channel (forest, &
    n_channel, active, sqrts, x, factor, volume, ok)
call phs_forest_evaluate_other_channels (forest, &
    n_channel, active, sqrts, x, factor, combine=.true.)
call phs_forest_get_prt_out (forest, int)
write (u, "(A)") "    Output values:"
do ch = 1, 4
    write (u, "(3x,5(1x," // FMT_12 // "))") x(:,ch)
end do
call int%basic_write (u)
write (u, "(A)") "    Factors:"
write (u, "(3x,5(1x," // FMT_12 // "))") factor
write (u, "(A)") "    Volume:"
write (u, "(3x,5(1x," // FMT_12 // "))") volume
call phs_forest_write (forest, u)

write (u, "(A)")
write (u, "(A)") " * Compute equivalences"

n_channel = 4
allocate (channel (n_channel))
call phs_forest_get_equivalences (forest, &
    channel, .true.)
do i = 1, n_channel
    write (u, "(1x,I0,':')", advance = "no") ch
    call channel(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)") " * Cleanup"

call model%final ()
call phs_forest_final (forest)
call syntax_phs_forest_final ()

write (u, "(A)")
write (u, "(A)") " * Test output end: phs_forest_1"

end subroutine phs_forest_1

```

Resonance histories

Read a suitably nontrivial forest from file and recover the set of resonance histories.

```
(PHS forests: execute tests)+≡
  call test (phs_forest_2, "phs_forest_2", &
    "handle phs forest resonance content", &
    u, results)

(PHS forests: test declarations)+≡
  public :: phs_forest_2

(PHS forests: tests)+≡
  subroutine phs_forest_2 (u)
    use os_interface
    integer, intent(in) :: u
    integer :: unit_fix
    type(phs_forest_t) :: forest
    type(model_data_t), target :: model
    type(string_t) :: process_id
    type(string_t) :: filename
    logical :: found_process
    type(resonance_history_set_t) :: res_set
    integer :: i

    write (u, "(A)")  "* Test output: phs_forest_2"
    write (u, "(A)")  "* Purpose: test PHS forest routines"
    write (u, "(A)")

    write (u, "(A)")  "* Reading model file"

    call model%init_sm_test ()

    write (u, "(A)")
    write (u, "(A)")  "* Create phase-space file 'phs_forest_2.phs'"
    write (u, "(A)")

    unit_fix = free_unit ()
    open (file="phs_forest_2.phs", unit=unit_fix, action="write")
    write (unit_fix, *) "process foo"
    write (unit_fix, *) 'md5sum_process      = "XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX"'
    write (unit_fix, *) 'md5sum_model_par   = "1A0B151EE6E2DEB92D880320355A3EAB"'
    write (unit_fix, *) 'md5sum_phs_config = "XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX"'
    write (unit_fix, *) "sqrts              = 100.00000000000000"
    write (unit_fix, *) "m_threshold_s    = 50.00000000000000"
    write (unit_fix, *) "m_threshold_t    = 100.00000000000000"
    write (unit_fix, *) "off_shell      = 2"
    write (unit_fix, *) "t_channel      = 6"
    write (unit_fix, *) "keep_nonresonant = F"
    write (unit_fix, *) ""
    write (unit_fix, *) "  grove"
    write (unit_fix, *) "    tree 3 7"
```

```

write (unit_fix, *) "      tree 3 7"
write (unit_fix, *) "      map 3 s_channel -24"
write (unit_fix, *) "      tree 5 7"
write (unit_fix, *) "      tree 3 7"
write (unit_fix, *) "      map 3 s_channel -24"
write (unit_fix, *) "      map 7 s_channel 23"
write (unit_fix, *) "      tree 5 7"
write (unit_fix, *) "      map 7 s_channel 25"
write (unit_fix, *) "      tree 3 11"
write (unit_fix, *) "      map 3 s_channel -24"
close (unit_fix)

write (u, "(A)")  "* Read phase-space file 'phs_forest_2.phs'"

call syntax_phs_forest_init ()
process_id = "foo"
filename = "phs_forest_2.phs"
call phs_forest_read &
      (forest, filename, process_id, 2, 3, model, found_process)

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"
write (u, "(A)")

call forest%extract_resonance_history_set (res_set)
call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call model%final ()
call phs_forest_final (forest)
call syntax_phs_forest_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_forest_2"

end subroutine phs_forest_2

```

19.9 Finding phase space parameterizations

If the phase space configuration is not found in the appropriate file, we should generate one.

The idea is to construct all Feynman diagrams subject to certain constraints which eliminate everything that is probably irrelevant for the integration. These Feynman diagrams (cascades) are grouped in groves by finding equivalence classes related by symmetry and ordered with respect to their importance (resonances). Finally, the result (or part of it) is written to file and used for the integration.

This module may eventually disappear and be replaced by CAML code. In particular, we need here a set of Feynman rules (vertices with particle codes,

but not the factors). Thus, the module works for the Standard Model only.

Note that this module is stand-alone, it communicates to the main program only via the generated ASCII phase-space configuration file.

```

<cascades.f90>≡
  <File header>

  module cascades

    <Use kinds>
      use kinds, only: TC, i8, i32
    <Use strings>
    <Use debug>
      use io_units
      use constants, only: one
      use format_defs, only: FMT_12, FMT_19
      use numeric_utils
      use diagnostics
      use hashes
      use sorting
      use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
      use physics_defs, only: UNDEFINED
      use model_data
      use flavors
      use lorentz

      use resonances, only: resonance_info_t
      use resonances, only: resonance_history_t
      use resonances, only: resonance_history_set_t
      use phs_forests

    <Standard module head>

    <Cascades: public>

    <Cascades: parameters>

    <Cascades: types>

    <Cascades: interfaces>

    contains

    <Cascades: procedures>

  end module cascades

```

19.9.1 The mapping modes

The valid mapping modes, to be used below. We will make use of the convention that mappings of internal particles have a positive value. Only for positive values, the flavor code is propagated when combining cascades.

```

<Mapping modes>≡
  integer, parameter :: &

```

```

& EXTERNAL_PRT = -1, &
& NO_MAPPING = 0, S_CHANNEL = 1, T_CHANNEL = 2, U_CHANNEL = 3, &
& RADIATION = 4, COLLINEAR = 5, INFRARED = 6, &
& STEP_MAPPING_E = 11, STEP_MAPPING_H = 12, &
& ON_SHELL = 99

```

$\langle \text{Cascades: parameters} \rangle \equiv$
 $\langle \text{Mapping modes} \rangle$

19.9.2 The cascade type

A cascade is essentially the same as a decay tree (both definitions may be merged in a later version). It contains a linked tree of nodes, each of which representing an internal particle. In contrast to decay trees, each node has a definite particle code. These nodes need not be modified, therefore we can use pointers and do not have to copy them. Thus, physically each cascades has only a single node, the mother particle. However, to be able to compare trees quickly, we store in addition an array of binary codes which is always sorted in ascending order. This is accompanied by a corresponding list of particle codes. The index is the location of the corresponding cascade in the cascade set, this may be used to access the daughters directly.

The real mass is the particle mass belonging to the particle code. The minimal mass is the sum of the real masses of all its daughters; this is the kinematical cutoff. The effective mass may be zero if the particle mass is below a certain threshold; it may be the real mass if the particle is resonant; or it may be some other value.

The logical `t_channel` is set if this a t -channel line, while `initial` is true only for an initial particle. Note that both initial particles are also `t_channel` by definition, and that they are distinguished by the direction of the tree: One of them decays and is the root of the tree, while the other one is one of the leaves.

The cascade is a list of nodes (particles) which are linked via the `daughter` entries. The node is the mother particle of the decay cascade. Much of the information in the nodes is repeated in arrays, to be accessible more easily. The arrays will be kept sorted by binary codes.

The counter `n_off_shell` is increased for each internal line that is neither resonant nor log-enhanced. It is set to zero if the current line is resonant, since this implies on-shell particle production and subsequent decay.

The counter `n_t_channel` is non-negative once an initial particle is included in the tree: then, it counts the number of t -channel lines.

The `multiplicity` is the number of branchings to follow until all daughters are on-shell. A resonant or non-decaying particle has multiplicity one. Merging nodes, the multiplicities add unless the mother is a resonance. An initial or final node has multiplicity zero.

The arrays correspond to the subnode tree `tree` of the current cascade. PDG codes are stored only for those positions which are resonant, with the exception of the last entry, i.e., the current node. Other positions, in particular external legs, are assigned undefined PDG code.

A cascade is uniquely identified by its tree, the tree of PDG codes, and the tree of mappings. The tree of resonances is kept only to mask the PDG tree as

described above.

<Cascades: types>≡

```

type :: cascade_t
  private
    ! counters
    integer :: index = 0
    integer :: grove = 0
    ! status
    logical :: active = .false.
    logical :: complete = .false.
    logical :: incoming = .false.
    ! this node
    integer(TC) :: bincode = 0
    type(flavor_t) :: flv
    integer :: pdg = UNDEFINED
    logical :: is_vector = .false.
    real(default) :: m_min = 0
    real(default) :: m_rea = 0
    real(default) :: m_eff = 0
    integer :: mapping = NO_MAPPING
    logical :: on_shell = .false.
    logical :: resonant = .false.
    logical :: log_enhanced = .false.
    logical :: t_channel = .false.
    ! global tree properties
    integer :: multiplicity = 0
    integer :: internal = 0
    integer :: n_off_shell = 0
    integer :: n_resonances = 0
    integer :: n_log_enhanced = 0
    integer :: n_t_channel = 0
    integer :: res_hash = 0
    ! the sub-node tree
    integer :: depth = 0
    integer(TC), dimension(:), allocatable :: tree
    integer, dimension(:), allocatable :: tree_pdg
    integer, dimension(:), allocatable :: tree_mapping
    logical, dimension(:), allocatable :: tree_resonant
    ! branch connections
    logical :: has_children = .false.
    type(cascade_t), pointer :: daughter1 => null ()
    type(cascade_t), pointer :: daughter2 => null ()
    type(cascade_t), pointer :: mother => null ()
    ! next in list
    type(cascade_t), pointer :: next => null ()
  contains
    <Cascades: cascade: TBP>
end type cascade_t

```

<Cascades: procedures>≡

```

subroutine cascade_init (cascade, depth)
  type(cascade_t), intent(out) :: cascade
  integer, intent(in) :: depth
  integer, save :: index = 0

```

```

index = cascade_index ()
cascade%index = index
cascade%depth = depth
cascade%active = .true.
allocate (cascade%tree (depth))
allocate (cascade%tree_pdg (depth))
allocate (cascade%tree_mapping (depth))
allocate (cascade%tree_resonant (depth))
end subroutine cascade_init

```

Keep and increment a global index

(Cascades: procedures)+≡

```

function cascade_index (seed) result (index)
integer :: index
integer, intent(in), optional :: seed
integer, save :: i = 0
if (present (seed)) i = seed
i = i + 1
index = i
end function cascade_index

```

We need three versions of writing cascades. This goes to the phase-space file.

For t/u channel mappings, we use the absolute value of the PDG code.

(Cascades: procedures)+≡

```

subroutine cascade_write_file_format (cascade, model, unit)
type(cascade_t), intent(in) :: cascade
class(model_data_t), intent(in), target :: model
integer, intent(in), optional :: unit
type(flavor_t) :: flv
integer :: u, i
2 format(3x,A,1x,I3,1x,A,1x,I9,1x,'!',1x,A)
u = given_output_unit (unit); if (u < 0) return
call write_reduced (cascade%tree, u)
write (u, "(A)")
do i = 1, cascade%depth
call flv%init (cascade%tree_pdg(i), model)
select case (cascade%tree_mapping(i))
case (NO_MAPPING, EXTERNAL_PRT)
case (S_CHANNEL)
write(u,2) 'map', &
cascade%tree(i), 's_channel', cascade%tree_pdg(i), &
char (flv%get_name ())
case (T_CHANNEL)
write(u,2) 'map', &
cascade%tree(i), 't_channel', abs (cascade%tree_pdg(i)), &
char (flv%get_name ())
case (U_CHANNEL)
write(u,2) 'map', &
cascade%tree(i), 'u_channel', abs (cascade%tree_pdg(i)), &
char (flv%get_name ())
case (RADIATION)
write(u,2) 'map', &
cascade%tree(i), 'radiation', cascade%tree_pdg(i), &
char (flv%get_name ())

```

```

        case (COLLINEAR)
            write(u,2) 'map', &
                cascade%tree(i), 'collinear', cascade%tree_pdg(i), &
                char (flv%get_name ())
        case (INFRARED)
            write(u,2) 'map', &
                cascade%tree(i), 'infrared ', cascade%tree_pdg(i), &
                char (flv%get_name ())
        case (ON_SHELL)
            write(u,2) 'map', &
                cascade%tree(i), 'on_shell ', cascade%tree_pdg(i), &
                char (flv%get_name ())
        case default
            call msg_bug (" Impossible mapping mode encountered")
        end select
    end do
contains
    subroutine write_reduced (array, unit)
        integer(TC), dimension(:), intent(in) :: array
        integer, intent(in) :: unit
        integer :: i
        write (u, "(3x,A,1x)", advance="no") "tree"
        do i = 1, size (array)
            if (decay_level (array(i)) > 1) then
                write (u, "(1x,I0)", advance="no") array(i)
            end if
        end do
    end subroutine write_reduced

    elemental function decay_level (k) result (l)
        integer(TC), intent(in) :: k
        integer :: l
        integer :: i
        l = 0
        do i = 0, bit_size(k) - 1
            if (btest(k,i)) l = l + 1
        end do
    end function decay_level

    subroutine start_comment (u)
        integer, intent(in) :: u
        write(u, '(1x,A)', advance='no') '!'
    end subroutine start_comment
end subroutine cascade_write_file_format

```

This creates metapost source for graphical display:

(Cascades: procedures)+≡

```

subroutine cascade_write_graph_format (cascade, count, unit)
    type(cascade_t), intent(in) :: cascade
    integer, intent(in) :: count
    integer, intent(in), optional :: unit
    integer :: u
    integer(TC) :: mask
    type(string_t) :: left_str, right_str
    u = given_output_unit (unit); if (u < 0) return

```

```

mask = 2**((cascade%depth+3)/2) - 1
left_str = ""
right_str = ""
write (u, '(A)') "\begin{minipage}{105pt}"
write (u, '(A)') "\vspace{30pt}"
write (u, '(A)') "\begin{center}"
write (u, '(A)') "\begin{fmfgraph*}(55,55)"
call graph_write (cascade, mask)
write (u, '(A)') "\fmfleft{" // char (extract (left_str, 2)) // "}"
write (u, '(A)') "\fmfright{" // char (extract (right_str, 2)) // "}"
write (u, '(A)') "\end{fmfgraph*}\\"
write (u, '(A,I5,A)') "\fbox{$", count, "$}"
write (u, '(A)') "\end{center}"
write (u, '(A)') "\end{minipage}"
write (u, '(A)') "%"
contains
recursive subroutine graph_write (cascade, mask, reverse)
  type(cascade_t), intent(in) :: cascade
  integer(TC), intent(in) :: mask
  logical, intent(in), optional :: reverse
  type(flavor_t) :: anti
  logical :: rev
  rev = .false.; if (present(reverse)) rev = reverse
  if (cascade%has_children) then
    if (.not.rev) then
      call vertex_write (cascade, cascade%daughter1, mask)
      call vertex_write (cascade, cascade%daughter2, mask)
    else
      call vertex_write (cascade, cascade%daughter2, mask, .true.)
      call vertex_write (cascade, cascade%daughter1, mask, .true.)
    end if
    if (cascade%complete) then
      call vertex_write (cascade, cascade%mother, mask, .true.)
      write (u, '(A,I0,A)') "\fmfv{d.shape=square}{v0}"
    end if
  else
    if (cascade%incoming) then
      anti = cascade%flv%anti ()
      call external_write (cascade%bincode, anti%get_tex_name (), &
        left_str)
    else
      call external_write (cascade%bincode, cascade%flv%get_tex_name (), &
        right_str)
    end if
  end if
end subroutine graph_write
recursive subroutine vertex_write (cascade, daughter, mask, reverse)
  type(cascade_t), intent(in) :: cascade, daughter
  integer(TC), intent(in) :: mask
  logical, intent(in), optional :: reverse
  integer :: bincode
  if (cascade%complete) then
    bincode = 0
  else

```

```

        bincode = cascade%bincode
    end if
    call graph_write (daughter, mask, reverse)
    if (daughter%has_children) then
        call line_write (bincode, daughter%bincode, daughter%flv, &
            mapping=daughter%mapping)
    else
        call line_write (bincode, daughter%bincode, daughter%flv)
    end if
end subroutine vertex_write
subroutine line_write (i1, i2, flv, mapping)
    integer(TC), intent(in) :: i1, i2
    type(flavor_t), intent(in) :: flv
    integer, intent(in), optional :: mapping
    integer :: k1, k2
    type(string_t) :: prt_type
    select case (flv%get_spin_type ())
    case (SCALAR);          prt_type = "plain"
    case (SPINOR);          prt_type = "fermion"
    case (VECTOR);          prt_type = "boson"
    case (VECTORSPINOR);    prt_type = "fermion"
    case (TENSOR);          prt_type = "dbl_wiggly"
    case default;           prt_type = "dashes"
    end select
    if (flv%is_antiparticle ()) then
        k1 = i2; k2 = i1
    else
        k1 = i1; k2 = i2
    end if
    if (present (mapping)) then
        select case (mapping)
        case (S_CHANNEL)
            write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
                & ",f=blue,lab=\sm\blue$" // &
                & char (flv%get_tex_name ()) // "$}" // &
                & "{v", k1, ",v", k2, "}"
        case (T_CHANNEL, U_CHANNEL)
            write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
                & ",f=cyan,lab=\sm\cyan$" // &
                & char (flv%get_tex_name ()) // "$}" // &
                & "{v", k1, ",v", k2, "}"
        case (RADIATION)
            write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
                & ",f=green,lab=\sm\green$" // &
                & char (flv%get_tex_name ()) // "$}" // &
                & "{v", k1, ",v", k2, "}"
        case (COLLINEAR)
            write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
                & ",f=magenta,lab=\sm\magenta$" // &
                & char (flv%get_tex_name ()) // "$}" // &
                & "{v", k1, ",v", k2, "}"
        case (INFRARED)
            write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
                & ",f=red,lab=\sm\red$" // &

```

```

        & char (flv%get_tex_name ()) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    case default
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=black}" // &
        & "{v", k1, ",v", k2, "}"
    end select
else
    write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
    & "}" // &
    & "{v", k1, ",v", k2, "}"
end if
end subroutine line_write
subroutine external_write (bincode, name, ext_str)
    integer(TC), intent(in) :: bincode
    type(string_t), intent(in) :: name
    type(string_t), intent(inout) :: ext_str
    character(len=20) :: str
    write (str, '(A2,I0)') ",v", bincode
    ext_str = ext_str // trim (str)
    write (u, '(A,I0,A,I0,A)') "\fmflabel{\sm$" &
    // char (name) &
    // "\",(" , bincode, ")" &
    // "$}{v", bincode, "}"
end subroutine external_write
end subroutine cascade_write_graph_format

```

This is for screen/debugging output:

(Cascades: procedures)+≡

```

subroutine cascade_write (cascade, unit)
    type(cascade_t), intent(in) :: cascade
    integer, intent(in), optional :: unit
    integer :: u
    character(9) :: depth
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(A,(1x,I7))") 'Cascade #', cascade%index
    write (u, "(A,(1x,I7))") ' Grove:      ', cascade%grove
    write (u, "(A,3(1x,L1))") ' act/cmp/inc: ', &
        cascade%active, cascade%complete, cascade%incoming
    write (u, "(A,I0)") ' Bincode:      ', cascade%bincode
    write (u, "(A)", advance="no") ' Flavor:      '
    call cascade%flv%write (unit)
    write (u, "(A,I9)") ' Active flavor:', cascade%pdg
    write (u, "(A,L1)") ' Is vector:    ', cascade%is_vector
    write (u, "(A,3(1x," // FMT_19 // "))") ' Mass (m/r/e): ', &
        cascade%m_min, cascade%m_rea, cascade%m_eff
    write (u, "(A,I1)") ' Mapping:      ', cascade%mapping
    write (u, "(A,3(1x,L1))") ' res/log/tch: ', &
        cascade%resonant, cascade%log_enhanced, cascade%t_channel
    write (u, "(A,(1x,I7))") ' Multiplicity: ', cascade%multiplicity
    write (u, "(A,2(1x,I7))") ' n intern/off: ', &
        cascade%internal, cascade%n_off_shell
    write (u, "(A,3(1x,I7))") ' n res/log/tch:', &
        cascade%n_resonances, cascade%n_log_enhanced, cascade%n_t_channel

```



```

write (u, "(A,I7)" ) ' Depth:          ', cascade%depth
write (depth, "(I7)" cascade%depth
write (u, "(A," // depth // "(1x,I7))" ) &
' Tree:          ', cascade%tree
write (u, "(A," // depth // "(1x,I7))" ) &
' Tree(PDG):     ', cascade%tree_pdg
write (u, "(A," // depth // "(1x,I7))" ) &
' Tree(mapping):', cascade%tree_mapping
write (u, "(A," // depth // "(1x,L1))" ) &
' Tree(res):     ', cascade%tree_resonant
if (cascade%has_children) then
write (u, "(A,I7,1x,I7)" ) ' Daughter1/2: ', &
cascade%daughter1%index, cascade%daughter2%index
end if
if (associated (cascade%mother)) then
write (u, "(A,I7)" ) ' Mother:          ', cascade%mother%index
end if
end subroutine cascade_write

```

19.9.3 Creating new cascades

This initializes a single-particle cascade (external, final state). The PDG entry in the tree is set undefined because the cascade is not resonant. However, the flavor entry is set, so the cascade flavor is identified nevertheless.

```

(Cascades: procedures)+≡
subroutine cascade_init_outgoing (cascade, flv, pos, m_thr)
type(cascade_t), intent(out) :: cascade
type(flavor_t), intent(in) :: flv
integer, intent(in) :: pos
real(default), intent(in) :: m_thr
call cascade_init (cascade, 1)
cascade%bincode = ibset (0_TC, pos-1)
cascade%flv = flv
cascade%pdg = cascade%flv%get_pdg ()
cascade%is_vector = flv%get_spin_type () == VECTOR
cascade%m_min = flv%get_mass ()
cascade%m_rea = cascade%m_min
if (cascade%m_rea >= m_thr) then
cascade%m_eff = cascade%m_rea
end if
cascade%on_shell = .true.
cascade%multiplicity = 1
cascade%tree(1) = cascade%bincode
cascade%tree_pdg(1) = cascade%pdg
cascade%tree_mapping(1) = EXTERNAL_PRT
cascade%tree_resonant(1) = .false.
end subroutine cascade_init_outgoing

```

The same for an incoming line:

```

(Cascades: procedures)+≡
subroutine cascade_init_incoming (cascade, flv, pos, m_thr)
type(cascade_t), intent(out) :: cascade

```

```

type(flavor_t), intent(in) :: flv
integer, intent(in) :: pos
real(default), intent(in) :: m_thr
call cascade_init (cascade, 1)
cascade%incoming = .true.
cascade%bincode = ibset (0_TC, pos-1)
cascade%flv = flv%anti ()
cascade%pdg = cascade%flv%get_pdg ()
cascade%is_vector = flv%get_spin_type () == VECTOR
cascade%m_min = flv%get_mass ()
cascade%m_rea = cascade%m_min
if (cascade%m_rea >= m_thr) then
    cascade%m_eff = cascade%m_rea
end if
cascade%on_shell = .true.
cascade%n_t_channel = 0
cascade%n_off_shell = 0
cascade%tree(1) = cascade%bincode
cascade%tree_pdg(1) = cascade%pdg
cascade%tree_mapping(1) = EXTERNAL_PRT
cascade%tree_resonant(1) = .false.
end subroutine cascade_init_incoming

```

19.9.4 Tools

This function returns true if the two cascades share no common external particle. This is a requirement for joining them.

```

<Cascades: interfaces>≡
interface operator(.disjunct.)
    module procedure cascade_disjunct
end interface

<Cascades: procedures>+≡
function cascade_disjunct (cascade1, cascade2) result (flag)
    logical :: flag
    type(cascade_t), intent(in) :: cascade1, cascade2
    flag = iand (cascade1%bincode, cascade2%bincode) == 0
end function cascade_disjunct

```

Compute a hash code for the resonance pattern of a cascade. We count the number of times each particle appears as a resonance.

We pack the PDG codes of the resonances in two arrays (s-channel and t-channel), sort them both, concatenate the results, transfer to i8 integers, and compute the hash code from this byte stream.

For t/u-channel, we remove the sign for antiparticles since this is not well-defined.

```

<Cascades: procedures>+≡
subroutine cascade_assign_resonance_hash (cascade)
    type(cascade_t), intent(inout) :: cascade
    integer(i8), dimension(1) :: mold
    cascade%res_hash = hash (transfer &

```

```

        ([sort (pack (cascade%tree_pdg, &
                     cascade%tree_resonant)), &
         sort (pack (abs (cascade%tree_pdg), &
                     cascade%tree_mapping == T_CHANNEL .or. &
                     cascade%tree_mapping == U_CHANNEL))), &
        mold))
end subroutine cascade_assign_resonance_hash

```

19.9.5 Hash entries for cascades

We will set up a hash array which contains keys of and pointers to cascades. We hold a list of cascade (pointers) within each bucket. This is not for collision resolution, but for keeping similar, but unequal cascades together.

```

<Cascades: types>+≡
  type :: cascade_p
    type(cascade_t), pointer :: cascade => null ()
    type(cascade_p), pointer :: next => null ()
  end type cascade_p

```

Here is the bucket or hash entry type:

```

<Cascades: types>+≡
  type :: hash_entry_t
    integer(i32) :: hashval = 0
    integer(i8), dimension(:), allocatable :: key
    type(cascade_p), pointer :: first => null ()
    type(cascade_p), pointer :: last => null ()
  end type hash_entry_t

```

```

<Cascades: public>≡
  public :: hash_entry_init

```

```

<Cascades: procedures>+≡
  subroutine hash_entry_init (entry, entry_in)
    type(hash_entry_t), intent(out) :: entry
    type(hash_entry_t), intent(in) :: entry_in
    type(cascade_p), pointer :: casc_iter, casc_copy
    entry%hashval = entry_in%hashval
    entry%key = entry_in%key
    casc_iter => entry_in%first
    do while (associated (casc_iter))
      allocate (casc_copy)
      casc_copy = casc_iter
      casc_copy%next => null ()
      if (associated (entry%first)) then
        entry%last%next => casc_copy
      else
        entry%first => casc_copy
      end if
      entry%last => casc_copy
      casc_iter => casc_iter%next
    end do
  end subroutine hash_entry_init

```

Finalize: just deallocate the list; the contents are just pointers.

```

<Cascades: procedures>+=
subroutine hash_entry_final (hash_entry)
  type(hash_entry_t), intent(inout) :: hash_entry
  type(cascade_p), pointer :: current
  do while (associated (hash_entry%first))
    current => hash_entry%first
    hash_entry%first => current%next
    deallocate (current)
  end do
end subroutine hash_entry_final

```

Output: concise format for debugging, just list cascade indices.

```

<Cascades: procedures>+=
subroutine hash_entry_write (hash_entry, unit)
  type(hash_entry_t), intent(in) :: hash_entry
  integer, intent(in), optional :: unit
  type(cascade_p), pointer :: current
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)", advance="no") "Entry:"
  do i = 1, size (hash_entry%key)
    write (u, "(1x,I0)", advance="no") hash_entry%key(i)
  end do
  write (u, "(1x,A)", advance="no") "->"
  current => hash_entry%first
  do while (associated (current))
    write (u, "(1x,I7)", advance="no") current%cascade%index
    current => current%next
  end do
  write (u, *)
end subroutine hash_entry_write

```

This function adds a cascade pointer to the bucket. If ok is present, check first if it is already there and return failure if yes. If cascade_ptr is also present, set it to the current cascade if successful. If not, set it to the cascade that is already there.

```

<Cascades: procedures>+=
subroutine hash_entry_add_cascade_ptr (hash_entry, cascade, ok, cascade_ptr)
  type(hash_entry_t), intent(inout) :: hash_entry
  type(cascade_t), intent(in), target :: cascade
  logical, intent(out), optional :: ok
  type(cascade_t), optional, pointer :: cascade_ptr
  type(cascade_p), pointer :: current
  if (present (ok)) then
    call hash_entry_check_cascade (hash_entry, cascade, ok, cascade_ptr)
    if (.not. ok) return
  end if
  allocate (current)
  current%cascade => cascade
  if (associated (hash_entry%last)) then

```

```

        hash_entry%last%next => current
    else
        hash_entry%first => current
    end if
    hash_entry%last => current
end subroutine hash_entry_add_cascade_ptr

```

This function checks whether a cascade is already in the bucket. For incomplete cascades, we look for an exact match. It should suffice to verify the tree, the PDG codes, and the mapping modes. This is the information that is written to the phase space file.

For complete cascades, we ignore the PDG code at positions with mappings infrared, collinear, or t/u-channel. Thus a cascade which is distinguished only by PDG code at such places, is flagged existent. If the convention is followed that light particles come before heavier ones (in the model definition), this ensures that the lightest particle is kept in the appropriate place, corresponding to the strongest peak.

For external cascades (incoming/outgoing) we take the PDG code into account even though it is zeroed in the PDG-code tree.

```

(Cascades: procedures)+≡
subroutine hash_entry_check_cascade (hash_entry, cascade, ok, cascade_ptr)
    type(hash_entry_t), intent(in), target :: hash_entry
    type(cascade_t), intent(in), target :: cascade
    logical, intent(out) :: ok
    type(cascade_t), optional, pointer :: cascade_ptr
    type(cascade_p), pointer :: current
    integer, dimension(:), allocatable :: tree_pdg
    ok = .true.
    allocate (tree_pdg (size (cascade%tree_pdg)))
    if (cascade%complete) then
        where (cascade%tree_mapping == INFRARED .or. &
             cascade%tree_mapping == COLLINEAR .or. &
             cascade%tree_mapping == T_CHANNEL .or. &
             cascade%tree_mapping == U_CHANNEL)
            tree_pdg = 0
        elsewhere
            tree_pdg = cascade%tree_pdg
        end where
    else
        tree_pdg = cascade%tree_pdg
    end if
    current => hash_entry%first
    do while (associated (current))
        if (current%cascade%depth == cascade%depth) then
            if (all (current%cascade%tree == cascade%tree)) then
                if (all (current%cascade%tree_mapping == cascade%tree_mapping)) &
                    then
                    if (all (current%cascade%tree_pdg .match. tree_pdg)) then
                        if (present (cascade_ptr)) cascade_ptr => current%cascade
                        ok = .false.; return
                    end if
                end if
            end if
        end if
    end if
end if

```

```

        end if
        current => current%next
    end do
    if (present (cascade_ptr)) cascade_ptr => cascade
end subroutine hash_entry_check_cascade

```

For PDG codes, we specify that the undefined code matches any code. This is already defined for flavor objects, but here we need it for the codes themselves.

```

<Cascades: interfaces>+=
    interface operator(.match.)
        module procedure pdg_match
    end interface

<Cascades: procedures>+=
    elemental function pdg_match (pdg1, pdg2) result (flag)
        logical :: flag
        integer(TC), intent(in) :: pdg1, pdg2
        select case (pdg1)
        case (0)
            flag = .true.
        case default
            select case (pdg2)
            case (0)
                flag = .true.
            case default
                flag = pdg1 == pdg2
            end select
        end select
    end function pdg_match

```

19.9.6 The cascade set

The cascade set will later be transformed into the decay forest. It is set up as a linked list. In addition to the usual **first** and **last** pointers, there is a **first_t** pointer which points to the first t-channel cascade (after all s-channel cascades), and a **first_k** pointer which points to the first final cascade (with a keystone).

As an auxiliary device, the object contains a hash array with associated parameters where an additional pointer is stored for each cascade. The keys are made from the relevant cascade data. This hash is used for fast detection (and thus avoidance) of double entries in the cascade list.

```

<Cascades: public>+=
    public :: cascade_set_t

<Cascades: types>+=
    type :: cascade_set_t
        private
        class(model_data_t), pointer :: model
        integer :: n_in, n_out, n_tot
        type(flavor_t), dimension(:, :), allocatable :: flv
        integer :: depth_out, depth_tot
        real(default) :: sqrts = 0
        real(default) :: m_threshold_s = 0
    end type

```

```

real(default) :: m_threshold_t = 0
integer :: off_shell = 0
integer :: t_channel = 0
logical :: keep_nonresonant
integer :: n_groves = 0
! The cascade list
type(cascade_t), pointer :: first => null ()
type(cascade_t), pointer :: last => null ()
type(cascade_t), pointer :: first_t => null ()
type(cascade_t), pointer :: first_k => null ()
! The hashtable
integer :: n_entries = 0
real :: fill_ratio = 0
integer :: n_entries_max = 0
integer(i32) :: mask = 0
logical :: fatal_beam_decay = .true.
type(hash_entry_t), dimension(:), allocatable :: entry
end type cascade_set_t

```

```

<Cascades: public>+≡
interface cascade_set_init
  module procedure cascade_set_init_base
  module procedure cascade_set_init_from_cascade
end interface

```

This might be broken. Test before using.

```

<Cascades: procedures>+≡
subroutine cascade_set_init_from_cascade (cascade_set, cascade_set_in)
  type(cascade_set_t), intent(out) :: cascade_set
  type(cascade_set_t), intent(in), target :: cascade_set_in
  type(cascade_t), pointer :: casc_iter, casc_copy
  cascade_set%model => cascade_set_in%model
  cascade_set%n_in = cascade_set_in%n_in
  cascade_set%n_out = cascade_set_in%n_out
  cascade_set%n_tot = cascade_set_in%n_tot
  cascade_set%flv = cascade_set_in%flv
  cascade_set%depth_out = cascade_set_in%depth_out
  cascade_set%depth_tot = cascade_set_in%depth_tot
  cascade_set%sqrts = cascade_set_in%sqrts
  cascade_set%m_threshold_s = cascade_set_in%m_threshold_s
  cascade_set%m_threshold_t = cascade_set_in%m_threshold_t
  cascade_set%off_shell = cascade_set_in%off_shell
  cascade_set%t_channel = cascade_set_in%t_channel
  cascade_set%keep_nonresonant = cascade_set_in%keep_nonresonant
  cascade_set%n_groves = cascade_set_in%n_groves

  casc_iter => cascade_set_in%first
  do while (associated (casc_iter))
    allocate (casc_copy)
    casc_copy = casc_iter
    casc_copy%next => null ()
    if (associated (cascade_set%first)) then
      cascade_set%last%next => casc_copy
    else

```

```

        cascade_set%first => casc_copy
    end if
    cascade_set%last => casc_copy
    casc_iter => casc_iter%next
end do

cascade_set%n_entries = cascade_set_in%n_entries
cascade_set%fill_ratio = cascade_set_in%fill_ratio
cascade_set%n_entries_max = cascade_set_in%n_entries_max
cascade_set%mask = cascade_set_in%mask
cascade_set%fatal_beam_decay = cascade_set_in%fatal_beam_decay
allocate (cascade_set%entry (0:cascade_set%mask))
cascade_set%entry = cascade_set_in%entry
end subroutine cascade_set_init_from_cascade

```

Return true if there are cascades which are active and complete, so the phase space file would be nonempty.

```

<Cascades: public>+=
    public :: cascade_set_is_valid

<Cascades: procedures>+=
    function cascade_set_is_valid (cascade_set) result (flag)
        logical :: flag
        type(cascade_set_t), intent(in) :: cascade_set
        type(cascade_t), pointer :: cascade
        flag = .false.
        cascade => cascade_set%first_k
        do while (associated (cascade))
            if (cascade%active .and. cascade%complete) then
                flag = .true.
                return
            end if
            cascade => cascade%next
        end do
    end function cascade_set_is_valid

```

The initializer sets up the hash table with some initial size guessed by looking at the number of external particles. We choose 256 for 3 external particles and a factor of 4 for each additional particle, limited at $2^{30}=1\text{G}$.

```

<Cascades: parameters>+=
    real, parameter, public :: CASCADE_SET_FILL_RATIO = 0.1

<Cascades: procedures>+=
    subroutine cascade_set_init_base (cascade_set, model, n_in, n_out, phs_par, &
        fatal_beam_decay, flv)
        type(cascade_set_t), intent(out) :: cascade_set
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in, n_out
        type(phs_parameters_t), intent(in) :: phs_par
        logical, intent(in) :: fatal_beam_decay
        type(flavor_t), dimension(:,,:), intent(in), optional :: flv
        integer :: size_guess
        integer :: i, j
        cascade_set%model => model

```



```

cascade_set%n_in = n_in
cascade_set%n_out = n_out
cascade_set%n_tot = n_in + n_out
if (present (flv)) then
    allocate (cascade_set%flv (size (flv, 1), size (flv, 2)))
    do i = 1, size (flv, 2)
        do j = 1, size (flv, 1)
            call cascade_set%flv(j,i)%init (flv(j,i)%get_pdg (), model)
        end do
    end do
end if
select case (n_in)
case (1); cascade_set%depth_out = 2 * n_out - 3
case (2); cascade_set%depth_out = 2 * n_out - 1
end select
cascade_set%depth_tot = 2 * cascade_set%n_tot - 3
cascade_set%sqrts = phs_par%sqrts
cascade_set%m_threshold_s = phs_par%m_threshold_s
cascade_set%m_threshold_t = phs_par%m_threshold_t
cascade_set%off_shell = phs_par%off_shell
cascade_set%t_channel = phs_par%t_channel
cascade_set%keep_nonresonant = phs_par%keep_nonresonant
cascade_set%fill_ratio = CASCADE_SET_FILL_RATIO
size_guess = ishft (256, min (2 * (cascade_set%n_tot - 3), 22))
cascade_set%n_entries_max = size_guess * cascade_set%fill_ratio
cascade_set%mask = size_guess - 1
allocate (cascade_set%entry (0:cascade_set%mask))
cascade_set%fatal_beam_decay = fatal_beam_decay
end subroutine cascade_set_init_base

```

The finalizer has to delete both the hash and the list.

```

<Cascades: public>+≡
    public :: cascade_set_final

<Cascades: procedures>+≡
    subroutine cascade_set_final (cascade_set)
        type(cascade_set_t), intent(inout), target :: cascade_set
        type(cascade_t), pointer :: current
        integer :: i
        if (allocated (cascade_set%entry)) then
            do i = 0, cascade_set%mask
                call hash_entry_final (cascade_set%entry(i))
            end do
            deallocate (cascade_set%entry)
        end if
        do while (associated (cascade_set%first))
            current => cascade_set%first
            cascade_set%first => cascade_set%first%next
            deallocate (current)
        end do
    end subroutine cascade_set_final

```

Write the process in ASCII format, in columns that are headed by the corresponding bincode.

```

<Cascades: public>+=
    public :: cascade_set_write_process_bincode_format

<Cascades: procedures>+=
    subroutine cascade_set_write_process_bincode_format (cascade_set, unit)
        type(cascade_set_t), intent(in), target :: cascade_set
        integer, intent(in), optional :: unit
        integer, dimension(:), allocatable :: bincode, field_width
        integer :: n_in, n_out, n_tot, n_flv
        integer :: u, f, i, bc
        character(20) :: str
        type(string_t) :: fmt_head
        type(string_t), dimension(:), allocatable :: fmt_proc
        u = given_output_unit (unit); if (u < 0) return
        if (.not. allocated (cascade_set%flv)) return
        write (u, "('!',1x,A)") "List of subprocesses with particle bincodes:"
        n_in = cascade_set%n_in
        n_out = cascade_set%n_out
        n_tot = cascade_set%n_tot
        n_flv = size (cascade_set%flv, 2)
        allocate (bincode (n_tot), field_width (n_tot), fmt_proc (n_tot))
        bc = 1
        do i = 1, n_out
            bincode(n_in + i) = bc
            bc = 2 * bc
        end do
        do i = n_in, 1, -1
            bincode(i) = bc
            bc = 2 * bc
        end do
        do i = 1, n_tot
            write (str, "(I0)") bincode(i)
            field_width(i) = len_trim (str)
            do f = 1, n_flv
                field_width(i) = max (field_width(i), &
                    len (cascade_set%flv(i,f)%get_name ()))
            end do
        end do
        fmt_head = "('!',)"
        do i = 1, n_tot
            fmt_head = fmt_head // ",1x,"
            fmt_proc(i) = "(1x,"
            write (str, "(I0)") field_width(i)
            fmt_head = fmt_head // "I" // trim(str)
            fmt_proc(i) = fmt_proc(i) // "A" // trim(str)
            if (i == n_in) then
                fmt_head = fmt_head // ",1x,' '"
            end if
        end do
        do i = 1, n_tot
            fmt_proc(i) = fmt_proc(i) // ")"
        end do
        fmt_head = fmt_head // ")"
        write (u, char (fmt_head)) bincode
        do f = 1, n_flv

```

```

write (u, "('!')", advance="no")
do i = 1, n_tot
  write (u, char (fmt_proc(i)), advance="no") &
    char (cascade_set%flv(i,f)%get_name ())
  if (i == n_in) write (u, "(ix,'=>')", advance="no")
end do
write (u, *)
end do
write (u, char (fmt_head)) bincode
end subroutine cascade_set_write_process_bincode_format

```

Write the process as a L^AT_EX expression.

```

<Cascades: procedures>+≡
subroutine cascade_set_write_process_tex_format (cascade_set, unit)
  type(cascade_set_t), intent(in), target :: cascade_set
  integer, intent(in), optional :: unit
  integer :: u, f, i
  u = given_output_unit (unit); if (u < 0) return
  if (.not. allocated (cascade_set%flv)) return
  write (u, "(A)") "\begin{align*}"
  do f = 1, size (cascade_set%flv, 2)
    do i = 1, cascade_set%n_in
      if (i > 1) write (u, "(A)", advance="no") "\quad "
      write (u, "(A)", advance="no") &
        char (cascade_set%flv(i,f)%get_tex_name ())
    end do
    write (u, "(A)", advance="no") "\quad &\to\quad "
    do i = cascade_set%n_in + 1, cascade_set%n_tot
      if (i > cascade_set%n_in + 1) write (u, "(A)", advance="no") "\quad "
      write (u, "(A)", advance="no") &
        char (cascade_set%flv(i,f)%get_tex_name ())
    end do
    if (f < size (cascade_set%flv, 2)) then
      write (u, "(A)") "\\ "
    else
      write (u, "(A)") ""
    end if
  end do
  write (u, "(A)") "\end{align*}"
end subroutine cascade_set_write_process_tex_format

```

Three output routines: phase-space file, graph source code, and screen output.

This version generates the phase space file. It deals only with complete cascades.

```

<Cascades: public>+≡
public :: cascade_set_write_file_format

<Cascades: procedures>+≡
subroutine cascade_set_write_file_format (cascade_set, unit)
  type(cascade_set_t), intent(in), target :: cascade_set
  integer, intent(in), optional :: unit
  type(cascade_t), pointer :: cascade
  integer :: u, grove, count

```

```

logical :: first_in_grove
u = given_output_unit (unit); if (u < 0) return
count = 0
do grove = 1, cascade_set%n_groves
  first_in_grove = .true.
  cascade => cascade_set%first_k
  do while (associated (cascade))
    if (cascade%active .and. cascade%complete) then
      if (cascade%grove == grove) then
        if (first_in_grove) then
          first_in_grove = .false.
          write (u, "(A)")
          write (u, "(1x,'!',1x,A,1x,I0,A)", advance='no') &
            'Multiplicity =', cascade%multiplicity, ","
          select case (cascade%n_resonances)
            case (0)
              write (u, '(1x,A)', advance='no') 'no resonances, '
            case (1)
              write (u, '(1x,A)', advance='no') '1 resonance, '
            case default
              write (u, '(1x,I0,1x,A)', advance='no') &
                cascade%n_resonances, 'resonances, '
          end select
          write (u, '(1x,I0,1x,A)', advance='no') &
            cascade%n_log_enhanced, 'logs, '
          write (u, '(1x,I0,1x,A)', advance='no') &
            cascade%n_off_shell, 'off-shell, '
          select case (cascade%n_t_channel)
            case (0); write (u, '(1x,A)') 's-channel graph'
            case (1); write (u, '(1x,A)') '1 t-channel line'
            case default
              write(u,'(1x,I0,1x,A)') &
                cascade%n_t_channel, 't-channel lines'
          end select
          write (u, '(1x,A,I0)') 'grove #', grove
        end if
        count = count + 1
        write (u, "(1x,'!',1x,A,I0)") "Channel #", count
        call cascade_write_file_format (cascade, cascade_set%model, u)
      end if
    end if
    cascade => cascade%next
  end do
end do
end subroutine cascade_set_write_file_format

```

This is the graph output format, the driver-file

```

<Cascades: public>+=
  public :: cascade_set_write_graph_format

<Cascades: procedures>+=
  subroutine cascade_set_write_graph_format &
    (cascade_set, filename, process_id, unit)
    type(cascade_set_t), intent(in), target :: cascade_set

```

```

type(string_t), intent(in) :: filename, process_id
integer, intent(in), optional :: unit
type(cascade_t), pointer :: cascade
integer :: u, grove, count, pgcount
logical :: first_in_grove
u = given_output_unit (unit); if (u < 0) return
write (u, '(A)') "\documentclass[10pt]{article}"
write (u, '(A)') "\usepackage{amsmath}"
write (u, '(A)') "\usepackage{feynmp}"
write (u, '(A)') "\usepackage{url}"
write (u, '(A)') "\usepackage{color}"
write (u, *)
write (u, '(A)') "\textwidth 18.5cm"
write (u, '(A)') "\evensidemargin -1.5cm"
write (u, '(A)') "\oddsidemargin -1.5cm"
write (u, *)
write (u, '(A)') "\newcommand{\blue}{\color{blue}}"
write (u, '(A)') "\newcommand{\green}{\color{green}}"
write (u, '(A)') "\newcommand{\red}{\color{red}}"
write (u, '(A)') "\newcommand{\magenta}{\color{magenta}}"
write (u, '(A)') "\newcommand{\cyan}{\color{cyan}}"
write (u, '(A)') "\newcommand{\sm}{\footnotesize}"
write (u, '(A)') "\setlength{\parindent}{0pt}"
write (u, '(A)') "\setlength{\parsep}{20pt}"
write (u, *)
write (u, '(A)') "\begin{document}"
write (u, '(A)') "\begin{fmffile}{ " // char (filename) // "}"
write (u, '(A)') "\fmfcmd{color magenta; magenta = red + blue;}"
write (u, '(A)') "\fmfcmd{color cyan; cyan = green + blue;}"
write (u, '(A)') "\begin{fmfshrink}{0.5}"
write (u, '(A)') "\begin{flushleft}"
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{\large\texttt{WHIZARD} phase space channels}" // &
& "\hfill\today"
write (u, *)
write (u, '(A)') "\vspace{10pt}"
write (u, '(A)') "\noindent" // &
& "\textbf{Process:} \url{ " // char (process_id) // "}"
call cascade_set_write_process_tex_format (cascade_set, u)
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{Note:} These are pseudo Feynman graphs that "
write (u, '(A)') "visualize phase-space parameterizations " // &
& "(‘‘integration channels’’). "
write (u, '(A)') "They do \emph{not} indicate Feynman graphs used for the " // &
& "matrix element."
write (u, *)
write (u, '(A)') "\textbf{Color code:} " // &
& "{\blue resonance,} " // &
& "{\cyan t-channel,} " // &
& "{\green radiation,} "
write (u, '(A)') "{\red infrared,} " // &
& "{\magenta collinear,} " // &

```

```

        & "external/off-shell"
write (u, *)
write (u, '(A)') "\noindent" // &
        & "\textbf{Black square:} Keystone, indicates ordering of " // &
        & "phase space parameters."
write (u, *)
write (u, '(A)') "\vspace{-20pt}"
count = 0
pgcount = 0
do grove = 1, cascade_set%n_groves
    first_in_grove = .true.
    cascade => cascade_set%first
    do while (associated (cascade))
        if (cascade%active .and. cascade%complete) then
            if (cascade%grove == grove) then
                if (first_in_grove) then
                    first_in_grove = .false.
                    write (u, *)
                    write (u, '(A)') "\vspace{20pt}"
                    write (u, '(A)') "\begin{tabular}{l}"
                    write (u, '(A,I5,A)') &
                        & "\fbox{\bf Grove \boldmath$", grove, "$} \\[10pt]"
                    write (u, '(A,I1,A)') "Multiplicity: ", &
                        cascade%multiplicity, "\\"
                    write (u, '(A,I1,A)') "Resonances:   ", &
                        cascade%n_resonances, "\\"
                    write (u, '(A,I1,A)') "Log-enhanced: ", &
                        cascade%n_log_enhanced, "\\"
                    write (u, '(A,I1,A)') "Off-shell:    ", &
                        cascade%n_off_shell, "\\"
                    write (u, '(A,I1,A)') "t-channel:    ", &
                        cascade%n_t_channel, ""
                    write (u, '(A)') "\end{tabular}"
                end if
                count = count + 1
                call cascade_write_graph_format (cascade, count, unit)
                if (pgcount >= 250) then
                    write (u, '(A)') "\clearpage"
                    pgcount = 0
                end if
            end if
        end if
        cascade => cascade%next
    end do
end do
write (u, '(A)') "\end{flushleft}"
write (u, '(A)') "\end{fmfshrink}"
write (u, '(A)') "\end{fmffile}"
write (u, '(A)') "\end{document}"
end subroutine cascade_set_write_graph_format

```

This is for screen output and debugging:

(Cascades: public)+≡

```

public :: cascade_set_write

(Cascades: procedures)+≡
subroutine cascade_set_write (cascade_set, unit, active_only, complete_only)
  type(cascade_set_t), intent(in), target :: cascade_set
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: active_only, complete_only
  logical :: active, complete
  type(cascade_t), pointer :: cascade
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  active = .true.; if (present (active_only)) active = active_only
  complete = .false.; if (present (complete_only)) complete = complete_only
  write (u, "(A)") "Cascade set:"
  write (u, "(3x,A)", advance="no") "Model:"
  if (associated (cascade_set%model)) then
    write (u, "(1x,A)") char (cascade_set%model%get_name ())
  else
    write (u, "(1x,A)") "[none]"
  end if
  write (u, "(3x,A)", advance="no") "n_in/out/tot ="
  write (u, "(3(1x,I7))") &
    cascade_set%n_in, cascade_set%n_out, cascade_set%n_tot
  write (u, "(3x,A)", advance="no") "depth_out/tot ="
  write (u, "(2(1x,I7))") cascade_set%depth_out, cascade_set%depth_tot
  write (u, "(3x,A)", advance="no") "mass thr(s/t) ="
  write (u, "(2(1x," // FMT_19 // ")") &
    cascade_set%m_threshold_s, cascade_set%m_threshold_t
  write (u, "(3x,A)", advance="no") "off shell ="
  write (u, "(1x,I7)") cascade_set%off_shell
  write (u, "(3x,A)", advance="no") "keep_nonreson ="
  write (u, "(1x,L1)") cascade_set%keep_nonresonant
  write (u, "(3x,A)", advance="no") "n_groves ="
  write (u, "(1x,I7)") cascade_set%n_groves
  write (u, "(A)")
  write (u, "(A)") "Cascade list:"
  if (associated (cascade_set%first)) then
    cascade => cascade_set%first
    do while (associated (cascade))
      if (active .and. .not. cascade%active) cycle
      if (complete .and. .not. cascade%complete) cycle
      call cascade_write (cascade, unit)
      cascade => cascade%next
    end do
  else
    write (u, "(A)") "[empty]"
  end if
  write (u, "(A)") "Hash array"
  write (u, "(3x,A)", advance="no") "n_entries ="
  write (u, "(1x,I7)") cascade_set%n_entries
  write (u, "(3x,A)", advance="no") "fill_ratio ="
  write (u, "(1x," // FMT_12 // ")") cascade_set%fill_ratio
  write (u, "(3x,A)", advance="no") "n_entries_max ="
  write (u, "(1x,I7)") cascade_set%n_entries_max
  write (u, "(3x,A)", advance="no") "mask ="

```

```

write (u, "(1x,I0)") cascade_set%mask
do i = 0, ubound (cascade_set%entry, 1)
  if (allocated (cascade_set%entry(i)%key)) then
    write (u, "(1x,I7)") i
    call hash_entry_write (cascade_set%entry(i), u)
  end if
end do
end subroutine cascade_set_write

```

19.9.7 Adding cascades

Add a deep copy of a cascade to the set. The copy has all content of the original, but the pointers are nullified. We do not care whether insertion was successful or not. The pointer argument, if present, is assigned to the input cascade, or to the hash entry if it is already present.

The procedure is recursive: any daughter or mother entries are also deep-copied and added to the cascade set before the current copy is added.

(Cascades: procedures)+≡

```

recursive subroutine cascade_set_add_copy &
  (cascade_set, cascade_in, cascade_ptr)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in) :: cascade_in
  type(cascade_t), optional, pointer :: cascade_ptr
  type(cascade_t), pointer :: cascade
  logical :: ok
  allocate (cascade)
  cascade = cascade_in
  if (associated (cascade_in%daughter1)) call cascade_set_add_copy &
    (cascade_set, cascade_in%daughter1, cascade%daughter1)
  if (associated (cascade_in%daughter2)) call cascade_set_add_copy &
    (cascade_set, cascade_in%daughter2, cascade%daughter2)
  if (associated (cascade_in%mother)) call cascade_set_add_copy &
    (cascade_set, cascade_in%mother, cascade%mother)
  cascade%next => null ()
  call cascade_set_add (cascade_set, cascade, ok, cascade_ptr)
  if (.not. ok) deallocate (cascade)
end subroutine cascade_set_add_copy

```

Add a cascade to the set. This does not deep-copy. We first try to insert it in the hash array. If successful, add it to the list. Failure indicates that it is already present, and we drop it.

The hash key is built solely from the tree array, so neither particle codes nor resonances count, just topology.

Technically, hash and list receive only pointers, so the cascade can be considered as being in either of both. We treat it as part of the list.

(Cascades: procedures)+≡

```

subroutine cascade_set_add (cascade_set, cascade, ok, cascade_ptr)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in), target :: cascade
  logical, intent(out) :: ok
  type(cascade_t), optional, pointer :: cascade_ptr

```



```

integer(i8), dimension(1) :: mold
call cascade_set_hash_insert &
    (cascade_set, transfer (cascade%tree, mold), cascade, ok, cascade_ptr)
if (ok) call cascade_set_list_add (cascade_set, cascade)
end subroutine cascade_set_add

```

Add a new cascade to the list:

```

<Cascades: procedures>+=
subroutine cascade_set_list_add (cascade_set, cascade)
type(cascade_set_t), intent(inout) :: cascade_set
type(cascade_t), intent(in), target :: cascade
if (associated (cascade_set%last)) then
    cascade_set%last%next => cascade
else
    cascade_set%first => cascade
end if
cascade_set%last => cascade
end subroutine cascade_set_list_add

```

Add a cascade entry to the hash array:

```

<Cascades: procedures>+=
subroutine cascade_set_hash_insert &
    (cascade_set, key, cascade, ok, cascade_ptr)
type(cascade_set_t), intent(inout), target :: cascade_set
integer(i8), dimension(:), intent(in) :: key
type(cascade_t), intent(in), target :: cascade
logical, intent(out) :: ok
type(cascade_t), optional, pointer :: cascade_ptr
integer(i32) :: h
if (cascade_set%n_entries >= cascade_set%n_entries_max) &
    call cascade_set_hash_expand (cascade_set)
h = hash (key)
call cascade_set_hash_insert_rec &
    (cascade_set, h, h, key, cascade, ok, cascade_ptr)
end subroutine cascade_set_hash_insert

```

Double the hashtable size when necessary:

```

<Cascades: procedures>+=
subroutine cascade_set_hash_expand (cascade_set)
type(cascade_set_t), intent(inout), target :: cascade_set
type(hash_entry_t), dimension(:), allocatable, target :: table_tmp
type(cascade_p), pointer :: current
integer :: i, s
allocate (table_tmp (0:cascade_set%mask))
table_tmp = cascade_set%entry
deallocate (cascade_set%entry)
s = 2 * size (table_tmp)
cascade_set%n_entries = 0
cascade_set%n_entries_max = s * cascade_set%fill_ratio
cascade_set%mask = s - 1
allocate (cascade_set%entry (0:cascade_set%mask))
do i = 0, ubound (table_tmp, 1)

```

```

        current => table_tmp(i)%first
    do while (associated (current))
        call cascade_set_hash_insert_rec &
            (cascade_set, table_tmp(i)%hashval, table_tmp(i)%hashval, &
             table_tmp(i)%key, current%cascade)
        current => current%next
    end do
end do
end subroutine cascade_set_hash_expand

```

Insert the cascade at the bucket determined by the hash value. If the bucket is filled, check first for a collision (unequal keys). In that case, choose the following bucket and repeat. Otherwise, add the cascade to the bucket.

If the bucket is empty, record the hash value, allocate and store the key, and then add the cascade to the bucket.

If ok is present, before insertion we check whether the cascade is already stored, and return failure if yes.

(*Cascades: procedures*) +=

```

recursive subroutine cascade_set_hash_insert_rec &
    (cascade_set, h, hashval, key, cascade, ok, cascade_ptr)
type(cascade_set_t), intent(inout) :: cascade_set
integer(i32), intent(in) :: h, hashval
integer(i8), dimension(:), intent(in) :: key
type(cascade_t), intent(in), target :: cascade
logical, intent(out), optional :: ok
type(cascade_t), optional, pointer :: cascade_ptr
integer(i32) :: i
i = iand (h, cascade_set%mask)
if (allocated (cascade_set%entry(i)%key)) then
    if (size (cascade_set%entry(i)%key) /= size (key)) then
        call cascade_set_hash_insert_rec &
            (cascade_set, h + 1, hashval, key, cascade, ok, cascade_ptr)
    else if (any (cascade_set%entry(i)%key /= key)) then
        call cascade_set_hash_insert_rec &
            (cascade_set, h + 1, hashval, key, cascade, ok, cascade_ptr)
    else
        call hash_entry_add_cascade_ptr &
            (cascade_set%entry(i), cascade, ok, cascade_ptr)
    end if
else
    cascade_set%entry(i)%hashval = hashval
    allocate (cascade_set%entry(i)%key (size (key)))
    cascade_set%entry(i)%key = key
    call hash_entry_add_cascade_ptr &
        (cascade_set%entry(i), cascade, ok, cascade_ptr)
    cascade_set%n_entries = cascade_set%n_entries + 1
end if
end subroutine cascade_set_hash_insert_rec

```

19.9.8 External particles

We want to initialize the cascade set with the outgoing particles. In case of multiple processes, initial cascades are prepared for all of them. The hash array check ensures that no particle appears more than once at the same place.

```

<Cascades: interfaces>+=
  interface cascade_set_add_outgoing
    module procedure cascade_set_add_outgoing1
    module procedure cascade_set_add_outgoing2
  end interface

<Cascades: procedures>+=
  subroutine cascade_set_add_outgoing2 (cascade_set, flv)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(flavor_t), dimension(:,:), intent(in) :: flv
    integer :: pos, prc, n_out, n_prc
    type(cascade_t), pointer :: cascade
    logical :: ok
    n_out = size (flv, dim=1)
    n_prc = size (flv, dim=2)
    do prc = 1, n_prc
      do pos = 1, n_out
        allocate (cascade)
        call cascade_init_outgoing &
          (cascade, flv(pos,prc), pos, cascade_set%m_threshold_s)
        call cascade_set_add (cascade_set, cascade, ok)
        if (.not. ok) then
          deallocate (cascade)
        end if
      end do
    end do
  end subroutine cascade_set_add_outgoing2

  subroutine cascade_set_add_outgoing1 (cascade_set, flv)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(flavor_t), dimension(:), intent(in) :: flv
    integer :: pos, n_out
    type(cascade_t), pointer :: cascade
    logical :: ok
    n_out = size (flv, dim=1)
    do pos = 1, n_out
      allocate (cascade)
      call cascade_init_outgoing &
        (cascade, flv(pos), pos, cascade_set%m_threshold_s)
      call cascade_set_add (cascade_set, cascade, ok)
      if (.not. ok) then
        deallocate (cascade)
      end if
    end do
  end subroutine cascade_set_add_outgoing1

```

The incoming particles are added one at a time. Nevertheless, we may have several processes which are looped over. At the first opportunity, we set the

pointer `first_t` in the cascade set which should point to the first t-channel cascade.

Return the indices of the first and last cascade generated.

(Cascades: interfaces)+≡

```
interface cascade_set_add_incoming
  module procedure cascade_set_add_incoming0
  module procedure cascade_set_add_incoming1
end interface
```

(Cascades: procedures)+≡

```
subroutine cascade_set_add_incoming1 (cascade_set, n1, n2, pos, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set
  integer, intent(out) :: n1, n2
  integer, intent(in) :: pos
  type(flavor_t), dimension(:), intent(in) :: flv
  integer :: prc, n_prc
  type(cascade_t), pointer :: cascade
  logical :: ok
  n1 = 0
  n2 = 0
  n_prc = size (flv)
  do prc = 1, n_prc
    allocate (cascade)
    call cascade_init_incoming &
      (cascade, flv(prc), pos, cascade_set%m_threshold_t)
    call cascade_set_add (cascade_set, cascade, ok)
    if (ok) then
      if (n1 == 0) n1 = cascade%index
      n2 = cascade%index
      if (.not. associated (cascade_set%first_t)) then
        cascade_set%first_t => cascade
      end if
    else
      deallocate (cascade)
    end if
  end do
end subroutine cascade_set_add_incoming1
```

```
subroutine cascade_set_add_incoming0 (cascade_set, n1, n2, pos, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set
  integer, intent(out) :: n1, n2
  integer, intent(in) :: pos
  type(flavor_t), intent(in) :: flv
  type(cascade_t), pointer :: cascade
  logical :: ok
  n1 = 0
  n2 = 0
  allocate (cascade)
  call cascade_init_incoming &
    (cascade, flv, pos, cascade_set%m_threshold_t)
  call cascade_set_add (cascade_set, cascade, ok)
  if (ok) then
    if (n1 == 0) n1 = cascade%index
```

```

n2 = cascade%index
if (.not. associated (cascade_set%first_t)) then
  cascade_set%first_t => cascade
end if
else
  deallocate (cascade)
end if
end subroutine cascade_set_add_incoming0

```

19.9.9 Cascade combination I: flavor assignment

We have two disjunct cascades, now use the vertex table to determine the possible flavors of the combination cascade. For each possibility, try to generate a new cascade. The total cascade depth has to be one less than the limit, because this is reached by setting the keystone.

```

<Cascades: procedures>+=
subroutine cascade_match_pair (cascade_set, cascade1, cascade2, s_channel)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in), target :: cascade1, cascade2
  logical, intent(in) :: s_channel
  integer, dimension(:), allocatable :: pdg3
  integer :: i, depth_max
  type(flavor_t) :: flv
  if (s_channel) then
    depth_max = cascade_set%depth_out
  else
    depth_max = cascade_set%depth_tot
  end if
  if (cascade1%depth + cascade2%depth < depth_max) then
    call cascade_set%model%match_vertex ( &
      cascade1%flv%get_pdg (), &
      cascade2%flv%get_pdg (), &
      pdg3)
    do i = 1, size (pdg3)
      call flv%init (pdg3(i), cascade_set%model)
      if (s_channel) then
        call cascade_combine_s (cascade_set, cascade1, cascade2, flv)
      else
        call cascade_combine_t (cascade_set, cascade1, cascade2, flv)
      end if
    end do
    deallocate (pdg3)
  end if
end subroutine cascade_match_pair

```

The triplet version takes a third cascade, and we check whether this triplet has a matching vertex in the database. If yes, we make a keystone cascade.

```

<Cascades: procedures>+=
subroutine cascade_match_triplet &
  (cascade_set, cascade1, cascade2, cascade3, s_channel)
  type(cascade_set_t), intent(inout), target :: cascade_set

```

```

type(cascade_t), intent(in), target :: cascade1, cascade2, cascade3
logical, intent(in) :: s_channel
integer :: depth_max
depth_max = cascade_set%depth_tot
if (cascade1%depth + cascade2%depth + cascade3%depth == depth_max) then
  if (cascade_set%model%check_vertex ( &
    cascade1%flv%get_pdg (), &
    cascade2%flv%get_pdg (), &
    cascade3%flv%get_pdg ())) then
    call cascade_combine_keystone &
      (cascade_set, cascade1, cascade2, cascade3, s_channel)
  end if
end if
end subroutine cascade_match_triplet

```

19.9.10 Cascade combination II: kinematics setup and check

Having three matching flavors, we start constructing the combination cascade. We look at the mass hierarchies and determine whether the cascade is to be kept. In passing we set mapping modes, resonance properties and such.

If successful, the cascade is finalized. For a resonant cascade, we prepare in addition a copy without the resonance.

```

(Cascades: procedures)+≡
subroutine cascade_combine_s (cascade_set, cascade1, cascade2, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in), target :: cascade1, cascade2
  type(flavor_t), intent(in) :: flv
  type(cascade_t), pointer :: cascade3, cascade4
  logical :: keep
  keep = .false.
  allocate (cascade3)
  call cascade_init (cascade3, cascade1%depth + cascade2%depth + 1)
  cascade3%bincode = ior (cascade1%bincode, cascade2%bincode)
  cascade3%flv = flv%anti ()
  cascade3%pdg = cascade3%flv%get_pdg ()
  cascade3%is_vector = flv%get_spin_type () == VECTOR
  cascade3%m_min = cascade1%m_min + cascade2%m_min
  cascade3%m_rea = flv%get_mass ()
  if (cascade3%m_rea > cascade_set%m_threshold_s) then
    cascade3%m_eff = cascade3%m_rea
  end if
  ! Potentially resonant cases [sqrts = m_rea for on-shell decay]
  if (cascade3%m_rea > cascade3%m_min &
    .and. cascade3%m_rea <= cascade_set%sqrts) then
    if (flv%get_width () /= 0) then
      if (cascade1%on_shell .or. cascade2%on_shell) then
        keep = .true.
        cascade3%mapping = S_CHANNEL
        cascade3%resonant = .true.
      end if
    else
      call warn_decay (flv)
    end if
  end if
end subroutine cascade_combine_s

```

```

        end if
! Collinear and IR singular cases
else if (cascade3%m_rea < cascade_set%sqrts) then
    ! Massless splitting
    if (cascade1%m_eff == 0 .and. cascade2%m_eff == 0 &
        .and. cascade3%depth <= 3) then
        keep = .true.
        cascade3%log_enhanced = .true.
        if (cascade3%is_vector) then
            if (cascade1%is_vector .and. cascade2%is_vector) then
                cascade3%mapping = COLLINEAR    ! three-vector-vertex
            else
                cascade3%mapping = INFRARED      ! vector splitting into matter
            end if
        else
            if (cascade1%is_vector .or. cascade2%is_vector) then
                cascade3%mapping = COLLINEAR    ! vector radiation off matter
            else
                cascade3%mapping = INFRARED      ! scalar radiation/splitting
            end if
        end if
! IR radiation off massive particle
else if (cascade3%m_eff > 0 .and. cascade1%m_eff > 0 &
        .and. cascade2%m_eff == 0 &
        .and. (cascade1%on_shell .or. cascade1%mapping == RADIATION) &
        .and. abs (cascade3%m_eff - cascade1%m_eff) &
            < cascade_set%m_threshold_s) &
        then
        keep = .true.
        cascade3%log_enhanced = .true.
        cascade3%mapping = RADIATION
    else if (cascade3%m_eff > 0 .and. cascade2%m_eff > 0 &
        .and. cascade1%m_eff == 0 &
        .and. (cascade2%on_shell .or. cascade2%mapping == RADIATION) &
        .and. abs (cascade3%m_eff - cascade2%m_eff) &
            < cascade_set%m_threshold_s) &
        then
        keep = .true.
        cascade3%log_enhanced = .true.
        cascade3%mapping = RADIATION
    end if
end if
! Non-singular cases, including failed resonances
if (.not. keep) then
    ! Two on-shell particles from a virtual mother
    if (cascade1%on_shell .or. cascade2%on_shell) then
        keep = .true.
        cascade3%m_eff = max (cascade3%m_min, &
            cascade1%m_eff + cascade2%m_eff)
        if (cascade3%m_eff < cascade_set%m_threshold_s) then
            cascade3%m_eff = 0
        end if
    end if
end if
end if
end if

```

```

! Complete and register the cascade (two in case of resonance)
if (keep) then
  cascade3%on_shell = cascade3%resonant .or. cascade3%log_enhanced
  if (cascade3%resonant) then
    cascade3%pdg = cascade3%flv%get_pdg ()
    if (cascade_set%keep_nonresonant) then
      allocate (cascade4)
      cascade4 = cascade3
      cascade4%index = cascade_index ()
      cascade4%pdg = UNDEFINED
      cascade4%mapping = NO_MAPPING
      cascade4%resonant = .false.
      cascade4%on_shell = .false.
    end if
    cascade3%m_min = cascade3%m_rea
    call cascade_fusion (cascade_set, cascade1, cascade2, cascade3)
    if (cascade_set%keep_nonresonant) then
      call cascade_fusion (cascade_set, cascade1, cascade2, cascade4)
    end if
  else
    call cascade_fusion (cascade_set, cascade1, cascade2, cascade3)
  end if
else
  deallocate (cascade3)
end if
contains
subroutine warn_decay (flv)
  type(flavor_t), intent(in) :: flv
  integer :: i
  integer, dimension(MAX_WARN_RESONANCE), save :: warned_code = 0
  LOOP_WARNED: do i = 1, MAX_WARN_RESONANCE
    if (warned_code(i) == 0) then
      warned_code(i) = flv%get_pdg ()
      write (msg_buffer, "(A)") &
        & " Intermediate decay of zero-width particle " &
        & // char (flv%get_name ()) &
        & // " may be possible."
      call msg_warning
      exit LOOP_WARNED
    else if (warned_code(i) == flv%get_pdg ()) then
      exit LOOP_WARNED
    end if
  end do LOOP_WARNED
end subroutine warn_decay
end subroutine cascade_combine_s

```

<Cascades: parameters>+≡

```
integer, parameter, public :: MAX_WARN_RESONANCE = 50
```

This is the t-channel version. `cascade1` is t-channel and contains the seed, `cascade2` is s-channel. We check for kinematically allowed beam decay (which is a fatal error), or massless splitting / soft radiation. The cascade is kept in all remaining cases and submitted for registration.

<Cascades: procedures>+≡


```

subroutine cascade_combine_t (cascade_set, cascade1, cascade2, flv)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in), target :: cascade1, cascade2
  type(flavor_t), intent(in) :: flv
  type(cascade_t), pointer :: cascade3
  allocate (cascade3)
  call cascade_init (cascade3, cascade1%depth + cascade2%depth + 1)
  cascade3%bincode = ior (cascade1%bincode, cascade2%bincode)
  cascade3%flv = flv%anti ()
  cascade3%pdg = abs (cascade3%flv%get_pdg ())
  cascade3%is_vector = flv%get_spin_type () == VECTOR
  if (cascade1%incoming) then
    cascade3%m_min = cascade2%m_min
  else
    cascade3%m_min = cascade1%m_min + cascade2%m_min
  end if
  cascade3%m_rea = flv%get_mass ()
  if (cascade3%m_rea > cascade_set%m_threshold_t) then
    cascade3%m_eff = max (cascade3%m_rea, cascade2%m_eff)
  else if (cascade2%m_eff > cascade_set%m_threshold_t) then
    cascade3%m_eff = cascade2%m_eff
  else
    cascade3%m_eff = 0
  end if
  ! Allowed decay of beam particle
  if (cascade1%incoming &
    .and. cascade1%m_rea > cascade2%m_rea + cascade3%m_rea) then
    call beam_decay (cascade_set%fatal_beam_decay)
  ! Massless splitting
  else if (cascade1%m_eff == 0 &
    .and. cascade2%m_eff < cascade_set%m_threshold_t &
    .and. cascade3%m_eff == 0) then
    cascade3%mapping = U_CHANNEL
    cascade3%log_enhanced = .true.
  ! IR radiation off massive particle
  else if (cascade1%m_eff /= 0 .and. cascade2%m_eff == 0 &
    .and. cascade3%m_eff /= 0 &
    .and. (cascade1%on_shell .or. cascade1%mapping == RADIATION) &
    .and. abs (cascade1%m_eff - cascade3%m_eff) &
      < cascade_set%m_threshold_t) &
    then
    cascade3%pdg = flv%get_pdg ()
    cascade3%log_enhanced = .true.
    cascade3%mapping = RADIATION
  end if
  cascade3%t_channel = .true.
  call cascade_fusion (cascade_set, cascade1, cascade2, cascade3)
contains
  subroutine beam_decay (fatal_beam_decay)
    logical, intent(in) :: fatal_beam_decay
    write (msg_buffer, "(1x,A,1x,'->',1x,A,1x,A)") &
      char (cascade1%flv%get_name ()), &
      char (cascade3%flv%get_name ()), &
      char (cascade2%flv%get_name ())

```

```

call msg_message
write (msg_buffer, "(1x,'mass(',A,')' =',1x,E17.10)") &
char (cascade1%flv%get_name()), cascade1%m_rea
call msg_message
write (msg_buffer, "(1x,'mass(',A,')' =',1x,E17.10)") &
char (cascade3%flv%get_name()), cascade3%m_rea
call msg_message
write (msg_buffer, "(1x,'mass(',A,')' =',1x,E17.10)") &
char (cascade2%flv%get_name()), cascade2%m_rea
call msg_message
if (fatal_beam_decay) then
call msg_fatal (" Phase space: Initial beam particle can decay")
else
call msg_warning (" Phase space: Initial beam particle can decay")
end if
end subroutine beam_decay
end subroutine cascade_combine_t

```

Here we complete a decay cascade. The third input is the single-particle cascade for the initial particle. There is no resonance or mapping assignment. The only condition for keeping the cascade is the mass sum of the final state, which must be less than the available energy.

Two modifications are necessary for scattering cascades: a pure s-channel diagram (cascade1 is the incoming particle) do not have a logarithmic mapping at top-level. And in a t-channel diagram, the last line exchanged is mapped t-channel, not u-channel. Finally, we can encounter the case of a $2 \rightarrow 1$ process, where cascade1 is incoming, and cascade2 is the outgoing particle. In all three cases we register a new cascade with the modified mapping.

(*Cascades: procedures*) +=

```

subroutine cascade_combine_keystone &
(cascade_set, cascade1, cascade2, cascade3, s_channel)
type(cascade_set_t), intent(inout), target :: cascade_set
type(cascade_t), intent(in), target :: cascade1, cascade2, cascade3
logical, intent(in) :: s_channel
type(cascade_t), pointer :: cascade4, cascade0
logical :: keep, ok
keep = .false.
allocate (cascade4)
call cascade_init &
(cascade4, cascade1%depth + cascade2%depth + cascade3%depth)
cascade4%complete = .true.
if (s_channel) then
cascade4%bincode = ior (cascade1%bincode, cascade2%bincode)
else
cascade4%bincode = cascade3%bincode
end if
cascade4%flv = cascade3%flv
cascade4%pdg = cascade3%pdg
cascade4%mapping = EXTERNAL_PRT
cascade4%is_vector = cascade3%is_vector
cascade4%m_min = cascade1%m_min + cascade2%m_min
cascade4%m_rea = cascade3%m_rea
cascade4%m_eff = cascade3%m_rea

```

```

if (cascade4%m_min < cascade_set%sqrts) then
    keep = .true.
end if
if (keep) then
    if (cascade1%incoming .and. cascade2%log_enhanced) then
        allocate (cascade0)
        cascade0 = cascade2
        cascade0%next => null ()
        cascade0%index = cascade_index ()
        cascade0%mapping = NO_MAPPING
        cascade0%log_enhanced = .false.
        cascade0%n_log_enhanced = cascade0%n_log_enhanced - 1
        cascade0%tree_mapping(cascade0%depth) = NO_MAPPING
        call cascade_keystone &
            (cascade_set, cascade1, cascade0, cascade3, cascade4, ok)
        if (ok) then
            call cascade_set_add (cascade_set, cascade0, ok)
        else
            deallocate (cascade0)
        end if
    else if (cascade1%t_channel .and. cascade1%mapping == U_CHANNEL) then
        allocate (cascade0)
        cascade0 = cascade1
        cascade0%next => null ()
        cascade0%index = cascade_index ()
        cascade0%mapping = T_CHANNEL
        cascade0%tree_mapping(cascade0%depth) = T_CHANNEL
        call cascade_keystone &
            (cascade_set, cascade0, cascade2, cascade3, cascade4, ok)
        if (ok) then
            call cascade_set_add (cascade_set, cascade0, ok)
        else
            deallocate (cascade0)
        end if
    else if (cascade1%incoming .and. cascade2%depth == 1) then
        allocate (cascade0)
        cascade0 = cascade2
        cascade0%next => null ()
        cascade0%index = cascade_index ()
        cascade0%mapping = ON_SHELL
        cascade0%tree_mapping(cascade0%depth) = ON_SHELL
        call cascade_keystone &
            (cascade_set, cascade1, cascade0, cascade3, cascade4, ok)
        if (ok) then
            call cascade_set_add (cascade_set, cascade0, ok)
        else
            deallocate (cascade0)
        end if
    else
        call cascade_keystone &
            (cascade_set, cascade1, cascade2, cascade3, cascade4, ok)
    end if
else
    deallocate (cascade4)

```

```

end if
end subroutine cascade_combine_keystone

```

19.9.11 Cascade combination III: node connections and tree fusion

Here we assign global tree properties. If the allowed number of off-shell lines is exceeded, discard the new cascade. Otherwise, assign the trees, sort them, and assign connections. Finally, append the cascade to the list. This may fail (because in the hash array there is already an equivalent cascade). On failure, discard the cascade.

```

(Cascades: procedures)+=
subroutine cascade_fusion (cascade_set, cascade1, cascade2, cascade3)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), intent(in), target :: cascade1, cascade2
  type(cascade_t), pointer :: cascade3
  integer :: i1, i2, i3, i4
  logical :: ok
  cascade3%internal = (cascade3%depth - 3) / 2
  if (cascade3%resonant) then
    cascade3%multiplicity = 1
    cascade3%n_resonances = &
      cascade1%n_resonances + cascade2%n_resonances + 1
  else
    cascade3%multiplicity = cascade1%multiplicity + cascade2%multiplicity
    cascade3%n_resonances = cascade1%n_resonances + cascade2%n_resonances
  end if
  if (cascade3%log_enhanced) then
    cascade3%n_log_enhanced = &
      cascade1%n_log_enhanced + cascade2%n_log_enhanced + 1
  else
    cascade3%n_log_enhanced = &
      cascade1%n_log_enhanced + cascade2%n_log_enhanced
  end if
  if (cascade3%resonant) then
    cascade3%n_off_shell = 0
  else if (cascade3%log_enhanced) then
    cascade3%n_off_shell = cascade1%n_off_shell + cascade2%n_off_shell
  else
    cascade3%n_off_shell = cascade1%n_off_shell + cascade2%n_off_shell + 1
  end if
  if (cascade3%t_channel) then
    cascade3%n_t_channel = cascade1%n_t_channel + 1
  end if
  if (cascade3%n_off_shell > cascade_set%off_shell) then
    deallocate (cascade3)
  else if (cascade3%n_t_channel > cascade_set%t_channel) then
    deallocate (cascade3)
  else
    i1 = cascade1%depth
    i2 = i1 + 1
    i3 = i1 + cascade2%depth
  end if
end subroutine

```

```

i4 = cascade3%depth
cascade3%tree(:i1) = cascade1%tree
where (cascade1%tree_mapping > NO_MAPPING)
    cascade3%tree_pdg(:i1) = cascade1%tree_pdg
elsewhere
    cascade3%tree_pdg(:i1) = UNDEFINED
end where
cascade3%tree_mapping(:i1) = cascade1%tree_mapping
cascade3%tree_resonant(:i1) = cascade1%tree_resonant
cascade3%tree(i2:i3) = cascade2%tree
where (cascade2%tree_mapping > NO_MAPPING)
    cascade3%tree_pdg(i2:i3) = cascade2%tree_pdg
elsewhere
    cascade3%tree_pdg(i2:i3) = UNDEFINED
end where
cascade3%tree_mapping(i2:i3) = cascade2%tree_mapping
cascade3%tree_resonant(i2:i3) = cascade2%tree_resonant
cascade3%tree(i4) = cascade3%bincode
cascade3%tree_pdg(i4) = cascade3%pdg
cascade3%tree_mapping(i4) = cascade3%mapping
cascade3%tree_resonant(i4) = cascade3%resonant
call tree_sort (cascade3%tree, &
    cascade3%tree_pdg, cascade3%tree_mapping, cascade3%tree_resonant)
cascade3%has_children = .true.
cascade3%daughter1 => cascade1
cascade3%daughter2 => cascade2
call cascade_set_add (cascade_set, cascade3, ok)
if (.not. ok) deallocate (cascade3)
end if
end subroutine cascade_fusion

```

Here we combine a cascade pair with an incoming particle, i.e., we set a keystone. Otherwise, this is similar. On the first opportunity, we set the `first_k` pointer in the cascade set.

(Cascades: procedures)+≡

```

subroutine cascade_keystone &
    (cascade_set, cascade1, cascade2, cascade3, cascade4, ok)
type(cascade_set_t), intent(inout), target :: cascade_set
type(cascade_t), intent(in), target :: cascade1, cascade2, cascade3
type(cascade_t), pointer :: cascade4
logical, intent(out) :: ok
integer :: i1, i2, i3, i4
cascade4%internal = (cascade4%depth - 3) / 2
cascade4%multiplicity = cascade1%multiplicity + cascade2%multiplicity
cascade4%n_resonances = cascade1%n_resonances + cascade2%n_resonances
cascade4%n_off_shell = cascade1%n_off_shell + cascade2%n_off_shell
cascade4%n_log_enhanced = &
    cascade1%n_log_enhanced + cascade2%n_log_enhanced
cascade4%n_t_channel = cascade1%n_t_channel + cascade2%n_t_channel
if (cascade4%n_off_shell > cascade_set%off_shell) then
    deallocate (cascade4)
    ok = .false.
else if (cascade4%n_t_channel > cascade_set%t_channel) then

```

```

        deallocate (cascade4)
        ok = .false.
    else
        i1 = cascade1%depth
        i2 = i1 + 1
        i3 = i1 + cascade2%depth
        i4 = cascade4%depth
        cascade4%tree(:i1) = cascade1%tree
        where (cascade1%tree_mapping > NO_MAPPING)
            cascade4%tree_pdg(:i1) = cascade1%tree_pdg
        elsewhere
            cascade4%tree_pdg(:i1) = UNDEFINED
        end where
        cascade4%tree_mapping(:i1) = cascade1%tree_mapping
        cascade4%tree_resonant(:i1) = cascade1%tree_resonant
        cascade4%tree(i2:i3) = cascade2%tree
        where (cascade2%tree_mapping > NO_MAPPING)
            cascade4%tree_pdg(i2:i3) = cascade2%tree_pdg
        elsewhere
            cascade4%tree_pdg(i2:i3) = UNDEFINED
        end where
        cascade4%tree_mapping(i2:i3) = cascade2%tree_mapping
        cascade4%tree_resonant(i2:i3) = cascade2%tree_resonant
        cascade4%tree(i4) = cascade4%bincode
        cascade4%tree_pdg(i4) = UNDEFINED
        cascade4%tree_mapping(i4) = cascade4%mapping
        cascade4%tree_resonant(i4) = .false.
        call tree_sort (cascade4%tree, &
            cascade4%tree_pdg, cascade4%tree_mapping, cascade4%tree_resonant)
        cascade4%has_children = .true.
        cascade4%daughter1 => cascade1
        cascade4%daughter2 => cascade2
        cascade4%mother => cascade3
        call cascade_set_add (cascade_set, cascade4, ok)
        if (ok) then
            if (.not. associated (cascade_set%first_k)) then
                cascade_set%first_k => cascade4
            end if
        else
            deallocate (cascade4)
        end if
    end if
end subroutine cascade_keystone

```

Sort a tree (array of binary codes) and particle code array simultaneously, by ascending binary codes. A convenient method is to use the `maxloc` function iteratively, to find and remove the largest entry in the tree array one by one.

(Cascades: procedures) +=

```

subroutine tree_sort (tree, pdg, mapping, resonant)
    integer(TC), dimension(:), intent(inout) :: tree
    integer, dimension(:), intent(inout) :: pdg, mapping
    logical, dimension(:), intent(inout) :: resonant
    integer(TC), dimension(size(tree)) :: tree_tmp

```

```

integer, dimension(size(pdg)) :: pdg_tmp, mapping_tmp
logical, dimension(size(resonant)) :: resonant_tmp
integer, dimension(1) :: pos
integer :: i
tree_tmp = tree
pdg_tmp = pdg
mapping_tmp = mapping
resonant_tmp = resonant
do i = size(tree),1,-1
    pos = maxloc (tree_tmp)
    tree(i) = tree_tmp (pos(1))
    pdg(i) = pdg_tmp (pos(1))
    mapping(i) = mapping_tmp (pos(1))
    resonant(i) = resonant_tmp (pos(1))
    tree_tmp(pos(1)) = 0
end do
end subroutine tree_sort

```

19.9.12 Cascade set generation

These procedures loop over cascades and build up the cascade set. After each iteration of the innermost loop, we set a breakpoint.

s-channel: We use a nested scan to combine all cascades with all other cascades.

```

(Cascades: procedures)+≡
subroutine cascade_set_generate_s (cascade_set)
    type(cascade_set_t), intent(inout), target :: cascade_set
    type(cascade_t), pointer :: cascade1, cascade2
    cascade1 => cascade_set%first
    LOOP1: do while (associated (cascade1))
        cascade2 => cascade_set%first
        LOOP2: do while (associated (cascade2))
            if (cascade2%index >= cascade1%index) exit LOOP2
            if (cascade1 .disjunct. cascade2) then
                call cascade_match_pair (cascade_set, cascade1, cascade2, .true.)
            end if
            call terminate_now_if_signal ()
            cascade2 => cascade2%next
        end do LOOP2
        cascade1 => cascade1%next
    end do LOOP1
end subroutine cascade_set_generate_s

```

The t-channel cascades are directed and have a seed (one of the incoming particles) and a target (the other one). We loop over all possible seeds and targets. Inside this, we loop over all t-channel cascades (*cascade1*) and s-channel cascades (*cascade2*) and try to combine them.

```

(Cascades: procedures)+≡
subroutine cascade_set_generate_t (cascade_set, pos_seed, pos_target)
    type(cascade_set_t), intent(inout), target :: cascade_set
    integer, intent(in) :: pos_seed, pos_target

```

```

type(cascade_t), pointer :: cascade_seed, cascade_target
type(cascade_t), pointer :: cascade1, cascade2
integer(TC) :: bc_seed, bc_target
bc_seed = ibset (0_TC, pos_seed-1)
bc_target = ibset (0_TC, pos_target-1)
cascade_seed => cascade_set%first_t
LOOP_SEED: do while (associated (cascade_seed))
  if (cascade_seed%bincode == bc_seed) then
    cascade_target => cascade_set%first_t
    LOOP_TARGET: do while (associated (cascade_target))
      if (cascade_target%bincode == bc_target) then
        cascade1 => cascade_set%first_t
        LOOP_T: do while (associated (cascade1))
          if ((cascade1 .disjunct. cascade_target) &
              .and. .not. (cascade1 .disjunct. cascade_seed)) then
            cascade2 => cascade_set%first
            LOOP_S: do while (associated (cascade2))
              if ((cascade2 .disjunct. cascade_target) &
                  .and. (cascade2 .disjunct. cascade1)) then
                call cascade_match_pair &
                  (cascade_set, cascade1, cascade2, .false.)
              end if
              call terminate_now_if_signal ()
              cascade2 => cascade2%next
            end do LOOP_S
          end if
          call terminate_now_if_signal ()
          cascade1 => cascade1%next
        end do LOOP_T
      end if
      call terminate_now_if_signal ()
      cascade_target => cascade_target%next
    end do LOOP_TARGET
  end if
  call terminate_now_if_signal ()
  cascade_seed => cascade_seed%next
end do LOOP_SEED
end subroutine cascade_set_generate_t

```

This part completes the phase space for decay processes. It is similar to s-channel cascade generation, but combines two cascade with the particular cascade of the incoming particle. This particular cascade is expected to be pointed at by `first_t`.

(Cascades: procedures) +=

```

subroutine cascade_set_generate_decay (cascade_set)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), pointer :: cascade1, cascade2
  type(cascade_t), pointer :: cascade_in
  cascade_in => cascade_set%first_t
  cascade1 => cascade_set%first
  do while (associated (cascade1))
    if (cascade1 .disjunct. cascade_in) then
      cascade2 => cascade1%next
    end if
  end do
end subroutine

```



```

do while (associated (cascade2))
  if ((cascade2 .disjunct. cascade1) &
      .and. (cascade2 .disjunct. cascade_in)) then
    call cascade_match_triplet (cascade_set, &
                              cascade1, cascade2, cascade_in, .true.)
  end if
  call terminate_now_if_signal ()
  cascade2 => cascade2%next
end do
end if
call terminate_now_if_signal ()
cascade1 => cascade1%next
end do
end subroutine cascade_set_generate_decay

```

This part completes the phase space for scattering processes. We combine a t-channel cascade (containing the seed) with a s-channel cascade and the target.

(Cascades: procedures)+≡

```

subroutine cascade_set_generate_scattering &
  (cascade_set, ns1, ns2, nt1, nt2, pos_seed, pos_target)
  type(cascade_set_t), intent(inout), target :: cascade_set
  integer, intent(in) :: pos_seed, pos_target
  integer, intent(in) :: ns1, ns2, nt1, nt2
  type(cascade_t), pointer :: cascade_seed, cascade_target
  type(cascade_t), pointer :: cascade1, cascade2
  integer(TC) :: bc_seed, bc_target
  bc_seed = ibset (0_TC, pos_seed-1)
  bc_target = ibset (0_TC, pos_target-1)
  cascade_seed => cascade_set%first_t
  LOOP_SEED: do while (associated (cascade_seed))
    if (cascade_seed%index < ns1) then
      cascade_seed => cascade_seed%next
      cycle LOOP_SEED
    else if (cascade_seed%index > ns2) then
      exit LOOP_SEED
    else if (cascade_seed%bincode == bc_seed) then
      cascade_target => cascade_set%first_t
      LOOP_TARGET: do while (associated (cascade_target))
        if (cascade_target%index < nt1) then
          cascade_target => cascade_target%next
          cycle LOOP_TARGET
        else if (cascade_target%index > nt2) then
          exit LOOP_TARGET
        else if (cascade_target%bincode == bc_target) then
          cascade1 => cascade_set%first_t
          LOOP_T: do while (associated (cascade1))
            if ((cascade1 .disjunct. cascade_target) &
                .and. .not. (cascade1 .disjunct. cascade_seed)) then
              cascade2 => cascade_set%first
              LOOP_S: do while (associated (cascade2))
                if ((cascade2 .disjunct. cascade_target) &
                    .and. (cascade2 .disjunct. cascade1)) then
                  call cascade_match_triplet (cascade_set, &

```

```

                                cascade1, cascade2, cascade_target, .false.)
                                end if
                                call terminate_now_if_signal ()
                                cascade2 => cascade2%next
                                end do LOOP_S
                                end if
                                call terminate_now_if_signal ()
                                cascade1 => cascade1%next
                                end do LOOP_T
                                end if
                                call terminate_now_if_signal ()
                                cascade_target => cascade_target%next
                                end do LOOP_TARGET
                                end if
                                call terminate_now_if_signal ()
                                cascade_seed => cascade_seed%next
                                end do LOOP_SEED
end subroutine cascade_set_generate_scattering

```

19.9.13 Groves

Before assigning groves, assign hashcodes to the resonance patterns, so they can easily be compared.

(Cascades: procedures) +=

```

subroutine cascade_set_assign_resonance_hash (cascade_set)
  type(cascade_set_t), intent(inout) :: cascade_set
  type(cascade_t), pointer :: cascade
  cascade => cascade_set%first_k
  do while (associated (cascade))
    call cascade_assign_resonance_hash (cascade)
    cascade => cascade%next
  end do
end subroutine cascade_set_assign_resonance_hash

```

After all cascades are recorded, we group the complete cascades in groves. A grove consists of cascades with identical multiplicity, number of resonances, log-enhanced, t-channel lines, and resonance flavors.

(Cascades: procedures) +=

```

subroutine cascade_set_assign_groves (cascade_set)
  type(cascade_set_t), intent(inout), target :: cascade_set
  type(cascade_t), pointer :: cascade1, cascade2
  integer :: multiplicity
  integer :: n_resonances, n_log_enhanced, n_t_channel, n_off_shell
  integer :: res_hash
  integer :: grove
  grove = 0
  cascade1 => cascade_set%first_k
  do while (associated (cascade1))
    if (cascade1%active .and. cascade1%complete &
      .and. cascade1%grove == 0) then
      grove = grove + 1
      cascade1%grove = grove
    end if
    cascade1 => cascade1%next
  end do
end subroutine cascade_set_assign_groves

```

```

multiplicity = cascade1%multiplicity
n_resonances = cascade1%n_resonances
n_log_enhanced = cascade1%n_log_enhanced
n_off_shell = cascade1%n_off_shell
n_t_channel = cascade1%n_t_channel
res_hash = cascade1%res_hash
cascade2 => cascade1%next
do while (associated (cascade2))
  if (cascade2%grove == 0) then
    if (cascade2%multiplicity == multiplicity &
        .and. cascade2%n_resonances == n_resonances &
        .and. cascade2%n_log_enhanced == n_log_enhanced &
        .and. cascade2%n_off_shell == n_off_shell &
        .and. cascade2%n_t_channel == n_t_channel &
        .and. cascade2%res_hash == res_hash) then
      cascade2%grove = grove
    end if
  end if
  call terminate_now_if_signal ()
  cascade2 => cascade2%next
end do
end if
call terminate_now_if_signal ()
cascade1 => cascade1%next
end do
cascade_set%n_groves = grove
end subroutine cascade_set_assign_groves

```

19.9.14 Generate the phase space file

Generate a complete phase space configuration.

For each flavor assignment: First, all s-channel graphs that can be built up from the outgoing particles. Then we distinguish (1) decay, where we complete the s-channel graphs by connecting to the input line, and (2) scattering, where we now generate t-channel graphs by introducing an incoming particle, and complete this by connecting to the other incoming particle.

After all cascade sets have been generated, merge them into a common set. This eliminates redundancies between flavor assignments.

```

<Cascades: public>+≡
  public :: cascade_set_generate

<Cascades: procedures>+≡
  subroutine cascade_set_generate &
    (cascade_set, model, n_in, n_out, flv, phs_par, fatal_beam_decay)
    type(cascade_set_t), intent(out) :: cascade_set
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: n_in, n_out
    type(flavor_t), dimension(:,:), intent(in) :: flv
    type(phs_parameters_t), intent(in) :: phs_par
    logical, intent(in) :: fatal_beam_decay
    type(cascade_set_t), dimension(:), allocatable :: cset
    type(cascade_t), pointer :: cascade

```

```

integer :: i
if (phase_space_vanishes (phs_par%sqrts, n_in, flv)) return
call cascade_set_init (cascade_set, model, n_in, n_out, phs_par, &
    fatal_beam_decay, flv)
allocate (cset (size (flv, 2)))
do i = 1, size (cset)
    call cascade_set_generate_single (cset(i), &
        model, n_in, n_out, flv(:,i), phs_par, fatal_beam_decay)
    cascade => cset(i)%first_k
    do while (associated (cascade))
        if (cascade%active .and. cascade%complete) then
            call cascade_set_add_copy (cascade_set, cascade)
        end if
        cascade => cascade%next
    end do
    call cascade_set_final (cset(i))
end do
cascade_set%first_k => cascade_set%first
call cascade_set_assign_resonance_hash (cascade_set)
call cascade_set_assign_groves (cascade_set)
end subroutine cascade_set_generate

```

This generates phase space for a single channel, without assigning groves.

(*Cascades: procedures*) +=

```

subroutine cascade_set_generate_single (cascade_set, &
    model, n_in, n_out, flv, phs_par, fatal_beam_decay)
type(cascade_set_t), intent(out) :: cascade_set
class(model_data_t), intent(in), target :: model
integer, intent(in) :: n_in, n_out
type(flavor_t), dimension(:), intent(in) :: flv
type(phs_parameters_t), intent(in) :: phs_par
logical, intent(in) :: fatal_beam_decay
integer :: n11, n12, n21, n22
call cascade_set_init (cascade_set, model, n_in, n_out, phs_par, &
    fatal_beam_decay)
call cascade_set_add_outgoing (cascade_set, flv(n_in+1:))
call cascade_set_generate_s (cascade_set)
select case (n_in)
case(1)
    call cascade_set_add_incoming &
        (cascade_set, n11, n12, n_out + 1, flv(1))
    call cascade_set_generate_decay (cascade_set)
case(2)
    call cascade_set_add_incoming &
        (cascade_set, n11, n12, n_out + 1, flv(2))
    call cascade_set_add_incoming &
        (cascade_set, n21, n22, n_out + 2, flv(1))
    call cascade_set_generate_t (cascade_set, n_out + 1, n_out + 2)
    call cascade_set_generate_t (cascade_set, n_out + 2, n_out + 1)
    call cascade_set_generate_scattering &
        (cascade_set, n11, n12, n21, n22, n_out + 1, n_out + 2)
    call cascade_set_generate_scattering &
        (cascade_set, n21, n22, n11, n12, n_out + 2, n_out + 1)

```

```

        end select
    end subroutine cascade_set_generate_single

```

Sanity check: Before anything else is done, check if there could possibly be any phase space.

```

<Cascades: public>+=
    public :: phase_space_vanishes

<Cascades: procedures>+=
    function phase_space_vanishes (sqrts, n_in, flv) result (flag)
        logical :: flag
        real(default), intent(in) :: squrts
        integer, intent(in) :: n_in
        type(flavor_t), dimension(:,:), intent(in) :: flv
        real(default), dimension(:,:), allocatable :: mass
        real(default), dimension(:), allocatable :: mass_in, mass_out
        integer :: n_prt, n_flv, i, j
        flag = .false.
        if (sqrts <= 0) then
            call msg_error ("Phase space vanishes (sqrts must be positive)")
            flag = .true.; return
        end if
        n_prt = size (flv, 1)
        n_flv = size (flv, 2)
        allocate (mass (n_prt, n_flv), mass_in (n_flv), mass_out (n_flv))
        mass = flv%get_mass ()
        mass_in = sum (mass(:n_in,:), 1)
        mass_out = sum (mass(n_in+1:,:), 1)
        if (any (mass_in > squrts)) then
            call msg_error ("Mass sum of incoming particles " &
                // "is more than available energy")
            flag = .true.; return
        end if
        if (any (mass_out > squrts)) then
            call msg_error ("Mass sum of outgoing particles " &
                // "is more than available energy")
            flag = .true.; return
        end if
    end function phase_space_vanishes

```

19.9.15 Return the resonance histories for subtraction

This appears to be essential (re-export of some imported assignment?)!

```

<Cascades: public>+=
    public :: assignment(=)

Extract the resonance set from a complete cascade.

<Cascades: cascade: TBP>=
    procedure :: extract_resonance_history => cascade_extract_resonance_history

<Cascades: procedures>+=
    subroutine cascade_extract_resonance_history &
        (cascade, res_hist, model, n_out)

```

```

class(cascade_t), intent(in), target :: cascade
type(resonance_history_t), intent(out) :: res_hist
class(model_data_t), intent(in), target :: model
integer, intent(in) :: n_out
type(resonance_info_t) :: resonance
integer :: i, mom_id, pdg
if (debug_on) call msg_debug2 (D_PHASESPACE, "cascade_extract_resonance_history")
if (cascade%n_resonances > 0) then
  if (cascade%has_children) then
    if (debug_on) call msg_debug2 (D_PHASESPACE, "cascade has resonances and children")
    do i = 1, size(cascade%tree_resonant)
      if (cascade%tree_resonant (i)) then
        mom_id = cascade%tree (i)
        pdg = cascade%tree_pdg (i)
        call resonance%init (mom_id, pdg, model, n_out)
        if (debug2_active (D_PHASESPACE)) then
          print *, 'D: Adding resonance'
          call resonance%write ()
        end if
        call res_hist%add_resonance (resonance)
      end if
    end do
  end if
end if
end subroutine cascade_extract_resonance_history

```

<Cascades: public>+≡

```
public :: cascade_set_get_n_trees
```

<Cascades: procedures>+≡

```

function cascade_set_get_n_trees (cascade_set) result (n)
  type(cascade_set_t), intent(in), target :: cascade_set
  integer :: n
  type(cascade_t), pointer :: cascade
  integer :: grove
  if (debug_on) call msg_debug (D_PHASESPACE, "cascade_set_get_n_trees")
  n = 0
  do grove = 1, cascade_set%n_groves
    cascade => cascade_set%first_k
    do while (associated (cascade))
      if (cascade%active .and. cascade%complete) then
        if (cascade%grove == grove) then
          n = n + 1
        end if
      end if
      cascade => cascade%next
    end do
  end do
  if (debug_on) call msg_debug (D_PHASESPACE, "n", n)
end function cascade_set_get_n_trees

```

Distill the set of resonance histories from the cascade set. The result is an array which contains each valid history exactly once.

<Cascades: public>+≡

```

public :: cascade_set_get_resonance_histories
<Cascades: procedures>+=
  subroutine cascade_set_get_resonance_histories (cascade_set, n_filter, res_hists)
    type(cascade_set_t), intent(in), target :: cascade_set
    integer, intent(in), optional :: n_filter
    type(resonance_history_t), dimension(:), allocatable, intent(out) :: res_hists
    type(resonance_history_t), dimension(:), allocatable :: tmp
    type(cascade_t), pointer :: cascade
    type(resonance_history_t) :: res_hist
    type(resonance_history_set_t) :: res_hist_set
    integer :: grove, i, n_hists
    logical :: included, add_to_list
    if (debug_on) call msg_debug (D_PHASESPACE, "cascade_set_get_resonance_histories")
    call res_hist_set%init (n_filter = n_filter)
    do grove = 1, cascade_set%n_groves
      cascade => cascade_set%first_k
      do while (associated (cascade))
        if (cascade%active .and. cascade%complete) then
          if (cascade%grove == grove) then
            if (debug_on) call msg_debug2 (D_PHASESPACE, "grove", grove)
            call cascade%extract_resonance_history &
              (res_hist, cascade_set%model, cascade_set%n_out)
            call res_hist_set%enter (res_hist)
          end if
        end if
        cascade => cascade%next
      end do
    end do
    call res_hist_set%freeze ()
    call res_hist_set%to_array (res_hists)
  end subroutine cascade_set_get_resonance_histories

```

19.9.16 Unit tests

Test module, followed by the corresponding implementation module.

```

<cascades_ut.f90>≡
  <File header>

  module cascades_ut
    use unit_tests
    use cascades_util

    <Standard module head>

    <Cascades: public test>

    contains

    <Cascades: test driver>

  end module cascades_ut

```

```

<cascades_uti.f90>≡
  <File header>

  module cascades_uti

    <Use kinds>
    <Use strings>
    use numeric_utils
    use flavors
    use model_data
    use phs_forests, only: phs_parameters_t
    use resonances, only: resonance_history_t

    use cascades

    <Standard module head>

    <Cascades: test declarations>

    contains

    <Cascades: tests>

  end module cascades_uti
API: driver for the unit tests below.
<Cascades: public test>≡
  public :: cascades_test
<Cascades: test driver>≡
  subroutine cascades_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Cascades: execute tests>
  end subroutine cascades_test

```

Check cascade setup

Checking the basic setup up of the phase space cascade parameterizations.

```

<Cascades: execute tests>≡
  call test (cascades_1, "cascades_1", &
    "check cascade setup", &
    u, results)
<Cascades: test declarations>≡
  public :: cascades_1
<Cascades: tests>≡
  subroutine cascades_1 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(flavor_t), dimension(5,2) :: flv
    type(cascade_set_t) :: cascade_set
    type(phs_parameters_t) :: phs_par

```



```

write (u, "(A)")  "* Test output: cascades_1"
write (u, "(A)")  "* Purpose: test cascade phase space functions"
write (u, "(A)")

write (u, "(A)")  "* Initializing"
write (u, "(A)")

call model%init_sm_test ()

call flv(1,1)%init ( 2, model)
call flv(2,1)%init (-2, model)
call flv(3,1)%init ( 1, model)
call flv(4,1)%init (-1, model)
call flv(5,1)%init (21, model)
call flv(1,2)%init ( 2, model)
call flv(2,2)%init (-2, model)
call flv(3,2)%init ( 2, model)
call flv(4,2)%init (-2, model)
call flv(5,2)%init (21, model)
phs_par%sqrts = 1000._default
phs_par%off_shell = 2

write (u, "(A)")
write (u, "(A)")  "* Generating the cascades"
write (u, "(A)")

call cascade_set_generate (cascade_set, model, 2, 3, flv, phs_par,.true.)
call cascade_set_write (cascade_set, u)
call cascade_set_write_file_format (cascade_set, u)

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call cascade_set_final (cascade_set)
call model%final ()

write (u, *)
write (u, "(A)")  "* Test output end: cascades_1"

end subroutine cascades_1

```

Check resonance history

```

<Cascades: execute tests>+≡
  call test(cascades_2, "cascades_2", &
    "Check resonance history", u, results)

<Cascades: test declarations>+≡
  public :: cascades_2

<Cascades: tests>+≡
  subroutine cascades_2 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model

```

```

type(flavor_t), dimension(5,1) :: flv
type(cascade_set_t) :: cascade_set
type(phs_parameters_t) :: phs_par
type(resonance_history_t), dimension(:), allocatable :: res_hists
integer :: n, i
write (u, "(A)")  "* Test output: cascades_2"
write (u, "(A)")  "* Purpose: Check resonance history"
write (u, "(A)")

write (u, "(A)")  "* Initializing"
write (u, "(A)")

call model%init_sm_test ()

call flv(1,1)%init ( 2, model)
call flv(2,1)%init (-2, model)
call flv(3,1)%init ( 1, model)
call flv(4,1)%init (-1, model)
call flv(5,1)%init (22, model)
phs_par%sqrts = 1000._default
phs_par%off_shell = 2

write (u, "(A)")
write (u, "(A)")  "* Generating the cascades"
write (u, "(A)")

call cascade_set_generate (cascade_set, model, 2, 3, flv, phs_par,.true.)
call cascade_set_get_resonance_histories (cascade_set, res_hists = res_hists)
n = cascade_set_get_n_trees (cascade_set)
call assert_equal (u, n, 24, "Number of trees")
do i = 1, size(res_hists)
    call res_hists(i)%write (u)
    write (u, "(A)")
end do

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call cascade_set_final (cascade_set)
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: cascades_2"
end subroutine cascades_2

```

19.10 WOOD phase space

This is the module that interfaces the `phs_forests` phase-space treatment and the `cascades` module for generating phase-space channels. As an extension of the `phs_base` abstract type, the phase-space configuration and instance implement the standard API.

(Currently, this is the only generic phase-space implementation of WHIZARD. For trivial two-particle phase space, there is `phs_wood` as an alternative.)

```

<phs_wood.f90>≡
  <File header>

  module phs_wood

    <Use kinds>
    <Use strings>
    use io_units
    use constants
    use numeric_utils
    use diagnostics
    use os_interface
    use md5
    use physics_defs
    use lorentz
    use model_data
    use flavors
    use process_constants
    use sf_mappings
    use sf_base
    use phs_base
    use mappings
    use resonances, only: resonance_history_set_t
    use phs_forests
    use cascades
    use cascades2

    <Standard module head>

    <PHS wood: public>

    <PHS wood: types>

    contains

    <PHS wood: procedures>

  end module phs_wood

```

19.10.1 Configuration

```

<PHS wood: public>≡
  public :: phs_wood_config_t

<PHS wood: types>≡
  type, extends (phs_config_t) :: phs_wood_config_t
    character(32) :: md5sum_forest = ""
    type(string_t) :: phs_path
    integer :: io_unit = 0
    logical :: io_unit_keep_open = .false.
    logical :: use_equivalences = .false.
    logical :: fatal_beam_decay = .true.

```

```

type(mapping_defaults_t) :: mapping_defaults
type(phs_parameters_t) :: par
type(string_t) :: run_id
type(cascade_set_t), allocatable :: cascade_set
logical :: use_cascades2 = .false.
type(feyngraph_set_t), allocatable :: feyngraph_set
type(phs_forest_t) :: forest
type(os_data_t) :: os_data
logical :: is_combined_integration = .false.
contains
<PHS wood: phs wood config: TBP>
end type phs_wood_config_t

```

Finalizer. We should delete the cascade set and the forest subobject.

Also close the I/O unit, just in case. (We assume that `io_unit` is not standard input/output.)

```

<PHS wood: phs wood config: TBP>≡
  procedure :: final => phs_wood_config_final

<PHS wood: procedures>≡
  subroutine phs_wood_config_final (object)
    class(phs_wood_config_t), intent(inout) :: object
    logical :: opened
    if (object%io_unit /= 0) then
      inquire (unit = object%io_unit, opened = opened)
      if (opened) close (object%io_unit)
    end if
    call object%clear_phase_space ()
    call phs_forest_final (object%forest)
  end subroutine phs_wood_config_final

<PHS wood: phs wood config: TBP>+≡
  procedure :: increase_n_par => phs_wood_config_increase_n_par

<PHS wood: procedures>+≡
  subroutine phs_wood_config_increase_n_par (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
    if (phs_config%is_combined_integration) then
      phs_config%n_par = phs_config%n_par + 3
    end if
  end subroutine phs_wood_config_increase_n_par

```

Output. The contents of the PHS forest are not printed explicitly.

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: write => phs_wood_config_write

<PHS wood: procedures>+≡
  subroutine phs_wood_config_write (object, unit, include_id)
    class(phs_wood_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: include_id
    integer :: u
    u = given_output_unit (unit)

```

```

write (u, "(1x,A)") &
    "Partonic phase-space configuration (phase-space forest):"
call object%base_write (unit)
write (u, "(1x,A)")    "Phase-space configuration parameters:"
call object%par%write (u)
call object%mapping_defaults%write (u)
write (u, "(3x,A,A,A)") "Run ID: '", char (object%run_id), "'"
end subroutine phs_wood_config_write

```

Print the PHS forest contents.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: write_forest => phs_wood_config_write_forest
<PHS wood: procedures>+≡
    subroutine phs_wood_config_write_forest (object, unit)
        class(phs_wood_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        call phs_forest_write (object%forest, u)
    end subroutine phs_wood_config_write_forest

```

Set the phase-space parameters that the configuration generator requests.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: set_parameters => phs_wood_config_set_parameters
<PHS wood: procedures>+≡
    subroutine phs_wood_config_set_parameters (phs_config, par)
        class(phs_wood_config_t), intent(inout) :: phs_config
        type(phs_parameters_t), intent(in) :: par
        phs_config%par = par
    end subroutine phs_wood_config_set_parameters

```

Enable the generation of channel equivalences (when calling configure).

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: enable_equivalences => phs_wood_config_enable_equivalences
<PHS wood: procedures>+≡
    subroutine phs_wood_config_enable_equivalences (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
        phs_config%use_equivalences = .true.
    end subroutine phs_wood_config_enable_equivalences

```

Set the phase-space mapping parameters that the configuration generator requests.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: set_mapping_defaults => phs_wood_config_set_mapping_defaults
<PHS wood: procedures>+≡
    subroutine phs_wood_config_set_mapping_defaults (phs_config, mapping_defaults)
        class(phs_wood_config_t), intent(inout) :: phs_config
        type(mapping_defaults_t), intent(in) :: mapping_defaults
        phs_config%mapping_defaults = mapping_defaults
    end subroutine phs_wood_config_set_mapping_defaults

```

Define the input stream for the phase-space file as an open logical unit. The unit must be connected.

```

(PHS wood: phs wood config: TBP)+≡
    procedure :: set_input => phs_wood_config_set_input

(PHS wood: procedures)+≡
    subroutine phs_wood_config_set_input (phs_config, unit)
        class(phs_wood_config_t), intent(inout) :: phs_config
        integer, intent(in) :: unit
        phs_config%io_unit = unit
        rewind (unit)
    end subroutine phs_wood_config_set_input

```

19.10.2 Phase-space generation

This subroutine generates a phase space configuration using the `cascades` module. Note that this may take time, and the `cascade_set` subobject may consume a large amount of memory.

```

(PHS wood: phs wood config: TBP)+≡
    procedure :: generate_phase_space => phs_wood_config_generate_phase_space

(PHS wood: procedures)+≡
    subroutine phs_wood_config_generate_phase_space (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
        integer :: off_shell, extra_off_shell
        logical :: valid
        integer :: unit_fds
        type(string_t) :: file_name
        logical :: file_exists
        call msg_message ("Phase space: generating configuration ...")
        off_shell = phs_config%par%off_shell
        if (phs_config%use_cascades2) then
            file_name = char (phs_config%id) // ".fds"
            inquire (file=char (file_name), exist=file_exists)
            if (.not. file_exists) call msg_fatal &
                ("The 0'Mega input file " // char (file_name) // &
                 " does not exist. " // "Please make sure that the " // &
                 "variable ?omega_write_phs_output has been set correctly.")
            unit_fds = free_unit ()
            open (unit=unit_fds, file=char(file_name), status='old', action='read')
            do extra_off_shell = 0, max (phs_config%n_tot - 3, 0)
                phs_config%par%off_shell = off_shell + extra_off_shell
                allocate (phs_config%feyngraph_set)
                call feyngraph_set_generate (phs_config%feyngraph_set, &
                    phs_config%model, phs_config%n_in, phs_config%n_out, &
                    phs_config%flv, &
                    phs_config%par, phs_config%fatal_beam_decay, unit_fds, &
                    phs_config%vis_channels)
                if (feyngraph_set_is_valid (phs_config%feyngraph_set)) then
                    exit
                else
                    call msg_message ("Phase space: ... failed. &
                        &Increasing phs_off_shell ...")
                end if
            end do
        end if
    end subroutine phs_wood_config_generate_phase_space

```

```

        call phs_config%feyngraph_set%final ()
        deallocate (phs_config%feyngraph_set)
    end if
end do
close (unit_fds)
else
    allocate (phs_config%cascade_set)
    do extra_off_shell = 0, max (phs_config%n_tot - 3, 0)
        phs_config%par%off_shell = off_shell + extra_off_shell
        call cascade_set_generate (phs_config%cascade_set, &
            phs_config%model, phs_config%n_in, phs_config%n_out, &
            phs_config%flv, &
            phs_config%par, phs_config%fatal_beam_decay)
        if (cascade_set_is_valid (phs_config%cascade_set)) then
            exit
        else
            call msg_message ("Phase space: ... failed. &
                &Increasing phs_off_shell ...")
        end if
    end do
end if
if (phs_config%use_cascades2) then
    valid = feyngraph_set_is_valid (phs_config%feyngraph_set)
else
    valid = cascade_set_is_valid (phs_config%cascade_set)
end if
if (valid) then
    call msg_message ("Phase space: ... success.")
else
    call msg_fatal ("Phase-space: generation failed")
end if
end subroutine phs_wood_config_generate_phase_space

```

Using the generated phase-space configuration, write an appropriate phase-space file to the stored (or explicitly specified) I/O unit.

(PHS wood: phs wood config: TBP)+≡

```

    procedure :: write_phase_space => phs_wood_config_write_phase_space

```

(PHS wood: procedures)+≡

```

    subroutine phs_wood_config_write_phase_space (phs_config, &
        filename_vis, unit)
        class(phs_wood_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        type(string_t), intent(in), optional :: filename_vis
        type(string_t) :: setenv_tex, setenv_mp, pipe, pipe_dvi
        integer :: u, unit_tex, unit_dev, status
        if (allocated (phs_config%cascade_set) .or. allocated (phs_config%feyngraph_set)) then
            if (present (unit)) then
                u = unit
            else
                u = phs_config%io_unit
            end if
            write (u, "(1x,A,A)") "process ", char (phs_config%id)
            write (u, "(A)")

```

```

if (phs_config%use_cascades2) then
  call feyngraph_set_write_process_bincode_format (phs_config%feyngraph_set, u)
else
  call cascade_set_write_process_bincode_format (phs_config%cascade_set, u)
end if
write (u, "(A)")
write (u, "(3x,A,A,A32,A)") "md5sum_process    = ", &
  '', phs_config%md5sum_process, ''
write (u, "(3x,A,A,A32,A)") "md5sum_model_par  = ", &
  '', phs_config%md5sum_model_par, ''
write (u, "(3x,A,A,A32,A)") "md5sum_phs_config = ", &
  '', phs_config%md5sum_phs_config, ''
call phs_config%par%write (u)
if (phs_config%use_cascades2) then
  call feyngraph_set_write_file_format (phs_config%feyngraph_set, u)
else
  call cascade_set_write_file_format (phs_config%cascade_set, u)
end if
if (phs_config%vis_channels) then
  unit_tex = free_unit ()
  open (unit=unit_tex, file=char(filename_vis // ".tex"), &
    action="write", status="replace")
  if (phs_config%use_cascades2) then
    call feyngraph_set_write_graph_format (phs_config%feyngraph_set, &
      filename_vis // "-graphs", phs_config%id, unit_tex)
  else
    call cascade_set_write_graph_format (phs_config%cascade_set, &
      filename_vis // "-graphs", phs_config%id, unit_tex)
  end if
  close (unit_tex)
  call msg_message ("Phase space: visualizing channels in file " &
    // char(trim(filename_vis)) // "...")
  if (phs_config%os_data%event_analysis_ps) then
    BLOCK: do
      unit_dev = free_unit ()
      open (file = "/dev/null", unit = unit_dev, &
        action = "write", iostat = status)
      if (status /= 0) then
        pipe = ""
        pipe_dvi = ""
      else
        pipe = " > /dev/null"
        pipe_dvi = " 2>/dev/null 1>/dev/null"
      end if
      close (unit_dev)
      if (phs_config%os_data%whizard_texpath /= "") then
        setenv_tex = "TEXINPUTS=" // &
          phs_config%os_data%whizard_texpath // " :$TEXINPUTS "
        setenv_mp = "MPINPUTS=" // &
          phs_config%os_data%whizard_texpath // " :$MPINPUTS "
      else
        setenv_tex = ""
        setenv_mp = ""
      end if
    end if
  end if

```



```

        call os_system_call (setenv_tex // &
            phs_config%os_data%latex // " " // &
            filename_vis // ".tex" // pipe, status)
    if (status /= 0) exit BLOCK
    if (phs_config%os_data%mpost /= "") then
        call os_system_call (setenv_mp // &
            phs_config%os_data%mpost // " " // &
            filename_vis // "-graphs.mp" // pipe, status)
    else
        call msg_fatal ("Could not use MetaPOST.")
    end if
    if (status /= 0) exit BLOCK
    call os_system_call (setenv_tex // &
        phs_config%os_data%latex // " " // &
        filename_vis // ".tex" // pipe, status)
    if (status /= 0) exit BLOCK
    call os_system_call &
        (phs_config%os_data%dvips // " -o " // filename_vis &
        // ".ps" // filename_vis // ".dvi" // pipe_dvi, status)
    if (status /= 0) exit BLOCK
    if (phs_config%os_data%event_analysis_pdf) then
        call os_system_call (phs_config%os_data%ps2pdf // " " // &
            filename_vis // ".ps", status)
        if (status /= 0) exit BLOCK
    end if
    exit BLOCK
end do BLOCK
if (status /= 0) then
    call msg_error ("Unable to compile analysis output file")
end if
end if
else
    call msg_fatal ("Phase-space configuration: &
        &no phase space object generated")
end if
end subroutine phs_wood_config_write_phase_space

```

Clear the phase-space configuration. This is useful since the object may become *really* large.

(PHS wood: phs wood config: TBP)+≡

```

    procedure :: clear_phase_space => phs_wood_config_clear_phase_space

```

(PHS wood: procedures)+≡

```

subroutine phs_wood_config_clear_phase_space (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
    if (allocated (phs_config%cascade_set)) then
        call cascade_set_final (phs_config%cascade_set)
        deallocate (phs_config%cascade_set)
    end if
    if (allocated (phs_config%feyngraph_set)) then
        call phs_config%feyngraph_set%final ()
        deallocate (phs_config%feyngraph_set)
    end if

```

```
end subroutine phs_wood_config_clear_phase_space
```

Extract the set of resonance histories

```
<PHS wood: phs wood config: TBP>+≡
  procedure :: extract_resonance_history_set &
    => phs_wood_config_extract_resonance_history_set

<PHS wood: procedures>+≡
  subroutine phs_wood_config_extract_resonance_history_set &
    (phs_config, res_set, include_trivial)
    class(phs_wood_config_t), intent(in) :: phs_config
    type(resonance_history_set_t), intent(out) :: res_set
    logical, intent(in), optional :: include_trivial
    call phs_config%forest%extract_resonance_history_set &
      (res_set, include_trivial)
  end subroutine phs_wood_config_extract_resonance_history_set
```

19.10.3 Phase-space configuration

We read the phase-space configuration from the stored I/O unit. If this is not set, we assume that we have to generate a phase space configuration. When done, we open a scratch file and write the configuration.

If `rebuild` is set, we should trash any existing phase space file and build a new one. Otherwise, we try to use an old one, which we check for existence and integrity. If `ignore_mismatch` is set, we reuse an existing file even if it does not match the current setup.

```
<PHS wood: phs wood config: TBP>+≡
  procedure :: configure => phs_wood_config_configure

<PHS wood: procedures>+≡
  subroutine phs_wood_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, ignore_mismatch, &
    nlo_type, subdir)
    class(phs_wood_config_t), intent(inout) :: phs_config
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: sqrts_fixed
    logical, intent(in), optional :: lab_is_cm
    logical, intent(in), optional :: azimuthal_dependence
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    integer, intent(in), optional :: nlo_type
    type(string_t), intent(in), optional :: subdir
    type(string_t) :: filename, filename_vis
    logical :: variable_limits
    logical :: ok, exist, found, check, match, rebuild_phs
    integer :: g, c0, c1, n
    if (present (nlo_type)) then
      phs_config%nlo_type = nlo_type
    else
      phs_config%nlo_type = BORN
    end if
    phs_config%sqrts = sqrts
```

```

phs_config%par%sqrts = sqrts
if (present (sqrts_fixed)) &
  phs_config%sqrts_fixed = sqrts_fixed
if (present (lab_is_cm)) &
  phs_config%lab_is_cm = lab_is_cm
if (present (azimuthal_dependence)) &
  phs_config%azimuthal_dependence = azimuthal_dependence
if (present (rebuild)) then
  rebuild_phs = rebuild
else
  rebuild_phs = .true.
end if
if (present (ignore_mismatch)) then
  check = .not. ignore_mismatch
  if (ignore_mismatch) &
    call msg_warning ("Reading phs file: MD5 sum check disabled")
else
  check = .true.
end if
phs_config%md5sum_forest = ""
call phs_config%compute_md5sum (include_id = .false.)
if (phs_config%io_unit == 0) then
  filename = phs_config%make_phs_filename (subdir)
  filename_vis = phs_config%make_phs_filename (subdir) // "-vis"
  if (.not. rebuild_phs) then
    if (check) then
      call phs_config%read_phs_file (exist, found, match, subdir=subdir)
      rebuild_phs = .not. (exist .and. found .and. match)
    else
      call phs_config%read_phs_file (exist, found, subdir=subdir)
      rebuild_phs = .not. (exist .and. found)
    end if
  end if
  if (.not. mpi_is_comm_master ()) then
    rebuild_phs = .false.
    call msg_message ("MPI: Workers do not build phase space configuration.")
  end if
  if (rebuild_phs) then
    call phs_config%generate_phase_space ()
    phs_config%io_unit = free_unit ()
    if (phs_config%id /= "") then
      call msg_message ("Phase space: writing configuration file '" &
        // char (filename) // "'")
      open (phs_config%io_unit, file = char (filename), &
        status = "replace", action = "readwrite")
    else
      open (phs_config%io_unit, status = "scratch", action = "readwrite")
    end if
    call phs_config%write_phase_space (filename_vis)
    rewind (phs_config%io_unit)
  else
    call msg_message ("Phase space: keeping configuration file '" &
      // char (filename) // "'")
  end if
end if

```

```

end if
if (phs_config%io_unit == 0) then
    ok = .true.
else
    call phs_forest_read (phs_config%forest, phs_config%io_unit, &
        phs_config%id, phs_config%n_in, phs_config%n_out, &
        phs_config%model, ok)
    if (.not. phs_config%io_unit_keep_open) then
        close (phs_config%io_unit)
        phs_config%io_unit = 0
    end if
end if
if (ok) then
    call phs_forest_set_flavors (phs_config%forest, phs_config%flv(:,1))
    variable_limits = .not. phs_config%lab_is_cm
    call phs_forest_set_parameters &
        (phs_config%forest, phs_config%mapping_defaults, variable_limits)
    call phs_forest_setup_prt_combinations (phs_config%forest)
    phs_config%n_channel = phs_forest_get_n_channels (phs_config%forest)
    phs_config%n_par = phs_forest_get_n_parameters (phs_config%forest)
    allocate (phs_config%channel (phs_config%n_channel))
    if (phs_config%use_equivalences) then
        call phs_forest_set_equivalences (phs_config%forest)
        call phs_forest_get_equivalences (phs_config%forest, &
            phs_config%channel, phs_config%azimuthal_dependence)
        phs_config%provides_equivalences = .true.
    end if
    call phs_forest_set_s_mappings (phs_config%forest)
    call phs_config%record_on_shell ()
    if (phs_config%mapping_defaults%enable_s_mapping) then
        call phs_config%record_s_mappings ()
    end if
    allocate (phs_config%chain (phs_config%n_channel), source = 0)
    do g = 1, phs_forest_get_n_groves (phs_config%forest)
        call phs_forest_get_grove_bounds (phs_config%forest, g, c0, c1, n)
        phs_config%chain (c0:c1) = g
    end do
    phs_config%provides_chains = .true.
    call phs_config%compute_md5sum_forest ()
else
    write (msg_buffer, "(A,A,A)" &
        "Phase space: process '", &
        char (phs_config%id), "' not found in configuration file"
    call msg_fatal ()
end if
end subroutine phs_wood_config_configure

```

The MD5 sum of the forest is computed in addition to the MD5 sum of the configuration. The reason is that the forest may depend on a user-provided external file. On the other hand, this MD5 sum encodes all information that is relevant for further processing. Therefore, the `get_md5sum` method returns this result, once it is available.

(PHS wood: phs wood config: TBP)+≡

```

        procedure :: compute_md5sum_forest => phs_wood_config_compute_md5sum_forest
<PHS wood: procedures>+≡
    subroutine phs_wood_config_compute_md5sum_forest (phs_config)
        class(phs_wood_config_t), intent(inout) :: phs_config
        integer :: u
        u = free_unit ()
        open (u, status = "scratch", action = "readwrite")
        call phs_config%write_forest (u)
        rewind (u)
        phs_config%md5sum_forest = md5sum (u)
        close (u)
    end subroutine phs_wood_config_compute_md5sum_forest

```

Create filenames according to standard conventions. The `id` is the process name including the suffix `_iX` where `X` stands for the component identifier (an integer). The `run_id` may be set or unset.

The convention for file names that include the run ID is to separate prefix, run ID, and any extensions by dots. We construct the file name by concatenating the individual elements accordingly. If there is no run ID, we nevertheless replace `_iX` by `.iX`.

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: make_phs_filename => phs_wood_make_phs_filename
<PHS wood: procedures>+≡
    function phs_wood_make_phs_filename (phs_config, subdir) result (filename)
        class(phs_wood_config_t), intent(in) :: phs_config
        type(string_t), intent(in), optional :: subdir
        type(string_t) :: filename
        type(string_t) :: basename, suffix, comp_code, comp_index
        basename = phs_config%id
        call split (basename, suffix, "_", back=.true.)
        comp_code = extract (suffix, 1, 1)
        comp_index = extract (suffix, 2)
        if (comp_code == "i" .and. verify (comp_index, "1234567890") == 0) then
            suffix = "." // comp_code // comp_index
        else
            basename = phs_config%id
            suffix = ""
        end if
        if (phs_config%run_id /= "") then
            filename = basename // "." // phs_config%run_id // suffix // ".phs"
        else
            filename = basename // suffix // ".phs"
        end if
        if (present (subdir)) then
            filename = subdir // "/" // filename
        end if
    end function phs_wood_make_phs_filename

```

```

<PHS wood: phs wood config: TBP>+≡
    procedure :: reshuffle_flavors => phs_wood_config_reshuffle_flavors

```

```

<PHS wood: procedures>+≡
  subroutine phs_wood_config_reshuffle_flavors (phs_config, reshuffle, flv_extra)
    class(phs_wood_config_t), intent(inout) :: phs_config
    integer, intent(in), dimension(:), allocatable :: reshuffle
    type(flavor_t), intent(in) :: flv_extra
    call phs_forest_set_flavors (phs_config%forest, phs_config%flv(:,1), reshuffle, flv_extra)
  end subroutine phs_wood_config_reshuffle_flavors

```

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: set_momentum_links => phs_wood_config_set_momentum_links

```

```

<PHS wood: procedures>+≡
  subroutine phs_wood_config_set_momentum_links (phs_config, reshuffle)
    class(phs_wood_config_t), intent(inout) :: phs_config
    integer, intent(in), dimension(:), allocatable :: reshuffle
    call phs_forest_set_momentum_links (phs_config%forest, reshuffle)
  end subroutine phs_wood_config_set_momentum_links

```

Identify resonances which are marked by s-channel mappings for the whole phase space and report them to the channel array.

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: record_s_mappings => phs_wood_config_record_s_mappings

<PHS wood: procedures>+≡
  subroutine phs_wood_config_record_s_mappings (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config
    logical :: flag
    real(default) :: mass, width
    integer :: c
    do c = 1, phs_config%n_channel
      call phs_forest_get_s_mapping (phs_config%forest, c, flag, mass, width)
      if (flag) then
        if (mass == 0) then
          call msg_fatal ("Phase space: s-channel resonance " &
            // " has zero mass")
        end if
        if (width == 0) then
          call msg_fatal ("Phase space: s-channel resonance " &
            // " has zero width")
        end if
        call phs_config%channel(c)%set_resonant (mass, width)
      end if
    end do
  end subroutine phs_wood_config_record_s_mappings

```

Identify on-shell mappings for the whole phase space and report them to the channel array.

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: record_on_shell => phs_wood_config_record_on_shell

<PHS wood: procedures>+≡
  subroutine phs_wood_config_record_on_shell (phs_config)
    class(phs_wood_config_t), intent(inout) :: phs_config

```

```

logical :: flag
real(default) :: mass
integer :: c
do c = 1, phs_config%n_channel
  call phs_forest_get_on_shell (phs_config%forest, c, flag, mass)
  if (flag) then
    call phs_config%channel(c)%set_on_shell (mass)
  end if
end do
end subroutine phs_wood_config_record_on_shell

```

Return the most relevant MD5 sum. This overrides the method of the base type.

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: get_md5sum => phs_wood_config_get_md5sum

<PHS wood: procedures>+≡
  function phs_wood_config_get_md5sum (phs_config) result (md5sum)
    class(phs_wood_config_t), intent(in) :: phs_config
    character(32) :: md5sum
    if (phs_config%md5sum_forest /= "") then
      md5sum = phs_config%md5sum_forest
    else
      md5sum = phs_config%md5sum_phs_config
    end if
  end function phs_wood_config_get_md5sum

```

Check whether a phase-space configuration for the current process exists. We look for the phase-space file that should correspond to the current process. If we find it, we check the MD5 sums stored in the file against the MD5 sums in the current configuration (if required).

If successful, read the PHS file.

```

<PHS wood: phs wood config: TBP>+≡
  procedure :: read_phs_file => phs_wood_read_phs_file

<PHS wood: procedures>+≡
  subroutine phs_wood_read_phs_file (phs_config, exist, found, match, subdir)
    class(phs_wood_config_t), intent(inout) :: phs_config
    logical, intent(out) :: exist
    logical, intent(out) :: found
    logical, intent(out), optional :: match
    type(string_t), intent(in), optional :: subdir
    type(string_t) :: filename
    integer :: u
    filename = phs_config%make_phs_filename (subdir)
    inquire (file = char (filename), exist = exist)
    if (exist) then
      u = free_unit ()
      open (u, file = char (filename), action = "read", status = "old")
      call phs_forest_read (phs_config%forest, u, &
        phs_config%id, phs_config%n_in, phs_config%n_out, &
        phs_config%model, found, &
        phs_config%md5sum_process, &

```

```

        phs_config%md5sum_model_par, &
        phs_config%md5sum_phs_config, &
        match = match)
    close (u)
else
    found = .false.
    if (present (match)) match = .false.
end if
end subroutine phs_wood_read_phs_file

```

Startup message, after configuration is complete.

<PHS wood: phs wood config: TBP>+≡

```

    procedure :: startup_message => phs_wood_config_startup_message

```

<PHS wood: procedures>+≡

```

subroutine phs_wood_config_startup_message (phs_config, unit)
    class(phs_wood_config_t), intent(in) :: phs_config
    integer, intent(in), optional :: unit
    integer :: n_groves, n_eq
    n_groves = phs_forest_get_n_groves (phs_config%forest)
    n_eq = phs_forest_get_n_equivalences (phs_config%forest)
    call phs_config%base_startup_message (unit)
    if (phs_config%n_channel == 1) then
        write (msg_buffer, "(A,2(I0,A))" &
            "Phase space: found ", phs_config%n_channel, &
            " channel, collected in ", n_groves, &
            " grove."
        )
    else if (n_groves == 1) then
        write (msg_buffer, "(A,2(I0,A))" &
            "Phase space: found ", phs_config%n_channel, &
            " channels, collected in ", n_groves, &
            " grove."
        )
    else
        write (msg_buffer, "(A,2(I0,A))" &
            "Phase space: found ", phs_config%n_channel, &
            " channels, collected in ", &
            phs_forest_get_n_groves (phs_config%forest), &
            " groves."
        )
    end if
    call msg_message (unit = unit)
    if (phs_config%use_equivalences) then
        if (n_eq == 1) then
            write (msg_buffer, "(A,I0,A)" &
                "Phase space: Using ", n_eq, &
                " equivalence between channels."
            )
        else
            write (msg_buffer, "(A,I0,A)" &
                "Phase space: Using ", n_eq, &
                " equivalences between channels."
            )
        end if
    else
        write (msg_buffer, "(A)" &
            "Phase space: no equivalences between channels used."
        )
    end if
end if

```



```

    call msg_message (unit = unit)
    write (msg_buffer, "(A,2(1x,I0,1x,A))") &
        "Phase space: wood"
    call msg_message (unit = unit)
end subroutine phs_wood_config_startup_message

```

Allocate an instance: the actual phase-space object.

```

<PHS wood: phs wood config: TBP>+≡
    procedure, nopass :: allocate_instance => phs_wood_config_allocate_instance

<PHS wood: procedures>+≡
    subroutine phs_wood_config_allocate_instance (phs)
        class(phs_t), intent(inout), pointer :: phs
        allocate (phs_wood_t :: phs)
    end subroutine phs_wood_config_allocate_instance

```

19.10.4 Kinematics implementation

We generate $\cos\theta$ and ϕ uniformly, covering the solid angle.

```

<PHS wood: public>+≡
    public :: phs_wood_t

<PHS wood: types>+≡
    type, extends (phs_t) :: phs_wood_t
        real(default) :: sqrts = 0
        type(phs_forest_t) :: forest
        real(default), dimension(3) :: r_real
        integer :: n_r_born = 0
    contains
        <PHS wood: phs wood: TBP>
    end type phs_wood_t

```

Output. The `verbose` setting is irrelevant, we just display the contents of the base object.

```

<PHS wood: phs wood: TBP>≡
    procedure :: write => phs_wood_write

<PHS wood: procedures>+≡
    subroutine phs_wood_write (object, unit, verbose)
        class(phs_wood_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u
        u = given_output_unit (unit)
        call object%base_write (u)
    end subroutine phs_wood_write

```

Write the forest separately.

```

<PHS wood: phs wood: TBP>+≡
    procedure :: write_forest => phs_wood_write_forest

```

```

<PHS wood: procedures>+≡
  subroutine phs_wood_write_forest (object, unit)
    class(phs_wood_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    call phs_forest_write (object%forest, u)
  end subroutine phs_wood_write_forest

```

Finalizer.

```

<PHS wood: phs wood: TBP>+≡
  procedure :: final => phs_wood_final

```

```

<PHS wood: procedures>+≡
  subroutine phs_wood_final (object)
    class(phs_wood_t), intent(inout) :: object
    call phs_forest_final (object%forest)
  end subroutine phs_wood_final

```

Initialization. We allocate arrays (`base_init`) and adjust the phase-space volume. The two-particle phase space volume is

$$\Phi_2 = \frac{1}{4(2\pi)^5} = 2.55294034614 \times 10^{-5} \quad (19.64)$$

independent of the particle masses.

```

<PHS wood: phs wood: TBP>+≡
  procedure :: init => phs_wood_init

<PHS wood: procedures>+≡
  subroutine phs_wood_init (phs, phs_config)
    class(phs_wood_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config
    call phs%base_init (phs_config)
    select type (phs_config)
    type is (phs_wood_config_t)
      phs%forest = phs_config%forest
      if (phs_config%is_combined_integration) then
        phs%n_r_born = phs_config%n_par - 3
      end if
    end select
  end subroutine phs_wood_init

```

19.10.5 Evaluation

We compute the outgoing momenta from the incoming momenta and the input parameter set `r_in` in channel `r_in`. We also compute the `r` parameters and Jacobians `f` for all other channels.

We do *not* need to apply a transformation from/to the c.m. frame, because in `phs_base` the momenta are already boosted to the c.m. frame before assigning them in the `phs` object, and inversely boosted when extracting them.

```

<PHS wood: phs wood: TBP>+≡

```

```

procedure :: evaluate_selected_channel => phs_wood_evaluate_selected_channel
procedure :: evaluate_other_channels => phs_wood_evaluate_other_channels

(PHS wood: procedures) +=
subroutine phs_wood_evaluate_selected_channel (phs, c_in, r_in)
  class(phs_wood_t), intent(inout) :: phs
  integer, intent(in) :: c_in
  real(default), intent(in), dimension(:) :: r_in
  logical :: ok
  phs%q_defined = .false.
  if (phs%p_defined) then
    call phs_forest_set_prt_in (phs%forest, phs%p)
    phs%r(:,c_in) = r_in
    call phs_forest_evaluate_selected_channel (phs%forest, &
      c_in, phs%active_channel, &
      phs%sqrts_hat, phs%r, phs%f, phs%volume, ok)
    select type (config => phs%config)
    type is (phs_wood_config_t)
      if (config%is_combined_integration) then
        if (phs%n_r_born >= 0) then
          phs%r_real = r_in (phs%n_r_born + 1 : phs%n_r_born + 3)
        else
          call msg_fatal ("n_r_born should be larger than 0!")
        end if
      end if
    end select
    if (ok) then
      phs%q = phs_forest_get_momenta_out (phs%forest)
      phs%q_defined = .true.
    end if
  end if
end subroutine phs_wood_evaluate_selected_channel

subroutine phs_wood_evaluate_other_channels (phs, c_in)
  class(phs_wood_t), intent(inout) :: phs
  integer, intent(in) :: c_in
  integer :: c
  if (phs%q_defined) then
    call phs_forest_evaluate_other_channels (phs%forest, &
      c_in, phs%active_channel, &
      phs%sqrts_hat, phs%r, phs%f, combine=.true.)
    select type (config => phs%config)
    type is (phs_wood_config_t)
      if (config%is_combined_integration) then
        if (phs%n_r_born >= 0) then
          do c = 1, size (phs%r, 2)
            phs%r(phs%n_r_born + 1 : phs%n_r_born + 3, c) = phs%r_real
          end do
        else
          phs%r_defined = .false.
        end if
      end if
    end select
    phs%r_defined = .true.
  end if
end if

```

```
end subroutine phs_wood_evaluate_other_channels
```

Inverse evaluation.

```
⟨PHS wood: phs wood: TBP⟩+≡
  procedure :: inverse => phs_wood_inverse
⟨PHS wood: procedures⟩+≡
  subroutine phs_wood_inverse (phs)
    class(phs_wood_t), intent(inout) :: phs
    if (phs%p_defined .and. phs%q_defined) then
      call phs_forest_set_prt_in (phs%forest, phs%p)
      call phs_forest_set_prt_out (phs%forest, phs%q)
      call phs_forest_recover_channel (phs%forest, &
        1, &
        phs%sqrts_hat, phs%r, phs%f, phs%volume)
      call phs_forest_evaluate_other_channels (phs%forest, &
        1, phs%active_channel, &
        phs%sqrts_hat, phs%r, phs%f, combine=.false.)
      phs%r_defined = .true.
    end if
  end subroutine phs_wood_inverse
```

19.10.6 Unit tests

Test module, followed by the corresponding implementation module.

```
⟨phs_wood.ut.f90⟩≡
  ⟨File header⟩

  module phs_wood_ut
    use unit_tests
    use phs_wood_uti

    ⟨Standard module head⟩

    ⟨PHS wood: public test⟩

    ⟨PHS wood: public test auxiliary⟩

    contains

    ⟨PHS wood: test driver⟩

  end module phs_wood_ut
⟨phs_wood.uti.f90⟩≡
  ⟨File header⟩

  module phs_wood_uti

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use io_units
    use os_interface
```

```

    use lorentz
    use flavors
    use model_data
    use process_constants
    use mappings
    use phs_base
    use phs_forests

    use phs_wood

    use phs_base_ut, only: init_test_process_data, init_test_decay_data

    <Standard module head>

    <PHS wood: public test auxiliary>

    <PHS wood: test declarations>

contains

    <PHS wood: tests>

    <PHS wood: test auxiliary>

end module phs_wood_ut
API: driver for the unit tests below.
<PHS wood: public test>≡
    public :: phs_wood_test
<PHS wood: test driver>≡
    subroutine phs_wood_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS wood: execute tests>
    end subroutine phs_wood_test

<PHS wood: public test>+≡
    public :: phs_wood_vis_test
<PHS wood: test driver>+≡
    subroutine phs_wood_vis_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <PHS wood: execute vis tests>
    end subroutine phs_wood_vis_test

```

Phase-space configuration data

Construct and display a test phase-space configuration object. Also check the `azimuthal_dependence` flag.

This auxiliary routine writes a phase-space configuration file to unit `u.phs`.

```

<PHS wood: public test auxiliary>≡
    public :: write_test_phs_file

```

```

<PHS wood: test auxiliary>≡
subroutine write_test_phs_file (u_phs, procname)
  integer, intent(in) :: u_phs
  type(string_t), intent(in), optional :: procname
  if (present (procname)) then
    write (u_phs, "(A,A)") "process ", char (procname)
  else
    write (u_phs, "(A)") "process testproc"
  end if
  write (u_phs, "(A,A)") "  md5sum_process   = ", '""'
  write (u_phs, "(A,A)") "  md5sum_model_par = ", '""'
  write (u_phs, "(A,A)") "  md5sum_phs_config = ", '""'
  write (u_phs, "(A)") "  sqrts           = 1000"
  write (u_phs, "(A)") "  m_threshold_s = 50"
  write (u_phs, "(A)") "  m_threshold_t = 100"
  write (u_phs, "(A)") "  off_shell = 2"
  write (u_phs, "(A)") "  t_channel = 6"
  write (u_phs, "(A)") "  keep_nonresonant = T"
  write (u_phs, "(A)") "  grove #1"
  write (u_phs, "(A)") "  tree 3"
end subroutine write_test_phs_file

<PHS wood: execute tests>≡
call test (phs_wood_1, "phs_wood_1", &
  "phase-space configuration", &
  u, results)

<PHS wood: test declarations>≡
public :: phs_wood_1

<PHS wood: tests>≡
subroutine phs_wood_1 (u)
  integer, intent(in) :: u
  type(model_data_t), target :: model
  type(process_constants_t) :: process_data
  class(phs_config_t), allocatable :: phs_data
  type(mapping_defaults_t) :: mapping_defaults
  real(default) :: sqrts
  integer :: u_phs, iostat
  character(32) :: buffer

  write (u, "(A)") "* Test output: phs_wood_1"
  write (u, "(A)") "* Purpose: initialize and display &
    &phase-space configuration data"
  write (u, "(A)")

  call model%init_test ()

  call syntax_phs_forest_init ()

  write (u, "(A)") "* Initialize a process"
  write (u, "(A)")

  call init_test_process_data (var_str ("phs_wood_1"), process_data)

```

```

write (u, "(A)")  "* Create a scratch phase-space file"
write (u, "(A)")

u_phs = free_unit ()
open (u_phs, status = "scratch", action = "readwrite")
call write_test_phs_file (u_phs, var_str ("phs_wood_1"))
rewind (u_phs)
do
  read (u_phs, "(A)", iostat = iostat)  buffer
  if (iostat /= 0)  exit
  write (u, "(A)") trim (buffer)
end do

write (u, "(A)")
write (u, "(A)")  "* Setup phase-space configuration object"
write (u, "(A)")

mapping_defaults%step_mapping = .false.

allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)
select type (phs_data)
type is (phs_wood_config_t)
  call phs_data%set_input (u_phs)
  call phs_data%set_mapping_defaults (mapping_defaults)
end select

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs_data%write (u)
write (u, "(A)")

select type (phs_data)
type is (phs_wood_config_t)
  call phs_data%write_forest (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

close (u_phs)
call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_1"

end subroutine phs_wood_1

```

Phase space evaluation

Compute kinematics for given parameters, also invert the calculation.

```

<PHS wood: execute tests>+≡
    call test (phs_wood_2, "phs_wood_2", &
        "phase-space evaluation", &
        u, results)

<PHS wood: test declarations>+≡
    public :: phs_wood_2

<PHS wood: tests>+≡
    subroutine phs_wood_2 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(flavor_t) :: flv
        type(process_constants_t) :: process_data
        real(default) :: sqrts, E
        class(phs_config_t), allocatable, target :: phs_data
        class(phs_t), pointer :: phs => null ()
        type(vector4_t), dimension(2) :: p, q
        integer :: u_phs

        write (u, "(A)")  "* Test output: phs_wood_2"
        write (u, "(A)")  "* Purpose: test simple single-channel phase space"
        write (u, "(A)")

        call model%init_test ()
        call flv%init (25, model)

        write (u, "(A)")  "* Initialize a process and a matching &
            &phase-space configuration"
        write (u, "(A)")

        call init_test_process_data (var_str ("phs_wood_2"), process_data)
        u_phs = free_unit ()
        open (u_phs, status = "scratch", action = "readwrite")
        call write_test_phs_file (u_phs, var_str ("phs_wood_2"))
        rewind (u_phs)

        allocate (phs_wood_config_t :: phs_data)
        call phs_data%init (process_data, model)
        select type (phs_data)
        type is (phs_wood_config_t)
            call phs_data%set_input (u_phs)
        end select

        sqrts = 1000._default
        call phs_data%configure (sqrts)

        call phs_data%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Initialize the phase-space instance"
        write (u, "(A)")

        call phs_data%allocate_instance (phs)
        call phs%init (phs_data)

```



```

call phs%write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

E = sqrt(s) / 2
p(1) = vector4_moving (E, sqrt (E**2 - flv%get_mass ()**2), 3)
p(2) = vector4_moving (E,-sqrt (E**2 - flv%get_mass ()**2), 3)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute phase-space point &
                  &for x = 0.125, 0.5"
write (u, "(A)")

call phs%evaluate_selected_channel (1, [0.125_default, 0.5_default])
call phs%evaluate_other_channels (1)
call phs%write (u)
write (u, "(A)")
select type (phs)
type is (phs_wood_t)
    call phs%write_forest (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
call phs%final ()
deallocate (phs)

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)
write (u, "(A)")
select type (phs)
type is (phs_wood_t)
    call phs%write_forest (u)
end select

call phs%final ()
deallocate (phs)

```

```

close (u_phs)
call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_2"

end subroutine phs_wood_2

```

Phase-space generation

Generate phase space for a simple process.

```

<PHS wood: execute tests>+≡
  call test (phs_wood_3, "phs_wood_3", &
    "phase-space generation", &
    u, results)

<PHS wood: test declarations>+≡
  public :: phs_wood_3

<PHS wood: tests>+≡
  subroutine phs_wood_3 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    type(phs_parameters_t) :: phs_par
    class(phs_config_t), allocatable :: phs_data
    integer :: iostat
    character(80) :: buffer

    write (u, "(A)")  "* Test output: phs_wood_3"
    write (u, "(A)")  "* Purpose: generate a phase-space configuration"
    write (u, "(A)")

    call model%init_test ()

    call syntax_phs_forest_init ()

    write (u, "(A)")  "* Initialize a process and phase-space parameters"
    write (u, "(A)")

    call init_test_process_data (var_str ("phs_wood_3"), process_data)
    allocate (phs_wood_config_t :: phs_data)
    call phs_data%init (process_data, model)

    phs_par%sqrts = 1000
    select type (phs_data)
    type is (phs_wood_config_t)
      call phs_data%set_parameters (phs_par)
      phs_data%io_unit_keep_open = .true.
    end select

    write (u, "(A)")

```

```

write (u, "(A)")  "* Generate a scratch phase-space file"
write (u, "(A)")

call phs_data%configure (phs_par%sqrts)

select type (phs_data)
type is (phs_wood_config_t)
  rewind (phs_data%io_unit)
  do
    read (phs_data%io_unit, "(A)", iostat = iostat)  buffer
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
  end do
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_3"

end subroutine phs_wood_3

```

Nontrivial process

Generate phase space for a $2 \rightarrow 3$ process.

```

<PHS wood: execute tests>+≡
  call test (phs_wood_4, "phs_wood_4", &
    "nontrivial process", &
    u, results)

<PHS wood: test declarations>+≡
  public :: phs_wood_4

<PHS wood: tests>+≡
  subroutine phs_wood_4 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    type(phs_parameters_t) :: phs_par
    class(phs_config_t), allocatable, target :: phs_data
    integer :: iostat
    character(80) :: buffer
    class(phs_t), pointer :: phs => null ()
    real(default) :: E, pL
    type(vector4_t), dimension(2) :: p
    type(vector4_t), dimension(3) :: q

    write (u, "(A)")  "* Test output: phs_wood_4"
    write (u, "(A)")  "* Purpose: generate a phase-space configuration"
    write (u, "(A)")

```

```

call model%init_test ()

call syntax_phs_forest_init ()

write (u, "(A)")  "* Initialize a process and phase-space parameters"
write (u, "(A)")

process_data%id = "phs_wood_4"
process_data%model_name = "Test"
process_data%n_in = 2
process_data%n_out = 3
process_data%n_flv = 1
allocate (process_data%flv_state (process_data%n_in + process_data%n_out, &
    process_data%n_flv))
process_data%flv_state(:,1) = [25, 25, 25, 6, -6]

allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)

phs_par%sqrts = 1000
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%io_unit_keep_open = .true.
end select

write (u, "(A)")
write (u, "(A)")  "* Generate a scratch phase-space file"
write (u, "(A)")

call phs_data%configure (phs_par%sqrts)

select type (phs_data)
type is (phs_wood_config_t)
    rewind (phs_data%io_unit)
    do
        read (phs_data%io_unit, "(A)", iostat = iostat)  buffer
        if (iostat /= 0) exit
        write (u, "(A)") trim (buffer)
    end do
end select

write (u, "(A)")
write (u, "(A)")  "* Initialize the phase-space instance"
write (u, "(A)")

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

write (u, "(A)")  "* Set incoming momenta"
write (u, "(A)")

select type (phs_data)

```

```

type is (phs_wood_config_t)
  E = phs_data%sqrts / 2
  pL = sqrt (E**2 - phs_data%flv(1,1)%get_mass ()**2)
end select
p(1) = vector4_moving (E, pL, 3)
p(2) = vector4_moving (E, -pL, 3)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()

write (u, "(A)")  "* Compute phase-space point &
  &for x = 0.1, 0.2, 0.3, 0.4, 0.5"
write (u, "(A)")

call phs%evaluate_selected_channel (1, &
  [0.1_default, 0.2_default, 0.3_default, 0.4_default, 0.5_default])
call phs%evaluate_other_channels (1)
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inverse kinematics"
write (u, "(A)")

call phs%get_outgoing_momenta (q)
call phs%final ()
deallocate (phs)

call phs_data%allocate_instance (phs)
call phs%init (phs_data)

call phs%set_incoming_momenta (p)
call phs%compute_flux ()
call phs%set_outgoing_momenta (q)

call phs%inverse ()
call phs%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call phs%final ()
deallocate (phs)

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_4"

end subroutine phs_wood_4

```

Equivalences

Generate phase space for a simple process, including channel equivalences.

```
<PHS wood: execute tests>+≡
    call test (phs_wood_5, "phs_wood_5", &
               "equivalences", &
               u, results)

<PHS wood: test declarations>+≡
    public :: phs_wood_5

<PHS wood: tests>+≡
    subroutine phs_wood_5 (u)
        integer, intent(in) :: u
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        type(phs_parameters_t) :: phs_par
        class(phs_config_t), allocatable :: phs_data

        write (u, "(A)")  "* Test output: phs_wood_5"
        write (u, "(A)")  "* Purpose: generate a phase-space configuration"
        write (u, "(A)")

        call model%init_test ()

        call syntax_phs_forest_init ()

        write (u, "(A)")  "* Initialize a process and phase-space parameters"
        write (u, "(A)")

        call init_test_process_data (var_str ("phs_wood_5"), process_data)
        allocate (phs_wood_config_t :: phs_data)
        call phs_data%init (process_data, model)

        phs_par%sqrts = 1000
        select type (phs_data)
        type is (phs_wood_config_t)
            call phs_data%set_parameters (phs_par)
            call phs_data%enable_equivalences ()
        end select

        write (u, "(A)")
        write (u, "(A)")  "* Generate a scratch phase-space file"
        write (u, "(A)")

        call phs_data%configure (phs_par%sqrts)
        call phs_data%write (u)
        write (u, "(A)")

        select type (phs_data)
        type is (phs_wood_config_t)
            call phs_data%write_forest (u)
        end select

        write (u, "(A)")
```

```

write (u, "(A)")  "* Cleanup"

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: phs_wood_5"

end subroutine phs_wood_5

```

MD5 sum checks

Generate phase space for a simple process. Repeat this with and without parameter change.

```

<PHS wood: execute tests>+≡
  call test (phs_wood_6, "phs_wood_6", &
    "phase-space generation", &
    u, results)

<PHS wood: test declarations>+≡
  public :: phs_wood_6

<PHS wood: tests>+≡
  subroutine phs_wood_6 (u)
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(process_constants_t) :: process_data
    type(phs_parameters_t) :: phs_par
    class(phs_config_t), allocatable :: phs_data
    logical :: exist, found, match
    integer :: u_phs
    character(*), parameter :: filename = "phs_wood_6.p.phs"

    write (u, "(A)")  "* Test output: phs_wood_6"
    write (u, "(A)")  "* Purpose: generate and check phase-space file"
    write (u, "(A)")

    call model%init_test ()

    call syntax_phs_forest_init ()

    write (u, "(A)")  "* Initialize a process and phase-space parameters"
    write (u, "(A)")

    call init_test_process_data (var_str ("phs_wood_6"), process_data)
    process_data%id = "phs_wood_6_p"
    process_data%md5sum = "1234567890abcdef1234567890abcdef"
    allocate (phs_wood_config_t :: phs_data)
    call phs_data%init (process_data, model)

    phs_par%sqrts = 1000
    select type (phs_data)
    type is (phs_wood_config_t)

```

```

        call phs_data%set_parameters (phs_par)
end select

write (u, "(A)")  "* Remove previous phs file, if any"
write (u, "(A)")

inquire (file = filename, exist = exist)
if (exist) then
    u_phs = free_unit ()
    open (u_phs, file = filename, action = "write")
    close (u_phs, status = "delete")
end if

write (u, "(A)")  "* Check phase-space file (should fail)"
write (u, "(A)")

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%read_phs_file (exist, found, match)
    write (u, "(1x,A,L1)")  "exist = ", exist
    write (u, "(1x,A,L1)")  "found = ", found
    write (u, "(1x,A,L1)")  "match = ", match
end select

write (u, "(A)")
write (u, "(A)")  "* Generate a phase-space file"
write (u, "(A)")

call phs_data%configure (phs_par%sqrts)

write (u, "(1x,A,A,A)")  "MD5 sum (process)    = '", &
    phs_data%md5sum_process, "'"
write (u, "(1x,A,A,A)")  "MD5 sum (model par) = '", &
    phs_data%md5sum_model_par, "'"
write (u, "(1x,A,A,A)")  "MD5 sum (phs config) = '", &
    phs_data%md5sum_phs_config, "'"

write (u, "(A)")
write (u, "(A)")  "* Check MD5 sum"
write (u, "(A)")

call phs_data%final ()
deallocate (phs_data)
allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)
phs_par%sqrts = 1000
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%sqrts = phs_par%sqrts
    phs_data%par%sqrts = phs_par%sqrts
end select
call phs_data%compute_md5sum ()

```



```

allocate (phs_wood_config_t :: phs_data)
call phs_data%init (process_data, model)
phs_par%sqrts = 1000
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%sqrts = phs_par%sqrts
    phs_data%par%sqrts = phs_par%sqrts
end select
call phs_data%compute_md5sum ()

write (u, "(1x,A,A,A)") "MD5 sum (process)      = '", &
    phs_data%md5sum_process, "'"
write (u, "(1x,A,A,A)") "MD5 sum (model par)   = '", &
    phs_data%md5sum_model_par, "'"
write (u, "(1x,A,A,A)") "MD5 sum (phs config) = '", &
    phs_data%md5sum_phs_config, "'"

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%read_phs_file (exist, found, match)
    write (u, "(1x,A,L1)") "exist = ", exist
    write (u, "(1x,A,L1)") "found = ", found
    write (u, "(1x,A,L1)") "match = ", match
end select

write (u, "(A)")
write (u, "(A)")  "* Modify phs parameter and check MD5 sum"
write (u, "(A)")

call phs_data%final ()
deallocate (phs_data)
allocate (phs_wood_config_t :: phs_data)
process_data%md5sum = "1234567890abcdef1234567890abcdef"
call phs_data%init (process_data, model)
phs_par%sqrts = 1000
phs_par%off_shell = 17
select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_parameters (phs_par)
    phs_data%sqrts = phs_par%sqrts
    phs_data%par%sqrts = phs_par%sqrts
end select
call phs_data%compute_md5sum ()

write (u, "(1x,A,A,A)") "MD5 sum (process)      = '", &
    phs_data%md5sum_process, "'"
write (u, "(1x,A,A,A)") "MD5 sum (model par)   = '", &
    phs_data%md5sum_model_par, "'"
write (u, "(1x,A,A,A)") "MD5 sum (phs config) = '", &
    phs_data%md5sum_phs_config, "'"

select type (phs_data)
type is (phs_wood_config_t)

```

```

        call phs_data%read_phs_file (exist, found, match)
        write (u, "(1x,A,L1)") "exist = ", exist
        write (u, "(1x,A,L1)") "found = ", found
        write (u, "(1x,A,L1)") "match = ", match
    end select

    write (u, "(A)")
    write (u, "(A)")  "* Modify model parameter and check MD5 sum"
    write (u, "(A)")

    call phs_data%final ()
    deallocate (phs_data)
    allocate (phs_wood_config_t :: phs_data)
    call model%set_par (var_str ("ms"), 100._default)
    call phs_data%init (process_data, model)
    phs_par%sqrts = 1000
    phs_par%off_shell = 1
    select type (phs_data)
    type is (phs_wood_config_t)
        call phs_data%set_parameters (phs_par)
        phs_data%sqrts = phs_par%sqrts
        phs_data%par%sqrts = phs_par%sqrts
    end select
    call phs_data%compute_md5sum ()

    write (u, "(1x,A,A,A)") "MD5 sum (process)    = '", &
        phs_data%md5sum_process, "'"
    write (u, "(1x,A,A,A)") "MD5 sum (model par) = '", &
        phs_data%md5sum_model_par, "'"
    write (u, "(1x,A,A,A)") "MD5 sum (phs config) = '", &
        phs_data%md5sum_phs_config, "'"

    select type (phs_data)
    type is (phs_wood_config_t)
        call phs_data%read_phs_file (exist, found, match)
        write (u, "(1x,A,L1)") "exist = ", exist
        write (u, "(1x,A,L1)") "found = ", found
        write (u, "(1x,A,L1)") "match = ", match
    end select

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call phs_data%final ()
    call model%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: phs_wood_6"

end subroutine phs_wood_6

```

(PHS wood: execute vis tests)≡

```

call test (phs_wood_vis_1, "phs_wood_vis_1", &
    "visualizing phase space channels", &

```

```

        u, results)
<PHS wood: test declarations>+≡
    public :: phs_wood_vis_1
<PHS wood: tests>+≡
    subroutine phs_wood_vis_1 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_data_t), target :: model
        type(process_constants_t) :: process_data
        class(phs_config_t), allocatable :: phs_data
        type(mapping_defaults_t) :: mapping_defaults
        type(string_t) :: vis_file, pdf_file, ps_file
        real(default) :: sqrts
        logical :: exist, exist_pdf, exist_ps
        integer :: u_phs, iostat, u_vis
        character(95) :: buffer

        write (u, "(A)")  "* Test output: phs_wood_vis_1"
        write (u, "(A)")  "* Purpose: visualizing the &
            &phase-space configuration"
        write (u, "(A)")

        call os_data%init ()
        call model%init_test ()

        call syntax_phs_forest_init ()

        write (u, "(A)")  "* Initialize a process"
        write (u, "(A)")

        call init_test_process_data (var_str ("phs_wood_vis_1"), process_data)

        write (u, "(A)")  "* Create a scratch phase-space file"
        write (u, "(A)")

        u_phs = free_unit ()
        open (u_phs, status = "scratch", action = "readwrite")
        call write_test_phs_file (u_phs, var_str ("phs_wood_vis_1"))
        rewind (u_phs)
        do
            read (u_phs, "(A)", iostat = iostat) buffer
            if (iostat /= 0) exit
            write (u, "(A)") trim (buffer)
        end do

        write (u, "(A)")
        write (u, "(A)")  "* Setup phase-space configuration object"
        write (u, "(A)")

        mapping_defaults%step_mapping = .false.

        allocate (phs_wood_config_t :: phs_data)
        call phs_data%init (process_data, model)

```

```

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%set_input (u_phs)
    call phs_data%set_mapping_defaults (mapping_defaults)
    phs_data%os_data = os_data
    phs_data%io_unit = 0
    phs_data%io_unit_keep_open = .true.
    phs_data%vis_channels = .true.
end select

sqrts = 1000._default
call phs_data%configure (sqrts)

call phs_data%write (u)
write (u, "(A)")

select type (phs_data)
type is (phs_wood_config_t)
    call phs_data%write_forest (u)
end select

vis_file = "phs_wood_vis_1.phs-vis.tex"
ps_file = "phs_wood_vis_1.phs-vis.ps"
pdf_file = "phs_wood_vis_1.phs-vis.pdf"
inquire (file = char (vis_file), exist = exist)
if (exist) then
    u_vis = free_unit ()
    open (u_vis, file = char (vis_file), action = "read", status = "old")
    iostat = 0
    do while (iostat == 0)
        read (u_vis, "(A)", iostat = iostat) buffer
        if (iostat == 0) write (u, "(A)") trim (buffer)
    end do
    close (u_vis)
else
    write (u, "(A)") "[Visualize LaTeX file is missing]"
end if
inquire (file = char (ps_file), exist = exist_ps)
if (exist_ps) then
    write (u, "(A)") "[Visualize Postscript file exists and is nonempty]"
else
    write (u, "(A)") "[Visualize Postscript file is missing/non-regular]"
end if
inquire (file = char (pdf_file), exist = exist_pdf)
if (exist_pdf) then
    write (u, "(A)") "[Visualize PDF file exists and is nonempty]"
else
    write (u, "(A)") "[Visualize PDF file is missing/non-regular]"
end if

write (u, "(A)")
write (u, "(A)") "* Cleanup"

close (u_phs)

```

```

call phs_data%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: phs_wood_vis_1"

end subroutine phs_wood_vis_1

```

19.11 The FKS phase space

```

<phs_fks.f90>=
<File header>

module phs_fks

  <Use kinds>
  <Use strings>
  <Use debug>
  use constants
  use diagnostics
  use io_units, only: given_output_unit, free_unit
  use format_utils, only: write_separator
  use lorentz
  use phs_points, only: phs_point_t
  use phs_points, only: assignment(=), size, sum
  use physics_defs
  use flavors
  use pdg_arrays, only: is_colored
  use models, only: model_t
  use sf_mappings
  use sf_base
  use phs_base
  use resonances, only: resonance_contributors_t, resonance_history_t
  use phs_forests, only: phs_forest_final
  use phs_wood
  use cascades
  use cascades2
  use process_constants
  use process_libraries
  use ttv_formfactors, only: generate_on_shell_decay_threshold, mis_to_mpole
  use format_defs, only: FMT_17

  <Standard module head>

  <phs_fks: public>

  <phs_fks: parameters>

  <phs_fks: types>

  <phs_fks: interfaces>

```

```
contains

<phs fks: procedures>

end module phs_fks
```

A container for the x_{\oplus} - and x_{\ominus} -values for initial-state phase spaces.

```
<phs fks: public>≡
  public :: isr_kinematics_t

<phs fks: types>≡
  type :: isr_kinematics_t
    integer :: n_in
    real(default), dimension(2) :: x = one
    real(default), dimension(2) :: z = zero
    real(default) :: sqrts_born = zero
    real(default), dimension(:), allocatable :: beam_energy
    real(default) :: fac_scale = zero
    real(default), dimension(2) :: jacobian = one
    integer :: isr_mode = SQRTS_FIXED
  contains
    <phs fks: isr kinematics: TBP>
    end type isr_kinematics_t

<phs fks: isr kinematics: TBP>≡
  procedure :: write => isr_kinematics_write

<phs fks: procedures>≡
  subroutine isr_kinematics_write (isr, unit)
    class(isr_kinematics_t), intent(in) :: isr
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u,"(A)") "ISR kinematics: "
    write (u,"(A," // FMT_17 // ",1X)") "x(+):          ", isr%x(1)
    write (u,"(A," // FMT_17 // ",1X)") "x(-):          ", isr%x(2)
    write (u,"(A," // FMT_17 // ",1X)") "z(+):          ", isr%z(1)
    write (u,"(A," // FMT_17 // ",1X)") "z(-):          ", isr%z(2)
    write (u,"(A," // FMT_17 // ",1X)") "sqrts (Born): ", isr%sqrts_born
    if (allocated (isr%beam_energy)) then
      do i = 1, size (isr%beam_energy)
        write (u,"(A," // FMT_17 // ",1X)") "Beam energy:  ", &
          isr%beam_energy(i)
      end do
    end if
    write (u,"(A," // FMT_17 // ",1X)") "Fac. scale:   ", isr%fac_scale
    do i = 1, 2
      write (u,"(A," // FMT_17 // ",1X)") "Jacobian:     ", isr%jacobian(i)
    end do
    write (u,"(A,I0,1X)") "ISR mode:      ", isr%isr_mode
  end subroutine isr_kinematics_write

<phs fks: public>+≡
  public :: phs_point_set_t
```

```

<phs fks: types>+≡
  type :: phs_point_set_t
    type(phs_point_t), dimension(:), allocatable :: phs_point
    logical :: initialized = .false.
  contains
    <phs fks: phs point set: TBP>
  end type phs_point_set_t

<phs fks: phs point set: TBP>≡
  procedure :: init => phs_point_set_init

<phs fks: procedures>+≡
  subroutine phs_point_set_init (phs_point_set, n_particles, n_phs)
    class(phs_point_set_t), intent(out) :: phs_point_set
    integer, intent(in) :: n_particles, n_phs
    integer :: i_phs
    allocate (phs_point_set%phs_point (n_phs))
    do i_phs = 1, n_phs
      phs_point_set%phs_point(i_phs) = n_particles
    end do
    phs_point_set%initialized = .true.
  end subroutine phs_point_set_init

<phs fks: phs point set: TBP>+≡
  procedure :: write => phs_point_set_write

<phs fks: procedures>+≡
  subroutine phs_point_set_write (phs_point_set, i_phs, contributors, unit, show_mass, &
    testflag, check_conservation, ultra, n_in)
    class(phs_point_set_t), intent(in) :: phs_point_set
    integer, intent(in), optional :: i_phs
    integer, intent(in), dimension(:), optional :: contributors
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_mass
    logical, intent(in), optional :: testflag, ultra
    logical, intent(in), optional :: check_conservation
    integer, intent(in), optional :: n_in
    integer :: i, u
    type(vector4_t) :: p_sum
    u = given_output_unit (unit); if (u < 0) return
    if (present (i_phs)) then
      call phs_point_set%phs_point(i_phs)%write &
        (unit = u, show_mass = show_mass, testflag = testflag, &
        check_conservation = check_conservation, ultra = ultra, n_in = n_in)
    else
      do i = 1, size(phs_point_set%phs_point)
        call phs_point_set%phs_point(i)%write &
          (unit = u, show_mass = show_mass, testflag = testflag, &
          check_conservation = check_conservation, ultra = ultra, n_in = n_in)
      end do
    end if
    if (present (contributors)) then
      if (debug_on) call msg_debug (D_SUBTRACTION, "Invariant masses for real emission: ")
      associate (pp => phs_point_set%phs_point(i_phs))

```



```

        p_sum = sum (pp, [contributors, size (pp)])
    end associate
    if (debug_active (D_SUBTRACTION)) &
        call vector4_write (p_sum, unit = unit, show_mass = show_mass, &
            testflag = testflag, ultra = ultra)
    end if
end subroutine phs_point_set_write

<phs fks: phs point set: TBP>+≡
    procedure :: get_n_momenta => phs_point_set_get_n_momenta

<phs fks: procedures>+≡
    elemental function phs_point_set_get_n_momenta (phs_point_set, i_res) result (n)
        integer :: n
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_res
        n = size (phs_point_set%phs_point(i_res))
    end function phs_point_set_get_n_momenta

<phs fks: phs point set: TBP>+≡
    procedure :: get_momenta => phs_point_set_get_momenta

<phs fks: procedures>+≡
    pure function phs_point_set_get_momenta (phs_point_set, i_phs, n_in) result (p)
        type(vector4_t), dimension(:), allocatable :: p
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs
        integer, intent(in), optional :: n_in
        integer :: i
        if (present (n_in)) then
            p = phs_point_set%phs_point(i_phs)%select ([(i, i=1, n_in)])
        else
            p = phs_point_set%phs_point(i_phs)
        end if
    end function phs_point_set_get_momenta

<phs fks: phs point set: TBP>+≡
    procedure :: get_momentum => phs_point_set_get_momentum

<phs fks: procedures>+≡
    pure function phs_point_set_get_momentum (phs_point_set, i_phs, i_mom) result (p)
        type(vector4_t) :: p
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs, i_mom
        p = phs_point_set%phs_point(i_phs)%select (i_mom)
    end function phs_point_set_get_momentum

<phs fks: phs point set: TBP>+≡
    procedure :: get_energy => phs_point_set_get_energy

<phs fks: procedures>+≡
    pure function phs_point_set_get_energy (phs_point_set, i_phs, i_mom) result (E)
        real(default) :: E
        class(phs_point_set_t), intent(in) :: phs_point_set

```

```

        integer, intent(in) :: i_phs, i_mom
        E = energy (phs_point_set%phs_point(i_phs)%select (i_mom))
    end function phs_point_set_get_energy

<phs fks: phs point set: TBP>+≡
    procedure :: get_sqrts => phs_point_set_get_sqrts

<phs fks: procedures>+≡
    function phs_point_set_get_sqrts (phs_point_set, i_phs) result (sqrts)
        real(default) :: sqrts
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in) :: i_phs
        sqrts = sqrt (phs_point_set%phs_point(i_phs)%get_msq ([1,2]))
    end function phs_point_set_get_sqrts

<phs fks: phs point set: TBP>+≡
    generic :: set_momenta => set_momenta_p, set_momenta_phs_point
    procedure :: set_momenta_p => phs_point_set_set_momenta_p

<phs fks: procedures>+≡
    subroutine phs_point_set_set_momenta_p (phs_point_set, i_phs, p)
        class(phs_point_set_t), intent(inout) :: phs_point_set
        integer, intent(in) :: i_phs
        type(vector4_t), intent(in), dimension(:) :: p
        phs_point_set%phs_point(i_phs) = p
    end subroutine phs_point_set_set_momenta_p

<phs fks: phs point set: TBP>+≡
    procedure :: set_momenta_phs_point => phs_point_set_set_momenta_phs_point

<phs fks: procedures>+≡
    subroutine phs_point_set_set_momenta_phs_point (phs_point_set, i_phs, p)
        class(phs_point_set_t), intent(inout) :: phs_point_set
        integer, intent(in) :: i_phs
        type(phs_point_t), intent(in) :: p
        phs_point_set%phs_point(i_phs) = p
    end subroutine phs_point_set_set_momenta_phs_point

<phs fks: phs point set: TBP>+≡
    procedure :: get_n_particles => phs_point_set_get_n_particles

<phs fks: procedures>+≡
    function phs_point_set_get_n_particles (phs_point_set, i) result (n_particles)
        integer :: n_particles
        class(phs_point_set_t), intent(in) :: phs_point_set
        integer, intent(in), optional :: i
        integer :: j
        j = 1; if (present (i)) j = i
        n_particles = size (phs_point_set%phs_point(j))
    end function phs_point_set_get_n_particles

<phs fks: phs point set: TBP>+≡
    procedure :: get_n_phs => phs_point_set_get_n_phs

```

```

<phs fks: procedures>+≡
function phs_point_set_get_n_phs (phs_point_set) result (n_phs)
  integer :: n_phs
  class(phs_point_set_t), intent(in) :: phs_point_set
  n_phs = size (phs_point_set%phs_point)
end function phs_point_set_get_n_phs

<phs fks: phs point set: TBP>+≡
procedure :: get_invariant_mass => phs_point_set_get_invariant_mass

<phs fks: procedures>+≡
function phs_point_set_get_invariant_mass (phs_point_set, i_phs, i_part) result (m2)
  real(default) :: m2
  class(phs_point_set_t), intent(in) :: phs_point_set
  integer, intent(in) :: i_phs
  integer, intent(in), dimension(:) :: i_part
  m2 = phs_point_set%phs_point(i_phs)%get_msq (i_part)
end function phs_point_set_get_invariant_mass

<phs fks: phs point set: TBP>+≡
procedure :: write_phs_point => phs_point_set_write_phs_point

<phs fks: procedures>+≡
subroutine phs_point_set_write_phs_point (phs_point_set, i_phs, unit, show_mass, &
  testflag, check_conservation, ultra, n_in)
  class(phs_point_set_t), intent(in) :: phs_point_set
  integer, intent(in) :: i_phs
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: show_mass
  logical, intent(in), optional :: testflag, ultra
  logical, intent(in), optional :: check_conservation
  integer, intent(in), optional :: n_in
  call phs_point_set%phs_point(i_phs)%write (unit, show_mass, testflag, &
    check_conservation, ultra, n_in)
end subroutine phs_point_set_write_phs_point

<phs fks: phs point set: TBP>+≡
procedure :: final => phs_point_set_final

<phs fks: procedures>+≡
subroutine phs_point_set_final (phs_point_set)
  class(phs_point_set_t), intent(inout) :: phs_point_set
  integer :: i
  deallocate (phs_point_set%phs_point)
  phs_point_set%initialized = .false.
end subroutine phs_point_set_final

<phs fks: public>+≡
public :: real_jacobian_t

<phs fks: types>+≡
type :: real_jacobian_t
  real(default), dimension(4) :: jac = 1._default
end type real_jacobian_t

```

```

<phs fks: public>+≡
  public :: real_kinematics_t

<phs fks: types>+≡
  type :: real_kinematics_t
    logical :: supply_xi_max = .true.
    real(default) :: xi_tilde
    real(default) :: phi
    real(default), dimension(:), allocatable :: xi_max, y
    real(default) :: xi_mismatch, y_mismatch
    type(real_jacobian_t), dimension(:), allocatable :: jac
    real(default) :: jac_mismatch
    type(phs_point_set_t) :: p_born_cms
    type(phs_point_set_t) :: p_born_lab
    type(phs_point_set_t) :: p_real_cms
    type(phs_point_set_t) :: p_real_lab
    type(phs_point_set_t) :: p_born_onshell
    type(phs_point_set_t), dimension(2) :: p_real_onshell
    integer, dimension(:), allocatable :: alr_to_i_phs
    real(default), dimension(3) :: x_rad
    real(default), dimension(:), allocatable :: jac_rand
    real(default), dimension(:), allocatable :: y_soft
    real(default) :: cms_energy2
    type(vector4_t), dimension(:), allocatable :: xi_ref_momenta
  contains
    <phs fks: real kinematics: TBP>
  end type real_kinematics_t

<phs fks: real kinematics: TBP>≡
  procedure :: init => real_kinematics_init

<phs fks: procedures>+≡
  subroutine real_kinematics_init (r, n_tot, n_phs, n_alr, n_contr)
    class(real_kinematics_t), intent(inout) :: r
    integer, intent(in) :: n_tot, n_phs, n_alr, n_contr
    allocate (r%xi_max (n_phs))
    allocate (r%y (n_phs))
    allocate (r%y_soft (n_phs))
    call r%p_born_cms%init (n_tot - 1, 1)
    call r%p_born_lab%init (n_tot - 1, 1)
    call r%p_real_cms%init (n_tot, n_phs)
    call r%p_real_lab%init (n_tot, n_phs)
    allocate (r%jac (n_phs), r%jac_rand (n_phs))
    allocate (r%alr_to_i_phs (n_alr))
    allocate (r%xi_ref_momenta (n_contr))
    r%alr_to_i_phs = 0
    r%xi_tilde = zero; r%xi_mismatch = zero
    r%xi_max = zero
    r%y = zero; r%y_mismatch = zero
    r%y_soft = zero
    r%phi = zero
    r%cms_energy2 = zero
    r%xi_ref_momenta = vector4_null
    r%jac_mismatch = one
    r%jac_rand = one
  end subroutine

```

```

end subroutine real_kinematics_init

<phs fks: real kinematics: TBP>+≡
  procedure :: init_onshell => real_kinematics_init_onshell

<phs fks: procedures>+≡
  subroutine real_kinematics_init_onshell (r, n_tot, n_phs)
    class(real_kinematics_t), intent(inout) :: r
    integer, intent(in) :: n_tot, n_phs
    call r%p_born_onshell%init (n_tot - 1, 1)
    call r%p_real_onshell(1)%init (n_tot, n_phs)
    call r%p_real_onshell(2)%init (n_tot, n_phs)
  end subroutine real_kinematics_init_onshell

<phs fks: real kinematics: TBP>+≡
  procedure :: write => real_kinematics_write

<phs fks: procedures>+≡
  subroutine real_kinematics_write (r, unit)
    class(real_kinematics_t), intent(in) :: r
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u,"(A)") "Real kinematics: "
    write (u,"(A," // FMT_17 // ",1X)") "xi_tilde: ", r%xi_tilde
    write (u,"(A," // FMT_17 // ",1X)") "phi: ", r%phi
    do i = 1, size (r%xi_max)
      write (u,"(A,I1,1X)") "i_phs: ", i
      write (u,"(A," // FMT_17 // ",1X)") "xi_max: ", r%xi_max(i)
      write (u,"(A," // FMT_17 // ",1X)") "y: ", r%y(i)
      write (u,"(A," // FMT_17 // ",1X)") "jac_rand: ", r%jac_rand(i)
      write (u,"(A," // FMT_17 // ",1X)") "y_soft: ", r%y_soft(i)
    end do
    write (u, "(A)") "Born Momenta: "
    write (u, "(A)") "CMS: "
    call r%p_born_cms%write (unit = u)
    write (u, "(A)") "Lab: "
    call r%p_born_lab%write (unit = u)
    write (u, "(A)") "Real Momenta: "
    write (u, "(A)") "CMS: "
    call r%p_real_cms%write (unit = u)
    write (u, "(A)") "Lab: "
    call r%p_real_lab%write (unit = u)
  end subroutine real_kinematics_write

```

The boost to the center-of-mass system only has a reasonable meaning above the threshold. Below the threshold, we do not apply boost at all, so that the top quarks stay in the rest frame. However, with top quarks exactly at rest, problems arise in the matrix elements (e.g. in the computation of angles). Therefore, we apply a boost which is not exactly 1, but has a tiny value differing from that.

```

<phs fks: public>+≡
  public :: get_boost_for_threshold_projection

```

```

<phs fks: procedures>+≡
function get_boost_for_threshold_projection (p, sqrts, mtop) result (L)
  type(lorentz_transformation_t) :: L
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(in) :: sqrts, mtop
  type(vector4_t) :: p_tmp
  type(vector3_t) :: dir
  real(default) :: scale_factor, arg
  p_tmp = p(THR_POS_WP) + p(THR_POS_B)
  arg = sqrts**2 - four * mtop**2
  if (arg > zero) then
    scale_factor = sqrt (arg) / two
  else
    scale_factor = tiny_07*1000
  end if
  dir = scale_factor * create_unit_vector (p_tmp)
  p_tmp = [sqrts / two, dir%p]
  L = boost (p_tmp, mtop)
end function get_boost_for_threshold_projection

```

This routine recomputes the value of ϕ used to generate the real phase space.

```

<phs fks: procedures>+≡
function get_generation_phi (p_born, p_real, emitter, i_gluon) result (phi)
  real(default) :: phi
  type(vector4_t), intent(in), dimension(:) :: p_born, p_real
  integer, intent(in) :: emitter, i_gluon
  type(vector4_t) :: p1, p2, pp
  type(lorentz_transformation_t) :: rot_to_gluon, rot_to_z
  type(vector3_t) :: dir, z
  real(default) :: cpsi
  pp = p_real(emitter) + p_real(i_gluon)
  cpsi = (space_part_norm (pp)**2 - space_part_norm (p_real(emitter))**2 &
    + space_part_norm (p_real(i_gluon))**2) / &
    (two * space_part_norm (pp) * space_part_norm (p_real(i_gluon)))
  dir = create_orthogonal (space_part (p_born(emitter)))
  rot_to_gluon = rotation (cpsi, sqrt (one - cpsi**2), dir)
  pp = rot_to_gluon * p_born(emitter)
  z%p = [0, 0, 1]
  rot_to_z = rotation_to_2nd &
    (space_part (p_born(emitter)) / space_part_norm (p_born(emitter)), z)
  p1 = rot_to_z * pp / space_part_norm (pp)
  p2 = rot_to_z * p_real(i_gluon)
  phi = azimuthal_distance (p1, p2)
  if (phi < zero) phi = twopi - abs(phi)
end function get_generation_phi

```

```

<phs fks: real kinematics: TBP>+≡
procedure :: apply_threshold_projection_real => real_kinematics_apply_threshold_projection_real

```

```

<phs fks: procedures>+≡
subroutine real_kinematics_apply_threshold_projection_real (r, i_phs, mtop, L_to_cms, invert)
  class(real_kinematics_t), intent(inout) :: r
  integer, intent(in) :: i_phs

```

```

real(default), intent(in) :: mtop
type(lorentz_transformation_t), intent(in), dimension(:) :: L_to_cms
logical, intent(in) :: invert
integer :: leg, other_leg
type(vector4_t), dimension(:), allocatable :: p_real
type(vector4_t), dimension(:), allocatable :: p_real_onshell
type(vector4_t), dimension(4) :: k_tmp
type(vector4_t), dimension(4) :: k_decay_onshell_real
type(vector4_t), dimension(3) :: k_decay_onshell_born
do leg = 1, 2
    other_leg = 3 - leg
    p_real = r%p_real_cms%phs_point(i_phs)
    allocate (p_real_onshell (size (p_real)))
    p_real_onshell(1:2) = p_real(1:2)
    k_tmp(1) = p_real(7)
    k_tmp(2) = p_real(ass_quark(leg))
    k_tmp(3) = p_real(ass_boson(leg))
    k_tmp(4) = [mtop, zero, zero, zero]
    call generate_on_shell_decay_threshold (k_tmp(1:3), &
        k_tmp(4), k_decay_onshell_real (2:4))
    k_decay_onshell_real (1) = k_tmp(4)
    k_tmp(1) = p_real(ass_quark(other_leg))
    k_tmp(2) = p_real(ass_boson(other_leg))
    k_decay_onshell_born = create_two_particle_decay (mtop**2, k_tmp(1), k_tmp(2))
    p_real_onshell(THR_POS_GLUON) = L_to_cms(leg) * k_decay_onshell_real (2)
    p_real_onshell(ass_quark(leg)) = L_to_cms(leg) * k_decay_onshell_real(3)
    p_real_onshell(ass_boson(leg)) = L_to_cms(leg) * k_decay_onshell_real(4)
    p_real_onshell(ass_quark(other_leg)) = L_to_cms(leg) * k_decay_onshell_born (2)
    p_real_onshell(ass_boson(other_leg)) = L_to_cms(leg) * k_decay_onshell_born (3)
    if (invert) then
        call vector4_invert_direction (p_real_onshell (ass_quark(other_leg)))
        call vector4_invert_direction (p_real_onshell (ass_boson(other_leg)))
    end if
    r%p_real_onshell(leg)%phs_point(i_phs) = p_real_onshell
    deallocate (p_real_onshell)
end do
end subroutine real_kinematics_apply_threshold_projection_real

```

<phs fks: public>+≡

```
public :: threshold_projection_born
```

<phs fks: procedures>+≡

```

subroutine threshold_projection_born (mtop, L_to_cms, p_in, p_onshell)
    real(default), intent(in) :: mtop
    type(lorentz_transformation_t), intent(in) :: L_to_cms
    type(vector4_t), intent(in), dimension(:) :: p_in
    type(vector4_t), intent(out), dimension(:) :: p_onshell
    type(vector4_t), dimension(3) :: k_decay_onshell
    type(vector4_t) :: p_tmp_1, p_tmp_2
    type(lorentz_transformation_t) :: L_to_cms_inv
    p_onshell(1:2) = p_in(1:2)
    L_to_cms_inv = inverse (L_to_cms)
    p_tmp_1 = L_to_cms_inv * p_in(THR_POS_B)
    p_tmp_2 = L_to_cms_inv * p_in(THR_POS_WP)

```

```

k_decay_onshell = create_two_particle_decay (mtop**2, &
    p_tmp_1, p_tmp_2)
p_onshell([THR_POS_B, THR_POS_WP]) = k_decay_onshell([2, 3])
p_tmp_1 = L_to_cms * p_in(THR_POS_BBAR)
p_tmp_2 = L_to_cms * p_in(THR_POS_WM)
k_decay_onshell = create_two_particle_decay (mtop**2, &
    p_tmp_1, p_tmp_2)
p_onshell([THR_POS_BBAR, THR_POS_WM]) = k_decay_onshell([2, 3])
p_onshell([THR_POS_WP, THR_POS_B]) = L_to_cms * p_onshell([THR_POS_WP, THR_POS_B])
p_onshell([THR_POS_WM, THR_POS_BBAR]) = L_to_cms_inv * p_onshell([THR_POS_WM, THR_POS_BBAR])
end subroutine threshold_projection_born

```

This routine computes the bounds of the Dalitz region for massive emitters. The corresponding derivation can be found in 1202.0465, App. A. It is also used for the POWHEG matching so the routine is public. The input parameter `m2` corresponds to the squared mass of the emitter.

```

<phs fks: public>+≡
public :: compute_dalitz_bounds

<phs fks: procedures>+≡
pure subroutine compute_dalitz_bounds (q0, m2, mrec2, z1, z2, k0_rec_max)
    real(default), intent(in) :: q0, m2, mrec2
    real(default), intent(out) :: z1, z2, k0_rec_max
    k0_rec_max = (q0**2 - m2 + mrec2) / (two * q0)
    z1 = (k0_rec_max + sqrt(k0_rec_max**2 - mrec2)) / q0
    z2 = (k0_rec_max - sqrt(k0_rec_max**2 - mrec2)) / q0
end subroutine compute_dalitz_bounds

```

Compute the `kt2` of a given emitter

```

<phs fks: real kinematics: TBP>+≡
procedure :: kt2 => real_kinematics_kt2

<phs fks: procedures>+≡
function real_kinematics_kt2 &
    (real_kinematics, i_phs, emitter, kt2_type, xi, y) result (kt2)
    real(default) :: kt2
    class(real_kinematics_t), intent(in) :: real_kinematics
    integer, intent(in) :: emitter, i_phs, kt2_type
    real(default), intent(in), optional :: xi, y
    real(default) :: xii, yy
    real(default) :: q, E_em, z, z1, z2, m2, mrec2, k0_rec_max
    type(vector4_t) :: p_emitter
    if (present(y)) then
        yy = y
    else
        yy = real_kinematics%y (i_phs)
    end if
    if (present(xi)) then
        xii = xi
    else
        xii = real_kinematics%xi_tilde * real_kinematics%xi_max (i_phs)
    end if
    select case (kt2_type)
    case (UBF_FSR_SIMPLE)

```



```

      kt2 = real_kinematics%cms_energy2 / two * xii**2 * (1 - yy)
case (UBF_FSR_MASSIVE)
  q = sqrt (real_kinematics%cms_energy2)
  p_emitter = real_kinematics%p_born_cms%phs_point(1)%select (emitter)
  mrec2 = (q - p_emitter%p(0))**2 - sum (p_emitter%p(1:3)**2)
  m2 = p_emitter**2
  E_em = energy (p_emitter)
  call compute_dalitz_bounds (q, m2, mrec2, z1, z2, k0_rec_max)
  z = z2 - (z2 - z1) * (one + yy) / two
  kt2 = xii**2 * q**3 * (one - z) / &
    (two * E_em - z * xii * q)
case (UBF_FSR_MASSLESS_RECOIL)
  kt2 = real_kinematics%cms_energy2 / two * xii**2 * (1 - yy**2) / two
case default
  kt2 = zero
  call msg_bug ("kt2_type must be set to a known value")
end select
end function real_kinematics_kt2

```

These are the possible values for upper_bound_func_type and will be used to decide which UBF object is allocated and which K_T scale for the matching is computed.

```

<phs fks: parameters>≡
  integer, parameter, public :: UBF_FSR_SIMPLE = 1
  integer, parameter, public :: UBF_FSR_MASSIVE = 2
  integer, parameter, public :: UBF_FSR_MASSLESS_RECOIL = 3

<phs fks: real kinematics: TBP>+≡
  procedure :: final => real_kinematics_final

<phs fks: procedures>+≡
  subroutine real_kinematics_final (real_kin)
    class(real_kinematics_t), intent(inout) :: real_kin
    if (allocated (real_kin%xi_max)) deallocate (real_kin%xi_max)
    if (allocated (real_kin%y)) deallocate (real_kin%y)
    if (allocated (real_kin%alr_to_i_phs)) deallocate (real_kin%alr_to_i_phs)
    if (allocated (real_kin%jac_rand)) deallocate (real_kin%jac_rand)
    if (allocated (real_kin%y_soft)) deallocate (real_kin%y_soft)
    if (allocated (real_kin%xi_ref_momenta)) deallocate (real_kin%xi_ref_momenta)
    call real_kin%p_born_cms%final (); call real_kin%p_born_lab%final ()
    call real_kin%p_real_cms%final (); call real_kin%p_real_lab%final ()
  end subroutine real_kinematics_final

<phs fks: parameters>+≡
  integer, parameter, public :: I_XI = 1
  integer, parameter, public :: I_Y = 2
  integer, parameter, public :: I_PHI = 3

  integer, parameter, public :: PHS_MODE_UNDEFINED = 0
  integer, parameter, public :: PHS_MODE_ADDITIONAL_PARTICLE = 1
  integer, parameter, public :: PHS_MODE_COLLINEAR_REMNANT = 2

<phs fks: public>+≡
  public :: phs_fks_config_t

```

```

<phs fks: types>+≡
type, extends (phs_wood_config_t) :: phs_fks_config_t
    integer :: mode = PHS_MODE_UNDEFINED
    character(32) :: md5sum_born_config
    logical :: born_2_to_1 = .false.
    logical :: make_dalitz_plot = .false.
contains
    <phs fks: fks config: TBP>
end type phs_fks_config_t

<phs fks: fks config: TBP>≡
procedure :: clear_phase_space => fks_config_clear_phase_space

<phs fks: procedures>+≡
subroutine fks_config_clear_phase_space (phs_config)
    class(phs_fks_config_t), intent(inout) :: phs_config
end subroutine fks_config_clear_phase_space

<phs fks: fks config: TBP>+≡
procedure :: write => phs_fks_config_write

<phs fks: procedures>+≡
subroutine phs_fks_config_write (object, unit, include_id)
    class(phs_fks_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: include_id
    integer :: u
    u = given_output_unit (unit)
    call object%phs_wood_config_t%write (u)
    write (u, "(3x,A,I0)") "NLO mode = ", object%mode
    write (u, "(3x,A,L1)") "2->1 proc = ", object%born_2_to_1
    write (u, "(3x,A,L1)") "Dalitz = ", object%make_dalitz_plot
    write (u, "(A,A)") "Extra Born md5sum: ", object%md5sum_born_config
end subroutine phs_fks_config_write

<phs fks: fks config: TBP>+≡
procedure :: set_mode => phs_fks_config_set_mode

<phs fks: procedures>+≡
subroutine phs_fks_config_set_mode (phs_config, mode)
    class(phs_fks_config_t), intent(inout) :: phs_config
    integer, intent(in) :: mode
    select case (mode)
    case (NLO_REAL, NLO_MISMATCH)
        phs_config%mode = PHS_MODE_ADDITIONAL_PARTICLE
    case (NLO_DGLAP)
        phs_config%mode = PHS_MODE_COLLINEAR_REMNANT
    end select
end subroutine phs_fks_config_set_mode

<phs fks: fks config: TBP>+≡
procedure :: configure => phs_fks_config_configure

```

```

<phs fks: procedures>+≡
subroutine phs_fks_config_configure (phs_config, sqrts, &
    sqrts_fixed, lab_is_cm, azimuthal_dependence, rebuild, &
    ignore_mismatch, nlo_type, subdir)
class(phs_fks_config_t), intent(inout) :: phs_config
real(default), intent(in) :: sqrts
logical, intent(in), optional :: sqrts_fixed
logical, intent(in), optional :: lab_is_cm
logical, intent(in), optional :: azimuthal_dependence
logical, intent(in), optional :: rebuild
logical, intent(in), optional :: ignore_mismatch
integer, intent(in), optional :: nlo_type
type(string_t), intent(in), optional :: subdir
if (present(nlo_type)) phs_config%nlo_type = nlo_type
if (.not. phs_config%is_combined_integration) then
    select case (phs_config%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
        phs_config%n_par = phs_config%n_par + 3
        if (phs_config%nlo_type == NLO_REAL .and. phs_config%n_out == 2) then
            phs_config%born_2_to_1 = .true.
        end if
    case (PHS_MODE_COLLINEAR_REMNANT)
        phs_config%n_par = phs_config%n_par + 1
    end select
end if
call phs_config%compute_md5sum ()
end subroutine phs_fks_config_configure

```

```

<phs fks: fks config: TBP>+≡
procedure :: startup_message => phs_fks_config_startup_message

```

```

<phs fks: procedures>+≡
subroutine phs_fks_config_startup_message (phs_config, unit)
class(phs_fks_config_t), intent(in) :: phs_config
integer, intent(in), optional :: unit
call phs_config%phs_wood_config_t%startup_message (unit)
end subroutine phs_fks_config_startup_message

```

```

<phs fks: fks config: TBP>+≡
procedure, nopass :: allocate_instance => phs_fks_config_allocate_instance

```

```

<phs fks: procedures>+≡
subroutine phs_fks_config_allocate_instance (phs)
class(phs_t), intent(inout), pointer :: phs
allocate (phs_fks_t :: phs)
end subroutine phs_fks_config_allocate_instance

```

If the phase space is generated from file, but we want to have resonance histories, we must force the cascade sets to be generated. However, it must be assured that Born flavors are used for this.

```

<phs fks: fks config: TBP>+≡
procedure :: generate_phase_space_extra => phs_fks_config_generate_phase_space_extra

```

(phs fks: procedures)+≡

```

subroutine phs_fks_config_generate_phase_space_extra (phs_config)
  class(phs_fks_config_t), intent(inout) :: phs_config
  integer :: off_shell, extra_off_shell
  type(flavor_t), dimension(:, :), allocatable :: flv_born
  integer :: i, j
  integer :: n_state, n_flv_born
  integer :: unit_fds
  logical :: valid
  type(string_t) :: file_name
  logical :: file_exists
  if (phs_config%use_cascades2) then
    allocate (phs_config%feyngraph_set)
  else
    allocate (phs_config%cascade_set)
  end if
  n_flv_born = size (phs_config%flv, 1) - 1
  n_state = size (phs_config%flv, 2)
  allocate (flv_born (n_flv_born, n_state))
  do i = 1, n_flv_born
    do j = 1, n_state
      flv_born(i, j) = phs_config%flv(i, j)
    end do
  end do
  if (phs_config%use_cascades2) then
    file_name = char (phs_config%id) // ".fds"
    inquire (file=char (file_name), exist=file_exists)
    if (.not. file_exists) call msg_fatal &
      ("The 0'Mega input file " // char (file_name) // &
       " does not exist. " // "Please make sure that the " // &
       "variable ?omega_write_phs_output has been set correctly.")
    unit_fds = free_unit ()
    open (unit=unit_fds, file=char(file_name), status='old', action='read')
  end if
  off_shell = phs_config%par%off_shell
  do extra_off_shell = 0, max (n_flv_born - 2, 0)
    phs_config%par%off_shell = off_shell + extra_off_shell
    if (phs_config%use_cascades2) then
      call feyngraph_set_generate (phs_config%feyngraph_set, &
        phs_config%model, phs_config%n_in, phs_config%n_out - 1, &
        flv_born, phs_config%par, phs_config%fatal_beam_decay, unit_fds, &
        phs_config%vis_channels)
      if (feyngraph_set_is_valid (phs_config%feyngraph_set)) exit
    else
      call cascade_set_generate (phs_config%cascade_set, &
        phs_config%model, phs_config%n_in, phs_config%n_out - 1, &
        flv_born, phs_config%par, phs_config%fatal_beam_decay)
      if (cascade_set_is_valid (phs_config%cascade_set)) exit
    end if
  end do
  if (phs_config%use_cascades2) then
    close (unit_fds)
    valid = feyngraph_set_is_valid (phs_config%feyngraph_set)
  else

```

```

        valid = cascade_set_is_valid (phs_config%cascade_set)
    end if
    if (.not. valid) &
        call msg_fatal ("Resonance extraction: Phase space generation failed")
    end subroutine phs_fks_config_generate_phase_space_extra

```

(phs fks: fks config: TBP)+≡

```

    procedure :: set_born_config => phs_fks_config_set_born_config

```

(phs fks: procedures)+≡

```

subroutine phs_fks_config_set_born_config (phs_config, phs_cfg_born)
    class(phs_fks_config_t), intent(inout) :: phs_config
    type(phs_wood_config_t), intent(in), target :: phs_cfg_born
    if (debug_on) &
        call msg_debug (D_PHASESPACE, "phs_fks_config_set_born_config")
    phs_config%forest = phs_cfg_born%forest
    phs_config%n_channel = phs_cfg_born%n_channel
    allocate (phs_config%channel (phs_config%n_channel))
    phs_config%channel = phs_cfg_born%channel
    phs_config%n_par = phs_cfg_born%n_par
    phs_config%n_state = phs_cfg_born%n_state
    phs_config%sqrts = phs_cfg_born%sqrts
    phs_config%par = phs_cfg_born%par
    phs_config%sqrts_fixed = phs_cfg_born%sqrts_fixed
    phs_config%azimuthal_dependence = phs_cfg_born%azimuthal_dependence
    phs_config%provides_chains = phs_cfg_born%provides_chains
    phs_config%lab_is_cm = phs_cfg_born%lab_is_cm
    phs_config%vis_channels = phs_cfg_born%vis_channels
    phs_config%provides_equivalences = phs_cfg_born%provides_equivalences
    allocate (phs_config%chain (size (phs_cfg_born%chain)))
    phs_config%chain = phs_cfg_born%chain
    phs_config%model => phs_cfg_born%model
    phs_config%use_cascades2 = phs_cfg_born%use_cascades2
    if (allocated (phs_cfg_born%cascade_set)) then
        allocate (phs_config%cascade_set)
        phs_config%cascade_set = phs_cfg_born%cascade_set
    end if
    if (allocated (phs_cfg_born%feyngraph_set)) then
        allocate (phs_config%feyngraph_set)
        phs_config%feyngraph_set = phs_cfg_born%feyngraph_set
    end if
    phs_config%md5sum_born_config = phs_cfg_born%md5sum_phs_config
end subroutine phs_fks_config_set_born_config

```

(phs fks: fks config: TBP)+≡

```

    procedure :: get_resonance_histories => phs_fks_config_get_resonance_histories

```

(phs fks: procedures)+≡

```

function phs_fks_config_get_resonance_histories (phs_config) result (resonance_histories)
    type(resonance_history_t), dimension(:), allocatable :: resonance_histories
    class(phs_fks_config_t), intent(inout) :: phs_config
    if (allocated (phs_config%cascade_set)) then
        call cascade_set_get_resonance_histories &
            (phs_config%cascade_set, n_filter = 2, res_hists = resonance_histories)
    end if
end function

```

```

else if (allocated (phs_config%feyngraph_set)) then
  call feyngraph_set_get_resonance_histories &
    (phs_config%feyngraph_set, n_filter = 2, res_hists = resonance_histories)
else
  if (debug_on) call msg_debug (D_PHASESPACE, "Have to rebuild phase space for resonance hist
  call phs_config%generate_phase_space_extra ()
  if (phs_config%use_cascades2) then
    call feyngraph_set_get_resonance_histories &
      (phs_config%feyngraph_set, n_filter = 2, res_hists = resonance_histories)
  else
    call cascade_set_get_resonance_histories &
      (phs_config%cascade_set, n_filter = 2, res_hists = resonance_histories)
  end if
end if
end function phs_fks_config_get_resonance_histories

<phs fks: public>+≡
public :: dalitz_plot_t

<phs fks: types>+≡
type :: dalitz_plot_t
  integer :: unit = -1
  type(string_t) :: filename
  logical :: active = .false.
  logical :: inverse = .false.
contains
  <phs fks: dalitz plot: TBP>
end type dalitz_plot_t

<phs fks: dalitz plot: TBP>≡
procedure :: init => dalitz_plot_init

<phs fks: procedures>+≡
subroutine dalitz_plot_init (plot, unit, filename, inverse)
  class(dalitz_plot_t), intent(inout) :: plot
  integer, intent(in) :: unit
  type(string_t), intent(in) :: filename
  logical, intent(in) :: inverse
  plot%active = .true.
  plot%unit = unit
  plot%inverse = inverse
  open (plot%unit, file = char (filename), action = "write")
end subroutine dalitz_plot_init

<phs fks: dalitz plot: TBP>+≡
procedure :: write_header => dalitz_plot_write_header

<phs fks: procedures>+≡
subroutine dalitz_plot_write_header (plot)
  class(dalitz_plot_t), intent(in) :: plot
  write (plot%unit, "(A36)") "### Dalitz plot generated by WHIZARD"
  if (plot%inverse) then
    write (plot%unit, "(A10,1x,A4)") "### k0_n+1", "k0_n"
  else

```

```

        write (plot%unit, "(A8,1x,A6)") "### k0_n", "k0_n+1"
    end if
end subroutine dalitz_plot_write_header

<phs fks: dalitz plot: TBP>+≡
    procedure :: register => dalitz_plot_register

<phs fks: procedures>+≡
    subroutine dalitz_plot_register (plot, k0_n, k0_np1)
        class(dalitz_plot_t), intent(in) :: plot
        real(default), intent(in) :: k0_n, k0_np1
        if (plot%inverse) then
            write (plot%unit, "(F8.4,1X,F8.4)") k0_np1, k0_n
        else
            write (plot%unit, "(F8.4,1X,F8.4)") k0_np1, k0_n
        end if
    end subroutine dalitz_plot_register

<phs fks: dalitz plot: TBP>+≡
    procedure :: final => dalitz_plot_final

<phs fks: procedures>+≡
    subroutine dalitz_plot_final (plot)
        class(dalitz_plot_t), intent(inout) :: plot
        logical :: opened
        plot%active = .false.
        plot%inverse = .false.
        if (plot%unit >= 0) then
            inquire (unit = plot%unit, opened = opened)
            if (opened) close (plot%unit)
        end if
        plot%filename = var_str ('')
        plot%unit = -1
    end subroutine dalitz_plot_final

<phs fks: parameters>+≡
    integer, parameter, public :: GEN_REAL_PHASE_SPACE = 1
    integer, parameter, public :: GEN_SOFT_MISMATCH = 2
    integer, parameter, public :: GEN_SOFT_LIMIT_TEST = 3
    integer, parameter, public :: GEN_COLL_LIMIT_TEST = 4
    integer, parameter, public :: GEN_ANTI_COLL_LIMIT_TEST = 5
    integer, parameter, public :: GEN_SOFT_COLL_LIMIT_TEST = 6
    integer, parameter, public :: GEN_SOFT_ANTI_COLL_LIMIT_TEST = 7

    integer, parameter, public :: SQRTS_FIXED = 1
    integer, parameter, public :: SQRTS_VAR = 2

    real(default), parameter :: xi_tilde_test_soft = 0.00001_default
    real(default), parameter :: xi_tilde_test_coll = 0.5_default
    real(default), parameter :: y_test_soft = 0.5_default
    real(default), parameter :: y_test_coll = 0.9999999_default
    !!! for testing EW singularities: y_test_coll = 0.99999999_default

```

Very soft or collinear phase-space points can become a problem for matrix elements providers, as some scalar products cannot be evaluated properly. Here, a nonsensical result can spoil the whole integration. We therefore check the scalar products appearing to be below a certain tolerance.

Naturally, this happens very rarely but for some processes, setting `?test_coll_limit = true` and/or `?test_soft_limit = true` leads to all phase space points being discarded by this routine.

```

<phs fks: public>+≡
    public :: check_scalar_products

<phs fks: procedures>+≡
    function check_scalar_products (p) result (valid)
        logical :: valid
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), parameter :: tolerance = 1E-7_default
        !!! for testing EW singularities: tolerance = 5E-9_default
        integer :: i, j
        valid = .true.
        do i = 1, size (p)
            do j = i, size (p)
                if (i /= j) then
                    if (abs(p(i) * p(j)) < tolerance) then
                        valid = .false.
                        exit
                    end if
                end if
            end do
        end do
    end function check_scalar_products

```

`xi_min` should be set to a non-zero value in order to avoid phase-space points with `p_real(emitter) = 0`.

```

<phs fks: public>+≡
    public :: phs_fks_generator_t

<phs fks: types>+≡
    type :: phs_fks_generator_t
        integer, dimension(:), allocatable :: emitters
        type(real_kinematics_t), pointer :: real_kinematics => null()
        type(isr_kinematics_t), pointer :: isr_kinematics => null()
        integer :: n_in
        real(default) :: xi_min
        real(default) :: y_max
        real(default) :: sqrts
        real(default) :: E_gluon
        real(default) :: mrec2
        real(default), dimension(:), allocatable :: m2
        logical :: massive_phsp = .false.
        logical, dimension(:), allocatable :: is_massive
        logical :: singular_jacobian = .false.
        integer :: i_fsr_first = -1
        type(resonance_contributors_t), dimension(:), allocatable :: resonance_contributors !!! Put so
        integer :: mode = GEN_REAL_PHASE_SPACE
    contains

```



```

    <phs fks: phs fks generator: TBP>
    end type phs_fks_generator_t

    <phs fks: phs fks generator: TBP>≡
    procedure :: connect_kinematics => phs_fks_generator_connect_kinematics

    <phs fks: procedures>+≡
    subroutine phs_fks_generator_connect_kinematics &
        (generator, isr_kinematics, real_kinematics, massive_phsp)
    class(phs_fks_generator_t), intent(inout) :: generator
    type(isr_kinematics_t), intent(in), pointer :: isr_kinematics
    type(real_kinematics_t), intent(in), pointer :: real_kinematics
    logical, intent(in) :: massive_phsp
    generator%real_kinematics => real_kinematics
    generator%isr_kinematics => isr_kinematics
    generator%massive_phsp = massive_phsp
    end subroutine phs_fks_generator_connect_kinematics

    <phs fks: phs fks generator: TBP>+≡
    procedure :: compute_isr_kinematics => phs_fks_generator_compute_isr_kinematics

    <phs fks: procedures>+≡
    subroutine phs_fks_generator_compute_isr_kinematics (generator, r, p_in)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: r
    type(vector4_t), dimension(2), intent(in), optional :: p_in
    integer :: em
    type(vector4_t), dimension(2) :: p

    if (present (p_in)) then
        p = p_in
    else
        p = generator%real_kinematics%p_born_lab%phs_point(1)%select ([1,2])
    end if

    associate (isr_kinematics => generator%isr_kinematics)
        do em = 1, 2
            isr_kinematics%x(em) = p(em)%p(0) / isr_kinematics%beam_energy(em)
            isr_kinematics%z(em) = one - (one - isr_kinematics%x(em)) * r
            isr_kinematics%jacobian(em) = one - isr_kinematics%x(em)
        end do
        isr_kinematics%sqrts_born = (p(1) + p(2))*1
    end associate
    end subroutine phs_fks_generator_compute_isr_kinematics

    <phs fks: phs fks generator: TBP>+≡
    procedure :: final => phs_fks_generator_final

    <phs fks: procedures>+≡
    subroutine phs_fks_generator_final (generator)
    class(phs_fks_generator_t), intent(inout) :: generator
    if (allocated (generator%emitters)) deallocate (generator%emitters)
    if (associated (generator%real_kinematics)) nullify (generator%real_kinematics)
    if (associated (generator%isr_kinematics)) nullify (generator%isr_kinematics)

```

```

    if (allocated (generator%m2)) deallocate (generator%m2)
    generator%massive_phsp = .false.
    if (allocated (generator%is_massive)) deallocate (generator%is_massive)
    generator%singular_jacobian = .false.
    generator%i_fsr_first = -1
    if (allocated (generator%resonance_contributors)) &
        deallocate (generator%resonance_contributors)
    generator%mode = GEN_REAL_PHASE_SPACE
end subroutine phs_fks_generator_final

```

A resonance phase space is uniquely specified via the resonance contributors and the corresponding emitters. The `phs_identifier` type also checks whether the given contributor-emitter configuration has already been evaluated to avoid duplicate computations.

```

<phs fks: public>+≡
    public :: phs_identifier_t

<phs fks: types>+≡
    type :: phs_identifier_t
        integer, dimension(:), allocatable :: contributors
        integer :: emitter = -1
        logical :: evaluated = .false.
    contains
    <phs fks: phs identifier: TBP>
    end type phs_identifier_t

<phs fks: phs identifier: TBP>≡
    generic :: init => init_from_emitter, init_from_emitter_and_contributors
    procedure :: init_from_emitter => phs_identifier_init_from_emitter
    procedure :: init_from_emitter_and_contributors &
        => phs_identifier_init_from_emitter_and_contributors

<phs fks: procedures>+≡
    subroutine phs_identifier_init_from_emitter (phs_id, emitter)
        class(phs_identifier_t), intent(out) :: phs_id
        integer, intent(in) :: emitter
        phs_id%emitter = emitter
    end subroutine phs_identifier_init_from_emitter

    subroutine phs_identifier_init_from_emitter_and_contributors &
        (phs_id, emitter, contributors)
        class(phs_identifier_t), intent(out) :: phs_id
        integer, intent(in) :: emitter
        integer, intent(in), dimension(:) :: contributors
        allocate (phs_id%contributors (size (contributors)))
        phs_id%contributors = contributors
        phs_id%emitter = emitter
    end subroutine phs_identifier_init_from_emitter_and_contributors

<phs fks: phs identifier: TBP>+≡
    procedure :: check => phs_identifier_check

<phs fks: procedures>+≡
    function phs_identifier_check (phs_id, emitter, contributors) result (check)

```

```

logical :: check
class(phs_identifier_t), intent(in) :: phs_id
integer, intent(in) :: emitter
integer, intent(in), dimension(:), optional :: contributors
check = phs_id%emitter == emitter
if (present (contributors)) then
    if (.not. allocated (phs_id%contributors)) &
        call msg_fatal ("Phs identifier: contributors not allocated!")
    check = check .and. all (phs_id%contributors == contributors)
end if
end function phs_identifier_check

```

<phs fks: phs identifier: TBP>+≡

```

procedure :: write => phs_identifier_write

```

<phs fks: procedures>+≡

```

subroutine phs_identifier_write (phs_id, unit)
    class(phs_identifier_t), intent(in) :: phs_id
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    write (u, '(A)') 'phs_identifier: '
    write (u, '(A,I1,I1)') 'Emitter: ', phs_id%emitter
    if (allocated (phs_id%contributors)) then
        write (u, '(A)', advance = 'no') 'Resonance contributors: '
        do i = 1, size (phs_id%contributors)
            write (u, '(I1,I1)', advance = 'no') phs_id%contributors(i)
        end do
    else
        write (u, '(A)') 'No Contributors allocated'
    end if
end subroutine phs_identifier_write

```

<phs fks: public>+≡

```

public :: check_for_phs_identifier

```

<phs fks: procedures>+≡

```

subroutine check_for_phs_identifier (phs_id, n_in, emitter, contributors, phs_exist, i_phs)
    type(phs_identifier_t), intent(in), dimension(:) :: phs_id
    integer, intent(in) :: n_in, emitter
    integer, intent(in), dimension(:), optional :: contributors
    logical, intent(out) :: phs_exist
    integer, intent(out) :: i_phs
    integer :: i
    phs_exist = .false.
    i_phs = -1
    do i = 1, size (phs_id)
        if (phs_id(i)%emitter < 0) then
            i_phs = i
            exit
        end if
        phs_exist = phs_id(i)%emitter == emitter
        if (present (contributors)) &
            phs_exist = phs_exist .and. all (phs_id(i)%contributors == contributors)
    end do

```

```

        if (phs_exist) then
            i_phs = i
            exit
        end if
    end do
end subroutine check_for_phs_identifier

```

The fks phase space type contains the wood phase space and separately the in- and outgoing momenta for the real process and the corresponding Born momenta. Additionally, there are the variables ξ, ξ_{max}, y and ϕ which are used to create the real phase space, as well as the jacobian and its corresponding soft and collinear limit. Lastly, the array `ch_to_em` connects each channel with an emitter.

```

<phs fks: public>+≡
    public :: phs_fks_t

<phs fks: types>+≡
    type, extends (phs_wood_t) :: phs_fks_t
        integer :: mode = PHS_MODE_UNDEFINED
        type(vector4_t), dimension(:), allocatable :: p_born
        type(vector4_t), dimension(:), allocatable :: q_born
        type(vector4_t), dimension(:), allocatable :: p_real
        type(vector4_t), dimension(:), allocatable :: q_real
        type(vector4_t), dimension(:), allocatable :: p_born_tot
        type(phs_fks_generator_t) :: generator
        real(default) :: r_isr
        type(phs_identifier_t), dimension(:), allocatable :: phs_identifiers
    contains
        <phs fks: phs fks: TBP>
        end type phs_fks_t

<phs fks: interfaces>≡

    interface compute_beta
        module procedure compute_beta_massless
        module procedure compute_beta_massive
    end interface

    interface get_xi_max_fsr
        module procedure get_xi_max_fsr_massless
        module procedure get_xi_max_fsr_massive
    end interface

<phs fks: phs fks: TBP>≡
    procedure :: write => phs_fks_write

<phs fks: procedures>+≡
    subroutine phs_fks_write (object, unit, verbose)
        class(phs_fks_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose
        integer :: u, i, n_id
        u = given_output_unit (unit)

```

```

call object%base_write ()
n_id = size (object%phs_identifiers)
if (n_id == 0) then
  write (u, "(A)") "No phs identifiers allocated! "
else
  do i = 1, n_id
    call object%phs_identifiers(i)%write (u)
  end do
end if
end subroutine phs_fks_write

```

Initializer for the phase space. Calls the initialization of the corresponding Born phase space, sets up the channel-emitter-association and allocates space for the momenta.

```

<phs fks: phs fks: TBP>+≡
  procedure :: init => phs_fks_init
<phs fks: procedures>+≡
  subroutine phs_fks_init (phs, phs_config)
    class(phs_fks_t), intent(out) :: phs
    class(phs_config_t), intent(in), target :: phs_config

    call phs%base_init (phs_config)
    select type (phs_config)
    type is (phs_fks_config_t)
      phs%config => phs_config
      phs%forest = phs_config%forest
    end select

    select type (phs)
    type is (phs_fks_t)
      select type (phs_config)
      type is (phs_fks_config_t)
        phs%mode = phs_config%mode
      end select

      select case (phs%mode)
      case (PHS_MODE_ADDITIONAL_PARTICLE)
        phs%n_r_born = phs%config%n_par - 3
      case (PHS_MODE_COLLINEAR_REMNANT)
        phs%n_r_born = phs%config%n_par - 1
      end select
    end select
  end subroutine phs_fks_init

```

For real components of $2 \rightarrow 1$ NLO processes we have to recompute the flux factor as this has to be the one of the underlying Born.

```

<phs fks: phs fks: TBP>+≡
  procedure :: compute_flux => phs_fks_compute_flux
<phs fks: procedures>+≡
  subroutine phs_fks_compute_flux (phs)
    class(phs_fks_t), intent(inout) :: phs
    call phs%compute_base_flux ()

```

```

select type (config => phs%config)
type is (phs_fks_config_t)
  if (config%born_2_to_1) then
    phs%flux = conv * twopi &
      / (2 * config%sqrts ** 2 * phs%m_out(1) ** 2)
  end if
end select
end subroutine phs_fks_compute_flux

```

```

<phs fks: phs fks: TBP>+≡
  procedure :: allocate_momenta => phs_fks_allocate_momenta

<phs fks: procedures>+≡
  subroutine phs_fks_allocate_momenta (phs, phs_config, data_is_born)
    class(phs_fks_t), intent(inout) :: phs
    class(phs_config_t), intent(in) :: phs_config
    logical, intent(in) :: data_is_born
    integer :: n_out_born
    allocate (phs%p_born (phs_config%n_in))
    allocate (phs%p_real (phs_config%n_in))
    select case (phs%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
      if (data_is_born) then
        n_out_born = phs_config%n_out
      else
        n_out_born = phs_config%n_out - 1
      end if
      allocate (phs%q_born (n_out_born))
      allocate (phs%q_real (n_out_born + 1))
      allocate (phs%p_born_tot (phs_config%n_in + n_out_born))
    end select
  end subroutine phs_fks_allocate_momenta

```

Evaluate selected channel. First, the subroutine calls the evaluation procedure of the underlying Born phase space, using $n_r - 3$ random numbers. Then, the remaining three random numbers are used to create ξ , y and ϕ , from which the real momenta are calculated from the Born momenta.

```

<phs fks: phs fks: TBP>+≡
  procedure :: evaluate_selected_channel => phs_fks_evaluate_selected_channel

<phs fks: procedures>+≡
  subroutine phs_fks_evaluate_selected_channel (phs, c_in, r_in)
    class(phs_fks_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    real(default), intent(in), dimension(:) :: r_in
    integer :: n_in

    call phs%phs_wood_t%evaluate_selected_channel (c_in, r_in)
    phs%r(:,c_in) = r_in

    phs%q_defined = phs%phs_wood_t%q_defined
    if (.not. phs%q_defined) return

    select case (phs%mode)

```

```

case (PHS_MODE_ADDITIONAL_PARTICLE)
  n_in = phs%config%n_in
  phs%p_born = phs%phs_wood_t%p
  phs%q_born = phs%phs_wood_t%q
  phs%p_born_tot (1: n_in) = phs%p_born
  phs%p_born_tot (n_in + 1 :) = phs%q_born
  call phs%set_reference_frames (.true.)
  call phs%set_isr_kinematics (.true.)
case (PHS_MODE_COLLINEAR_REMNANT)
  call phs%compute_isr_kinematics (r_in(phs%n_r_born + 1))
  phs%r_isr = r_in(phs%n_r_born + 1)
end select
end subroutine phs_fks_evaluate_selected_channel

```

```

<phs fks: phs fks: TBP>+≡
  procedure :: evaluate_other_channels => phs_fks_evaluate_other_channels

```

```

<phs fks: procedures>+≡
  subroutine phs_fks_evaluate_other_channels (phs, c_in)
    class(phs_fks_t), intent(inout) :: phs
    integer, intent(in) :: c_in
    call phs%phs_wood_t%evaluate_other_channels (c_in)
    phs%r_defined = .true.
  end subroutine phs_fks_evaluate_other_channels

```

```

<phs fks: phs fks: TBP>+≡
  procedure :: get_mcpair => phs_fks_get_mcpair

```

```

<phs fks: procedures>+≡
  subroutine phs_fks_get_mcpair (phs, c, r)
    class(phs_fks_t), intent(in) :: phs
    integer, intent(in) :: c
    real(default), dimension(:), intent(out) :: r
    r(1 : phs%n_r_born) = phs%r(1 : phs%n_r_born,c)
    select case (phs%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
      r(phs%n_r_born + 1 :) = phs%r_real
    case (PHS_MODE_COLLINEAR_REMNANT)
      r(phs%n_r_born + 1 :) = phs%r_isr
    end select
  end subroutine phs_fks_get_mcpair

```

```

<phs fks: phs fks: TBP>+≡
  procedure :: set_beam_energy => phs_fks_set_beam_energy

```

```

<phs fks: procedures>+≡
  subroutine phs_fks_set_beam_energy (phs)
    class(phs_fks_t), intent(inout) :: phs
    call phs%generator%set_sqrts_hat (phs%config%sqrts)
  end subroutine phs_fks_set_beam_energy

```

```

<phs fks: phs fks: TBP>+≡
  procedure :: set_emitters => phs_fks_set_emitters

```

```

<phs fks: procedures>+≡
  subroutine phs_fks_set_emitters (phs, emitters)
    class(phs_fks_t), intent(inout) :: phs
    integer, intent(in), dimension(:), allocatable :: emitters
    call phs%generator%set_emitters (emitters)
  end subroutine phs_fks_set_emitters

<phs fks: phs fks: TBP>+≡
  procedure :: set_momenta => phs_fks_set_momenta

<phs fks: procedures>+≡
  subroutine phs_fks_set_momenta (phs, p)
    class(phs_fks_t), intent(inout) :: phs
    type(vector4_t), intent(in), dimension(:) :: p
    integer :: n_in, n_tot_born
    select case (phs%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
      n_in = phs%config%n_in; n_tot_born = phs%config%n_tot - 1
      phs%p_born = p(1 : n_in)
      phs%q_born = p(n_in + 1 : n_tot_born)
      phs%p_born_tot = p
    end select
  end subroutine phs_fks_set_momenta

<phs fks: phs fks: TBP>+≡
  procedure :: setup_masses => phs_fks_setup_masses

<phs fks: procedures>+≡
  subroutine phs_fks_setup_masses (phs, n_tot)
    class(phs_fks_t), intent(inout) :: phs
    integer, intent(in) :: n_tot
    call phs%generator%setup_masses (n_tot)
  end subroutine phs_fks_setup_masses

<phs fks: phs fks: TBP>+≡
  procedure :: get_born_momenta => phs_fks_get_born_momenta

<phs fks: procedures>+≡
  subroutine phs_fks_get_born_momenta (phs, p)
    class(phs_fks_t), intent(inout) :: phs
    type(vector4_t), intent(out), dimension(:) :: p
    select case (phs%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
      p(1 : phs%config%n_in) = phs%p_born
      p(phs%config%n_in + 1 :) = phs%q_born
    case (PHS_MODE_COLLINEAR_REMNANT)
      p(1:phs%config%n_in) = phs%phs_wood_t%p
      p(phs%config%n_in + 1 :) = phs%phs_wood_t%q
    end select
    if (.not. phs%config%lab_is_cm) p = phs%lt_cm_to_lab * p
  end subroutine phs_fks_get_born_momenta

<phs fks: phs fks: TBP>+≡
  procedure :: get_outgoing_momenta => phs_fks_get_outgoing_momenta

```



```

<phs fks: procedures>+≡
  subroutine phs_fks_get_outgoing_momenta (phs, q)
    class(phs_fks_t), intent(in) :: phs
    type(vector4_t), intent(out), dimension(:) :: q
    select case (phs%mode)
    case (PHS_MODE_ADDITIONAL_PARTICLE)
      q = phs%q_real
    case (PHS_MODE_COLLINEAR_REMNANT)
      q = phs%phs_wood_t%q
    end select
  end subroutine phs_fks_get_outgoing_momenta

<phs fks: phs fks: TBP>+≡
  procedure :: get_incoming_momenta => phs_fks_get_incoming_momenta

<phs fks: procedures>+≡
  subroutine phs_fks_get_incoming_momenta (phs, p)
    class(phs_fks_t), intent(in) :: phs
    type(vector4_t), intent(inout), dimension(:), allocatable :: p
    p = phs%p_real
  end subroutine phs_fks_get_incoming_momenta

<phs fks: phs fks: TBP>+≡
  procedure :: set_isr_kinematics => phs_fks_set_isr_kinematics

<phs fks: procedures>+≡
  subroutine phs_fks_set_isr_kinematics (phs, requires_boost)
    class(phs_fks_t), intent(inout) :: phs
    logical, intent(in) :: requires_boost
    type(vector4_t), dimension(2) :: p
    if (phs%generator%isr_kinematics%isr_mode == SQRTS_VAR) then
      if (requires_boost) then
        p = phs%lt_cm_to_lab &
          * phs%generator%real_kinematics%p_born_cms%phs_point(1)%select ([1,2])
      else
        p = phs%generator%real_kinematics%p_born_lab%phs_point(1)%select ([1,2])
      end if
      call phs%generator%set_isr_kinematics (p)
    end if
  end subroutine phs_fks_set_isr_kinematics

<phs fks: phs fks: TBP>+≡
  procedure :: generate_radiation_variables => &
    phs_fks_generate_radiation_variables

<phs fks: procedures>+≡
  subroutine phs_fks_generate_radiation_variables (phs, r_in, threshold)
    class(phs_fks_t), intent(inout) :: phs
    real(default), intent(in), dimension(:) :: r_in
    logical, intent(in) :: threshold
    type(vector4_t), dimension(:), allocatable :: p_born
    if (size (r_in) /= 3) call msg_fatal &
      ("Real kinematics need to be generated using three random numbers!")
    select case (phs%mode)

```

```

case (PHS_MODE_ADDITIONAL_PARTICLE)
  allocate (p_born (size (phs%p_born_tot)))
  if (threshold) then
    p_born = phs%get_onshell_projected_momenta ()
  else
    p_born = phs%p_born_tot
  if (.not. phs%lab_is_cm ()) &
    p_born = inverse (phs%lt_cm_to_lab) * p_born
  end if
  call phs%generator%generate_radiation_variables &
    (r_in, p_born, phs%phs_identifiers, threshold)
  phs%r_real = r_in
end select
end subroutine phs_fks_generate_radiation_variables

```

<phs fks: phs fks: TBP>+≡

```

procedure :: compute_xi_ref_momenta => phs_fks_compute_xi_ref_momenta

```

<phs fks: procedures>+≡

```

subroutine phs_fks_compute_xi_ref_momenta (phs, p_in, contributors)
  class(phs_fks_t), intent(inout) :: phs
  type(vector4_t), intent(in), dimension(:), optional :: p_in
  type(resonance_contributors_t), intent(in), dimension(:), optional :: contributors
  if (phs%mode == PHS_MODE_ADDITIONAL_PARTICLE) then
    if (present (p_in)) then
      call phs%generator%compute_xi_ref_momenta (p_in, contributors)
    else
      call phs%generator%compute_xi_ref_momenta (phs%p_born_tot, contributors)
    end if
  end if
end subroutine phs_fks_compute_xi_ref_momenta

```

<phs fks: phs fks: TBP>+≡

```

procedure :: compute_xi_ref_momenta_threshold => phs_fks_compute_xi_ref_momenta_threshold

```

<phs fks: procedures>+≡

```

subroutine phs_fks_compute_xi_ref_momenta_threshold (phs)
  class(phs_fks_t), intent(inout) :: phs
  select case (phs%mode)
  case (PHS_MODE_ADDITIONAL_PARTICLE)
    call phs%generator%compute_xi_ref_momenta_threshold &
      (phs%get_onshell_projected_momenta ())
  end select
end subroutine phs_fks_compute_xi_ref_momenta_threshold

```

<phs fks: phs fks: TBP>+≡

```

procedure :: compute_cms_energy => phs_fks_compute_cms_energy

```

<phs fks: procedures>+≡

```

subroutine phs_fks_compute_cms_energy (phs)
  class(phs_fks_t), intent(inout) :: phs
  if (phs%mode == PHS_MODE_ADDITIONAL_PARTICLE) &
    call phs%generator%compute_cms_energy (phs%p_born_tot)
end subroutine phs_fks_compute_cms_energy

```

When initial-state radiation is involved, either due to beamstrahlung or QCD/QED corrections, it is important to have access to both the phase space points in the center-of-mass and lab frame.

```

<phs fks: phs fks: TBP>+≡
  procedure :: set_reference_frames => phs_fks_set_reference_frames

<phs fks: procedures>+≡
  subroutine phs_fks_set_reference_frames (phs, is_cms)
    class(phs_fks_t), intent(inout) :: phs
    logical, intent(in) :: is_cms
    associate (real_kinematics => phs%generator%real_kinematics)
      if (phs%config%lab_is_cm) then
        real_kinematics%p_born_cms%phs_point(1) = phs%p_born_tot
        real_kinematics%p_born_lab%phs_point(1) = phs%p_born_tot
      else
        if (is_cms) then
          real_kinematics%p_born_cms%phs_point(1) &
            = phs%p_born_tot
          real_kinematics%p_born_lab%phs_point(1) &
            = phs%lt_cm_to_lab * phs%p_born_tot
        else
          real_kinematics%p_born_cms%phs_point(1) &
            = inverse (phs%lt_cm_to_lab) * phs%p_born_tot
          real_kinematics%p_born_lab%phs_point(1) &
            = phs%p_born_tot
        end if
      end if
    end associate
  end subroutine phs_fks_set_reference_frames

<phs fks: phs fks: TBP>+≡
  procedure :: i_phs_is_isr => phs_fks_i_phs_is_isr

<phs fks: procedures>+≡
  function phs_fks_i_phs_is_isr (phs, i_phs) result (is_isr)
    logical :: is_isr
    class(phs_fks_t), intent(in) :: phs
    integer, intent(in) :: i_phs
    is_isr = phs%phs_identifiers(i_phs)%emitter <= phs%generator%n_in
  end function phs_fks_i_phs_is_isr

```

19.11.1 Creation of the real phase space - FSR

At this point, the Born phase space has been generated, as well as the three random variables ξ , y and ϕ . The question is how the real phase space is generated for a final-state emission configuration. We work with two different sets of momenta, the Born configuration $\{\bar{k}_\oplus, \bar{k}_\ominus, \bar{k}_1, \dots, \bar{k}_n\}$ and the real configuration $\{k_\oplus, k_\ominus, k_1, \dots, k_n, k_{n+1}\}$. We define the momentum of the emitter to be on the n -th position and the momentum of the radiated particle to be at position $n+1$. The magnitude of the spatial component of k is denoted by \underline{k} .

For final-state emissions, it is $\bar{k}_\oplus = k_\oplus$ and $\bar{k}_\ominus = k_\ominus$. Thus, the center-of-mass systems coincide and it is

$$q = \sum_{i=1}^n \bar{k}_i = \sum_{i=1}^{n+1} k_i, \quad (19.65)$$

with $\vec{q} = 0$ and $q^2 = (q^0)^2$.

We want to construct the real phase space from the Born phase space using three random numbers. They are defined as follows:

- $\xi = \frac{2k_{n+1}^0}{\sqrt{s}} \in [0, \xi_{max}]$, where k_{n+1} denotes the four-momentum of the radiated particle.
- $y = \cos \theta = \frac{\vec{k}_n \cdot \vec{k}_{n+1}}{k_n k_{n+1}}$ is the splitting angle.
- The angle between the two splitting particles in the transversal plane, $\phi \in [0, 2\pi]$.

Further, $k_{rec} = \sum_{i=1}^{n-1} k_i$ denotes the sum of all recoiling momenta.

```

<phs fks: phs fks generator: TBP>+≡
  generic :: generate_fsr => generate_fsr_default, generate_fsr_resonances

<phs fks: phs fks generator: TBP>+≡
  procedure :: generate_fsr_default => phs_fks_generator_generate_fsr_default

<phs fks: procedures>+≡
  subroutine phs_fks_generator_generate_fsr_default (generator, emitter, i_phs, &
    p_born, p_real, xi_y_phi, no_jacobians)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: emitter, i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(inout), dimension(:) :: p_real
    real(default), intent(in), dimension(3), optional :: xi_y_phi
    logical, intent(in), optional :: no_jacobians
    real(default) :: q0

    call generator%generate_fsr_in (p_born, p_real)
    q0 = sum (p_born(1:generator%n_in))**1
    generator%i_fsr_first = generator%n_in + 1
    call generator%generate_fsr_out (emitter, i_phs, p_born, p_real, q0, &
      xi_y_phi = xi_y_phi, no_jacobians = no_jacobians)
    if (debug_active (D_PHASESPACE)) then
      call vector4_check_momentum_conservation (p_real, generator%n_in, &
        rel_smallness = 1000 * tiny_07, abs_smallness = tiny_07)
    end if
  end subroutine phs_fks_generator_generate_fsr_default

<phs fks: phs fks generator: TBP>+≡
  procedure :: generate_fsr_resonances => phs_fks_generator_generate_fsr_resonances

```

(phs fks: procedures)+≡

```

subroutine phs_fks_generator_generate_fsr_resonances (generator, &
    emitter, i_phs, i_con, p_born, p_real, xi_y_phi, no_jacobians)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: emitter, i_phs
    integer, intent(in) :: i_con
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(inout), dimension(:) :: p_real
    real(default), intent(in), dimension(3), optional :: xi_y_phi
    logical, intent(in), optional :: no_jacobians
    integer, dimension(:), allocatable :: resonance_list
    integer, dimension(size(p_born)) :: inv_resonance_list
    type(vector4_t), dimension(:), allocatable :: p_tmp_born
    type(vector4_t), dimension(:), allocatable :: p_tmp_real
    type(vector4_t) :: p_resonance
    real(default) :: q0
    integer :: i, j, nlegborn, nlegreal
    integer :: i_emitter
    type(lorentz_transformation_t) :: boost_to_resonance
    integer :: n_resonant_particles
    if (debug_on) call msg_debug2 (D_PHASESPACE, "phs_fks_generator_generate_fsr_resonances")
    nlegborn = size (p_born); nlegreal = nlegborn + 1
    allocate (resonance_list (size (generator%resonance_contributors(i_con)%c)))
    resonance_list = generator%resonance_contributors(i_con)%c
    n_resonant_particles = size (resonance_list)

    if (.not. any (resonance_list == emitter)) then
        call msg_fatal ("Emitter must be included in the resonance list!")
    else
        do i = 1, n_resonant_particles
            if (resonance_list (i) == emitter) i_emitter = i
        end do
    end if

    inv_resonance_list = &
        create_inverse_resonance_list (nlegborn, resonance_list)

    allocate (p_tmp_born (n_resonant_particles))
    allocate (p_tmp_real (n_resonant_particles + 1))
    p_tmp_born = vector4_null
    p_tmp_real = vector4_null
    j = 1
    do i = 1, n_resonant_particles
        p_tmp_born(j) = p_born(resonance_list(i))
        j = j + 1
    end do

    call generator%generate_fsr_in (p_born, p_real)

    p_resonance = generator%real_kinematics%xi_ref_momenta(i_con)
    q0 = p_resonance**1

    boost_to_resonance = inverse (boost (p_resonance, q0))
    p_tmp_born = boost_to_resonance * p_tmp_born

```

```

generator%i_fsr_first = 1
call generator%generate_fsr_out (emitter, i_phs, p_tmp_born, p_tmp_real, &
    q0, i_emitter, xi_y_phi)
p_tmp_real = inverse (boost_to_resonance) * p_tmp_real

do i = generator%n_in + 1, nlegborn
    if (any (resonance_list == i)) then
        p_real(i) = p_tmp_real(inv_resonance_list (i))
    else
        p_real(i) = p_born (i)
    end if
end do
p_real(nlegreal) = p_tmp_real (n_resonant_particles + 1)

if (debug_active (D_PHASESPACE)) then
    call vector4_check_momentum_conservation (p_real, generator%n_in, &
        rel_smallness = 1000 * tiny_07, abs_smallness = tiny_07)
end if

```

contains

```

function create_inverse_resonance_list (nlegborn, resonance_list) &
    result (inv_resonance_list)
    integer, intent(in) :: nlegborn
    integer, intent(in), dimension(:) :: resonance_list
    integer, dimension(nlegborn) :: inv_resonance_list
    integer :: i, j
    inv_resonance_list = 0
    j = 1
    do i = 1, nlegborn
        if (any (i == resonance_list)) then
            inv_resonance_list (i) = j
            j = j + 1
        end if
    end do
end function create_inverse_resonance_list

function boosted_energy () result (E)
    real(default) :: E
    type(vector4_t) :: p_boost
    p_boost = boost_to_resonance * p_resonance
    E = p_boost%p(0)
end function boosted_energy
end subroutine phs_fks_generator_generate_fsr_resonances

```

<phs fks: phs fks generator: TBP>+≡

```

procedure :: generate_fsr_threshold => phs_fks_generator_generate_fsr_threshold

```

<phs fks: procedures>+≡

```

subroutine phs_fks_generator_generate_fsr_threshold (generator, &
    emitter, i_phs, p_born, p_real, xi_y_phi)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: emitter, i_phs

```

```

type(vector4_t), intent(in), dimension(:) :: p_born
type(vector4_t), intent(inout), dimension(:) :: p_real
real(default), intent(in), dimension(3), optional :: xi_y_phi
type(vector4_t), dimension(2) :: p_tmp_born
type(vector4_t), dimension(3) :: p_tmp_real
integer :: nlegborn, nlegreal
type(vector4_t) :: p_top
real(default) :: q0
type(lorentz_transformation_t) :: boost_to_top
integer :: leg, other_leg
real(default) :: sqrts, mtop
if (debug_on) call msg_debug2 (D_PHASESPACE, "phs_fks_generator_generate_fsr_resonances")
nlegborn = size (p_born); nlegreal = nlegborn + 1

leg = thr_leg(emitter); other_leg = 3 - leg

p_tmp_born(1) = p_born (ass_boson(leg))
p_tmp_born(2) = p_born (ass_quark(leg))

call generator%generate_fsr_in (p_born, p_real)

p_top = generator%real_kinematics%xi_ref_momenta(leg)

q0 = p_top**1
sqrts = two * p_born(1)%p(0)
mtop = m1s_to_mpole (sqrts)
if (sqrts**2 - four * mtop**2 > zero) then
    boost_to_top = inverse (boost (p_top, q0))
else
    boost_to_top = identity
end if
p_tmp_born = boost_to_top * p_tmp_born

generator%i_fsr_first = 1
call generator%generate_fsr_out (emitter, i_phs, p_tmp_born, &
    p_tmp_real, q0, 2, xi_y_phi)
p_tmp_real = inverse (boost_to_top) * p_tmp_real

p_real(ass_boson(leg)) = p_tmp_real(1)
p_real(ass_quark(leg)) = p_tmp_real(2)
p_real(ass_boson(other_leg)) = p_born(ass_boson(other_leg))
p_real(ass_quark(other_leg)) = p_born(ass_quark(other_leg))
p_real(THR_POS_GLUON) = p_tmp_real(3)

end subroutine phs_fks_generator_generate_fsr_threshold

<phs fks: phs fks generator: TBP>+≡
    procedure :: generate_fsr_in => phs_fks_generator_generate_fsr_in

<phs fks: procedures>+≡
    subroutine phs_fks_generator_generate_fsr_in (generator, p_born, p_real)
        class(phs_fks_generator_t), intent(inout) :: generator
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(inout), dimension(:) :: p_real

```

```

integer :: i
do i = 1, generator%n_in
    p_real(i) = p_born(i)
end do
end subroutine phs_fks_generator_generate_fsr_in

```

<phs fks: phs fks generator: TBP>+≡

```

procedure :: generate_fsr_out => phs_fks_generator_generate_fsr_out

```

<phs fks: procedures>+≡

```

subroutine phs_fks_generator_generate_fsr_out (generator, &
    emitter, i_phs, p_born, p_real, q0, p_emitter_index, xi_y_phi, no_jacobians)
class(phs_fks_generator_t), intent(inout) :: generator
integer, intent(in) :: emitter, i_phs
type(vector4_t), intent(in), dimension(:) :: p_born
type(vector4_t), intent(inout), dimension(:) :: p_real
real(default), intent(in) :: q0
integer, intent(in), optional :: p_emitter_index
real(default), intent(in), dimension(3), optional :: xi_y_phi
logical, intent(in), optional :: no_jacobians
real(default) :: xi, y, phi
integer :: nlegborn, nlegreal
real(default) :: uk_np1, uk_n
real(default) :: uk_rec, k_rec0
type(vector3_t) :: k_n_born, k
real(default) :: uk_n_born, uk, k2, k0_n
real(default) :: cpsi, beta
type(vector3_t) :: vec, vec_orth
type(lorentz_transformation_t) :: rot
integer :: i, p_em
logical :: compute_jac
p_em = emitter; if (present (p_emitter_index)) p_em = p_emitter_index
compute_jac = .true.
if (present (no_jacobians)) compute_jac = .not. no_jacobians
if (generator%i_fsr_first < 0) &
    call msg_fatal ("FSR generator is called for outgoing particles but "&
        &"i_fsr_first is not set!")

if (present (xi_y_phi)) then
    xi = xi_y_phi(I_XI)
    y = xi_y_phi(I_Y)
    phi = xi_y_phi(I_PHI)
else
    associate (rad_var => generator%real_kinematics)
        xi = rad_var%xi_tilde
        if (rad_var%supply_xi_max) xi = xi * rad_var%xi_max(i_phs)
        y = rad_var%y(i_phs)
        phi = rad_var%phi
    end associate
end if

nlegborn = size (p_born)
nlegreal = nlegborn + 1
generator%E_gluon = q0 * xi / two

```



```

uk_np1 = generator%E_gluon
k_n_born = p_born(p_em)%p(1:3)
uk_n_born = k_n_born**1

generator%mmrec2 = (q0 - p_born(p_em)%p(0))**2 &
- space_part_norm(p_born(p_em))**2
if (generator%is_massive(emitter)) then
  call generator%compute_emitter_kinematics (y, emitter, &
    i_phs, q0, k0_n, uk_n, uk, compute_jac)
else
  call generator%compute_emitter_kinematics (y, q0, uk_n, uk)
  generator%real_kinematics%y_soft(i_phs) = y
  k0_n = uk_n
end if

if (debug_on) call msg_debug2 (D_PHASESPACE, "phs_fks_generator_generate_fsr_out")
call debug_input_values ()

vec = uk_n / uk_n_born * k_n_born
vec_orth = create_orthogonal (vec)
p_real(p_em)%p(0) = k0_n
p_real(p_em)%p(1:3) = vec%p(1:3)
cpsi = (uk_n**2 + uk**2 - uk_np1**2) / (two * uk_n * uk)
!!! This is to catch the case where cpsi = 1, but numerically
!!! turns out to be slightly larger than 1.
call check_cpsi_bound (cpsi)
rot = rotation (cpsi, - sqrt (one - cpsi**2), vec_orth)
p_real(p_em) = rot * p_real(p_em)
vec = uk_np1 / uk_n_born * k_n_born
vec_orth = create_orthogonal (vec)
p_real(nlegreal)%p(0) = uk_np1
p_real(nlegreal)%p(1:3) = vec%p(1:3)
cpsi = (uk_np1**2 + uk**2 - uk_n**2) / (two * uk_np1 * uk)
call check_cpsi_bound (cpsi)
rot = rotation (cpsi, sqrt (one - cpsi**2), vec_orth)
p_real(nlegreal) = rot * p_real(nlegreal)
call construct_recoiling_momenta ()
if (compute_jac) call compute_jacobians ()

contains

<phs fks: generator generate_fsr_out_procedures>

end subroutine phs_fks_generator_generate_fsr_out

<phs fks: generator generate_fsr_out_procedures>≡
subroutine debug_input_values ()
  if (debug2_active (D_PHASESPACE)) then
    call generator%write ()
    print *, 'emitter = ', emitter
    print *, 'p_born:'
    call vector4_write_set (p_born)
    print *, 'p_real:'
    call vector4_write_set (p_real)
  end if
end subroutine

```

```

      print *, 'q0 = ', q0
      if (present(p_emitter_index)) then
        print *, 'p_emitter_index = ', p_emitter_index
      else
        print *, 'p_emitter_index not given'
      end if
    end if
  end if
end subroutine debug_input_values

```

(phs fks: generator generate fsr out procedures)+≡

```

subroutine check_cpsi_bound (cpsi)
  real(default), intent(inout) :: cpsi
  if (cpsi > one) then
    cpsi = one
  else if (cpsi < -one) then
    cpsi = - one
  end if
end subroutine check_cpsi_bound

```

Construction of the recoiling momenta. The reshuffling of momenta must not change the invariant mass of the recoiling system, which means $k_{\text{rec}}^2 = k_{\text{rec}}^{-2}$. Therefore, the momenta are related by a boost, $\bar{k}_i = \Lambda k_i$. The boost parameter is

$$\beta = \frac{q^2 - (k_{\text{rec}}^0 + k_{\text{rec}})^2}{q^2 + (k_{\text{rec}}^0 + k_{\text{rec}})^2}$$

(phs fks: generator generate fsr out procedures)+≡

```

subroutine construct_recoiling_momenta ()
  type(lorentz_transformation_t) :: lambda
  k_rec0 = q0 - p_real(p_em)%p(0) - p_real(nlegreal)%p(0)
  if (k_rec0**2 > generator%mrec2) then
    uk_rec = sqrt (k_rec0**2 - generator%mrec2)
  else
    uk_rec = 0
  end if
  if (generator%is_massive(emitter)) then
    beta = compute_beta (q0**2, k_rec0, uk_rec, &
      p_born(p_em)%p(0), uk_n_born)
  else
    beta = compute_beta (q0**2, k_rec0, uk_rec)
  end if
  k = p_real(p_em)%p(1:3) + p_real(nlegreal)%p(1:3)
  vec%p(1:3) = one / uk * k%p(1:3)
  lambda = boost (beta / sqrt(one - beta**2), vec)
  do i = generator%i_fsr_first, nlegborn
    if (i /= p_em) then
      p_real(i) = lambda * p_born(i)
    end if
  end do
  vec%p(1:3) = p_born(p_em)%p(1:3) / uk_n_born
  rot = rotation (cos(phi), sin(phi), vec)
  p_real(nlegreal) = rot * p_real(nlegreal)
  p_real(p_em) = rot * p_real(p_em)

```

```
end subroutine construct_recoiling_momenta
```

The factor $\frac{g^2}{(4\pi)^3}$ is not included here since it is supplied during phase space generation. Also, we already divide by ξ .

(phs fks: generator generate_fsr_out_procedures)+≡

```
subroutine compute_jacobians ()
  associate (jac => generator%real_kinematics%jac(i_phs))
    if (generator%is_massive(emitter)) then
      jac%jac(1) = jac%jac(1) * four / q0 / uk_n_born / xi
    else
      k2 = two * uk_n * uk_np1 * (one - y)
      jac%jac(1) = uk_n**2 / uk_n_born / (uk_n - k2 / (two * q0))
    end if
    jac%jac(2) = one
    jac%jac(3) = one - xi / two * q0 / uk_n_born
  end associate
end subroutine compute_jacobians
```

(phs fks: phs fks: TBP)+≡

```
procedure :: generate_fsr_in => phs_fks_generate_fsr_in
```

(phs fks: procedures)+≡

```
subroutine phs_fks_generate_fsr_in (phs)
  class(phs_fks_t), intent(inout) :: phs
  type(vector4_t), dimension(:), allocatable :: p
  p = phs%generator%real_kinematics%p_born_lab%get_momenta (1, phs%generator%n_in)
end subroutine phs_fks_generate_fsr_in
```

(phs fks: phs fks: TBP)+≡

```
procedure :: generate_fsr => phs_fks_generate_fsr
```

(phs fks: procedures)+≡

```
subroutine phs_fks_generate_fsr (phs, emitter, i_phs, p_real, i_con, &
  xi_y_phi, no_jacobians)
  class(phs_fks_t), intent(inout) :: phs
  integer, intent(in) :: emitter, i_phs
  type(vector4_t), intent(inout), dimension(:) :: p_real
  integer, intent(in), optional :: i_con
  real(default), intent(in), dimension(3), optional :: xi_y_phi
  logical, intent(in), optional :: no_jacobians
  type(vector4_t), dimension(:), allocatable :: p
  associate (generator => phs%generator)
    p = generator%real_kinematics%p_born_cms%phs_point(1)
    generator%real_kinematics%supply_xi_max = .true.
    if (present (i_con)) then
      call generator%generate_fsr (emitter, i_phs, i_con, p, p_real, &
        xi_y_phi, no_jacobians)
    else
      call generator%generate_fsr (emitter, i_phs, p, p_real, &
        xi_y_phi, no_jacobians)
    end if
    generator%real_kinematics%p_real_cms%phs_point(i_phs) = p_real
    if (.not. phs%config%lab_is_cm) p_real = phs%lt_cm_to_lab * p_real
  end associate
end subroutine
```

```

        generator%real_kinematics%p_real_lab%phs_point(i_phs) = p_real
    end associate
end subroutine phs_fks_generate_fsr

<phs fks: phs fks: TBP>+≡
    procedure :: get_onshell_projected_momenta => phs_fks_get_onshell_projected_momenta

<phs fks: procedures>+≡
    pure function phs_fks_get_onshell_projected_momenta (phs) result (p)
        type(vector4_t), dimension(:), allocatable :: p
        class(phs_fks_t), intent(in) :: phs
        p = phs%generator%real_kinematics%p_born_onshell%phs_point(1)
    end function phs_fks_get_onshell_projected_momenta

<phs fks: phs fks: TBP>+≡
    procedure :: generate_fsr_threshold => phs_fks_generate_fsr_threshold

<phs fks: procedures>+≡
    subroutine phs_fks_generate_fsr_threshold (phs, emitter, i_phs, p_real)
        class(phs_fks_t), intent(inout) :: phs
        integer, intent(in) :: emitter, i_phs
        type(vector4_t), intent(inout), dimension(:), optional :: p_real
        type(vector4_t), dimension(:), allocatable :: p_born
        type(vector4_t), dimension(:), allocatable :: pp
        integer :: leg
        associate (generator => phs%generator)
            generator%real_kinematics%supply_xi_max = .true.
            allocate (p_born (1 : generator%real_kinematics%p_born_cms%get_n_particles()))
            p_born = generator%real_kinematics%p_born_onshell%get_momenta (1)
            allocate (pp (size (p_born) + 1))
            call generator%generate_fsr_threshold (emitter, i_phs, p_born, pp)
            leg = thr_leg (emitter)
            call generator%real_kinematics%p_real_onshell(leg)%set_momenta (i_phs, pp)
            if (present (p_real)) p_real = pp
        end associate
    end subroutine phs_fks_generate_fsr_threshold

<phs fks: phs fks: TBP>+≡
    generic :: compute_xi_max => compute_xi_max_internal, compute_xi_max_with_output
    procedure :: compute_xi_max_internal => phs_fks_compute_xi_max_internal

<phs fks: procedures>+≡
    subroutine phs_fks_compute_xi_max_internal (phs, p, threshold)
        class(phs_fks_t), intent(inout) :: phs
        type(vector4_t), intent(in), dimension(:) :: p
        logical, intent(in) :: threshold
        integer :: i_phs, i_con, emitter
        do i_phs = 1, size (phs%phs_identifiers)
            associate (phs_id => phs%phs_identifiers(i_phs), generator => phs%generator)
                emitter = phs_id%emitter
                if (threshold) then
                    call generator%compute_xi_max (emitter, i_phs, p, &
                        generator%real_kinematics%xi_max(i_phs), i_con = thr_leg(emitter))
                else if (allocated (phs_id%contributors)) then

```

```

        do i_con = 1, size (phs_id%contributors)
            call generator%compute_xi_max (emitter, i_phs, p, &
                generator%real_kinematics%xi_max(i_phs), i_con = 1)
        end do
    else
        call generator%compute_xi_max (emitter, i_phs, p, &
            generator%real_kinematics%xi_max(i_phs))
    end if
end associate
end do
end subroutine phs_fks_compute_xi_max_internal

```

<phs fks: phs fks: TBP>+≡

```

    procedure :: compute_xi_max_with_output => phs_fks_compute_xi_max_with_output

```

<phs fks: procedures>+≡

```

    subroutine phs_fks_compute_xi_max_with_output (phs, emitter, i_phs, y, p, xi_max)
        class(phs_fks_t), intent(inout) :: phs
        integer, intent(in) :: i_phs, emitter
        real(default), intent(in) :: y
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), intent(out) :: xi_max
        call phs%generator%compute_xi_max (emitter, i_phs, p, xi_max, y_in = y)
    end subroutine phs_fks_compute_xi_max_with_output

```

<phs fks: phs fks generator: TBP>+≡

```

    generic :: compute_emitter_kinematics => &
        compute_emitter_kinematics_massless, &
        compute_emitter_kinematics_massive
    procedure :: compute_emitter_kinematics_massless => &
        phs_fks_generator_compute_emitter_kinematics_massless
    procedure :: compute_emitter_kinematics_massive => &
        phs_fks_generator_compute_emitter_kinematics_massive

```

<phs fks: procedures>+≡

```

    subroutine phs_fks_generator_compute_emitter_kinematics_massless &
        (generator, y, q0, uk_em, uk)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: y, q0
        real(default), intent(out) :: uk_em, uk
        real(default) :: k0_np1, q2

        k0_np1 = generator%E_gluon
        q2 = q0**2

        uk_em = (q2 - generator%mprec2 - two * q0 * k0_np1) / (two * (q0 - k0_np1 * (one - y)))
        uk = sqrt (uk_em**2 + k0_np1**2 + two * uk_em * k0_np1 * y)
    end subroutine phs_fks_generator_compute_emitter_kinematics_massless

    subroutine phs_fks_generator_compute_emitter_kinematics_massive &
        (generator, y, em, i_phs, q0, k0_em, uk_em, uk, compute_jac)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: y
        integer, intent(in) :: em, i_phs

```

```

real(default), intent(in) :: q0
real(default), intent(inout) :: k0_em, uk_em, uk
logical, intent(in) :: compute_jac
real(default) :: k0_np1, q2, mrec2, m2
real(default) :: k0_rec_max, k0_em_max, k0_rec, uk_rec
real(default) :: z, z1, z2

k0_np1 = generator%E_gluon
q2 = q0**2
mrec2 = generator%mrec2
m2 = generator%m2(em)

k0_rec_max = (q2 - m2 + mrec2) / (two * q0)
k0_em_max = (q2 + m2 - mrec2) / (two * q0)
z1 = (k0_rec_max + sqrt(k0_rec_max**2 - mrec2)) / q0
z2 = (k0_rec_max - sqrt(k0_rec_max**2 - mrec2)) / q0
z = z2 - (z2 - z1) * (one + y) / two
k0_em = k0_em_max - k0_np1 * z
k0_rec = q0 - k0_np1 - k0_em
uk_em = sqrt(k0_em**2 - m2)
uk_rec = sqrt(k0_rec**2 - mrec2)
uk = uk_rec
if (compute_jac) &
    generator%real_kinematics%jac(i_phs)%jac = q0 * (z1 - z2) / four * k0_np1
generator%real_kinematics%y_soft(i_phs) = &
    (two * q2 * z - q2 - mrec2 + m2) / (sqrt(k0_em_max**2 - m2) * q0) / two
end subroutine phs_fks_generator_compute_emitter_kinematics_massive

```

(phs fks: procedures)+≡

```

function recompute_xi_max (q0, mrec2, m2, y) result (xi_max)
    real(default) :: xi_max
    real(default), intent(in) :: q0, mrec2, m2, y
    real(default) :: q2, k0_np1_max, k0_rec_max
    real(default) :: z1, z2, z
    q2 = q0**2
    k0_rec_max = (q2 - m2 + mrec2) / (two * q0)
    z1 = (k0_rec_max + sqrt(k0_rec_max**2 - mrec2)) / q0
    z2 = (k0_rec_max - sqrt(k0_rec_max**2 - mrec2)) / q0
    z = z2 - (z2 - z1) * (one + y) / 2
    k0_np1_max = - (q2 * z**2 - two * q0 * k0_rec_max * z + mrec2) / (two * q0 * z * (one - z))
    xi_max = two * k0_np1_max / q0
end function recompute_xi_max

```

(phs fks: procedures)+≡

```

function compute_beta_massless (q2, k0_rec, uk_rec) result (beta)
    real(default), intent(in) :: q2, k0_rec, uk_rec
    real(default) :: beta
    beta = (q2 - (k0_rec + uk_rec)**2) / (q2 + (k0_rec + uk_rec)**2)
end function compute_beta_massless

function compute_beta_massive (q2, k0_rec, uk_rec, &
    k0_em_born, uk_em_born) result (beta)
    real(default), intent(in) :: q2, k0_rec, uk_rec

```

```

real(default), intent(in) :: k0_em_born, uk_em_born
real(default) :: beta
real(default) :: k0_rec_born, uk_rec_born, alpha
k0_rec_born = sqrt(q2) - k0_em_born
uk_rec_born = uk_em_born
alpha = (k0_rec + uk_rec) / (k0_rec_born + uk_rec_born)
beta = (one - alpha**2) / (one + alpha**2)
end function compute_beta_massive

```

The momentum of the radiated particle is computed according to

$$\underline{k}_n = \frac{q^2 - M_{\text{rec}}^2 - 2q^0 \underline{k}_{n+1}}{2(q^0 - \underline{k}_{n+1}(1 - y))}, \quad (19.66)$$

with $k = k_n + k_{n+1}$ and $M_{\text{rec}}^2 = k_{\text{rec}}^2 = (q - k)^2$. Because of $\bar{\mathbf{k}}_n \parallel \mathbf{k}_n + \mathbf{k}_{n+1}$ we find $M_{\text{rec}}^2 = (q - \bar{k}_n)^2$. Equation 19.66 follows from the fact that $(\mathbf{k} - \mathbf{k}_n)^2 = \mathbf{k}_{n+1}^2$, which is equivalent to $\mathbf{k}_n \cdot \mathbf{k} = \frac{1}{2}(\underline{k}_n^2 + \underline{k}^2 - \underline{k}_{n+1}^2)$. \mathbf{k}_n and \mathbf{k}_{n+1} are obtained by first setting up vectors parallel to $\bar{\mathbf{k}}_n$,

$$\mathbf{k}'_n = \underline{k}_n \frac{\bar{\mathbf{k}}_n}{\bar{k}_n}, \quad \mathbf{k}'_{n+1} = \underline{k}_{n+1} \frac{\bar{\mathbf{k}}_n}{\bar{k}_n},$$

and then rotating these vectors by an amount of $\cos \psi_n = \frac{\mathbf{k}_n \cdot \mathbf{k}}{\bar{k}_n \underline{k}}$. The emitted particle cannot have more momentum than the emitter has in the Born phase space. Thus, there is an upper bound for ξ , determined by the condition $k_{n+1}^0 = \bar{k}_n$, which is equal to

$$\xi_{\text{max}} = \frac{2}{\bar{k}_n} q^0.$$

(phs fks: procedures)+≡

```

pure function get_xi_max_fsr_massless (p_born, q0, emitter) result (xi_max)
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: q0
  integer, intent(in) :: emitter
  real(default) :: xi_max
  real(default) :: uk_n_born
  uk_n_born = space_part_norm (p_born(emitter))
  xi_max = two * uk_n_born / q0
end function get_xi_max_fsr_massless

```

The computation of ξ_{max} for massive emitters is described in arXiv:1202.0465. Let's recapitulate it here.

We consider the Dalitz-domain created by k_{n+1}^0 , k_n^0 and k_{rec}^0 and introduce the parameterization

$$k_n^0 = \bar{k}_n^0 - z k_{n+1}^0$$

Then, for each value of z , there exists a maximum value of \underline{k}_{n+1} from which ξ_{max} can be extracted via $\xi_{\text{max}} = 2k_{n+1}^0/q$. It is determined by the condition

$$\underline{k}_{n+1} \pm \underline{k}_n \pm \underline{k}_{\text{rec}} = 0.$$

This can be manipulated to yield

$$(\underline{k}_{n+1}^2 + \underline{k}_n^2 - \underline{k}_{\text{rec}}^2)^2 = 4\underline{k}_{n+1}^2 \underline{k}_n^2.$$

Here we can use $k_n^2 = (k_n^0)^2 - m^2$ and $k_{\text{rec}}^2 = (q - k_n^0 - k_{n+1}^0)^2 - M_{\text{rec}}^2$, as well as the above parameterization of k_n^0 , to obtain

$$4k_{n+1}^2 (2k_{n+1} q z (1 - z) + q^2 z^2 - 2q \bar{k}_{\text{rec}}^0 z + M_{\text{rec}}^2) = 0.$$

Solving for k_{n+1}^0 gives

$$k_{n+1}^0 = \frac{2q \bar{k}_{\text{rec}}^0 z - q^2 z^2 - M_{\text{rec}}^2}{2q z (1 - z)}. \quad (19.67)$$

It is still open how to compute z . For this, consider that the right-hand-side of equation (19.67) vanishes for

$$z_{1,2} = \left(\bar{k}_{\text{rec}}^0 \pm \sqrt{(\bar{k}_{\text{rec}}^0)^2 - M_{\text{rec}}^2} \right) / q,$$

which corresponds to the borders of the Dalitz-region where the gluon momentum vanishes. Thus we define

$$z = z_2 - \frac{1}{2}(z_2 - z_1)(1 + y).$$

(phs fks: procedures)+≡

```
pure function get_xi_max_fsr_massive (p_born, q0, emitter, m2, y) result (xi_max)
  real(default) :: xi_max
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: q0
  integer, intent(in) :: emitter
  real(default), intent(in) :: m2, y
  real(default) :: mrec2
  real(default) :: k0_rec_max
  real(default) :: z, z1, z2
  real(default) :: k0_np1_max
  associate (p => p_born(emitter)%p)
    mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
  end associate
  call compute_dalitz_bounds (q0, m2, mrec2, z1, z2, k0_rec_max)
  z = z2 - (z2 - z1) * (one + y) / two
  k0_np1_max = - (q0**2 * z**2 - two * q0 * k0_rec_max * z + mrec2) &
    / (two * q0 * z * (one - z))
  xi_max = two * k0_np1_max / q0
end function get_xi_max_fsr_massive
```

(phs fks: parameters)+≡

```
integer, parameter, public :: I_PLUS = 1
integer, parameter, public :: I_MINUS = 2
```

Computes ξ_{max} in the case of ISR as documented in eq. 27.39.

(phs fks: procedures)+≡

```
function get_xi_max_isr (xb, y) result (xi_max)
  real(default) :: xi_max
  real(default), dimension(2), intent(in) :: xb
  real(default), intent(in) :: y
  xi_max = one - max (xi_max_isr_plus (xb(I_PLUS), y), xi_max_isr_minus (xb(I_MINUS), y))
```



```

contains
  function xi_max_isr_plus (x, y)
    real(default) :: xi_max_isr_plus
    real(default), intent(in) :: x, y
    real(default) :: deno
    deno = sqrt ((one + x**2)**2 * (one - y)**2 + 16 * y * x**2) + (one - y) * (1 - x**2)
    xi_max_isr_plus = two * (one + y) * x**2 / deno
  end function xi_max_isr_plus

  function xi_max_isr_minus (x, y)
    real(default) :: xi_max_isr_minus
    real(default), intent(in) :: x, y
    real(default) :: deno
    deno = sqrt ((one + x**2)**2 * (one + y)**2 - 16 * y * x**2) + (one + y) * (1 - x**2)
    xi_max_isr_minus = two * (one - y) * x**2 / deno
  end function xi_max_isr_minus
end function get_xi_max_isr

```

```

<phs fks: procedures>+≡
recursive function get_xi_max_isr_decay (p) result (xi_max)
  real(default) :: xi_max
  type(vector4_t), dimension(:), intent(in) :: p
  integer :: n_tot
  type(vector4_t), dimension(:), allocatable :: p_dec_new
  n_tot = size (p)
  if (n_tot == 3) then
    xi_max = xi_max_one_to_two (p(1), p(2), p(3))
  else
    allocate (p_dec_new (n_tot - 1))
    p_dec_new(1) = sum (p (3 : ))
    p_dec_new(2 : n_tot - 1) = p (3 : n_tot)
    xi_max = min (xi_max_one_to_two (p(1), p(2), sum(p(3 : ))), &
      get_xi_max_isr_decay (p_dec_new))
  end if
contains
  function xi_max_one_to_two (p_in, p_out1, p_out2) result (xi_max)
    real(default) :: xi_max
    type(vector4_t), intent(in) :: p_in, p_out1, p_out2
    real(default) :: m_in, m_out1, m_out2
    m_in = p_in**1
    m_out1 = p_out1**1; m_out2 = p_out2**1
    xi_max = one - (m_out1 + m_out2)**2 / m_in**2
  end function xi_max_one_to_two
end function get_xi_max_isr_decay

```

19.11.2 Creation of the real phase space - ISR

```

<phs fks: phs fks: TBP>+≡
  procedure :: generate_isr => phs_fks_generate_isr

<phs fks: procedures>+≡
  subroutine phs_fks_generate_isr (phs, i_phs, p_real)
    class(phs_fks_t), intent(inout) :: phs

```

```

integer, intent(in) :: i_phs
type(vector4_t), intent(inout), dimension(:) :: p_real
type(vector4_t) :: p0, p1
type(lorentz_transformation_t) :: lt
real(default) :: sqrts_hat
type(vector4_t), dimension(:), allocatable :: p_work

associate (generator => phs%generator)
  select case (generator%n_in)
  case (1)
    p_work = generator%real_kinematics%p_born_cms%phs_point(1)
    call generator%generate_isr_fixed_beam_energy (i_phs, p_work, p_real)
    phs%config%lab_is_cm = .true.
  case (2)
    select case (generator%isr_kinematics%isr_mode)
    case (SQRTS_FIXED)
      p_work = generator%real_kinematics%p_born_cms%phs_point(1)
      call generator%generate_isr_fixed_beam_energy (i_phs, p_work, p_real)
    case (SQRTS_VAR)
      p_work = generator%real_kinematics%p_born_lab%phs_point(1)
      call generator%generate_isr (i_phs, p_work, p_real)
    end select
  end select
  generator%real_kinematics%p_real_lab%phs_point(i_phs) = p_real
  if (.not. phs%config%lab_is_cm) then
    sqrts_hat = (p_real(1) + p_real(2))*1
    p0 = p_real(1) + p_real(2)
    lt = boost (p0, sqrts_hat)
    p1 = inverse(lt) * p_real(1)
    lt = lt * rotation_to_2nd (3, space_part (p1))
    phs%generator%real_kinematics%p_real_cms%phs_point(i_phs) &
      = inverse (lt) * p_real
  else
    phs%generator%real_kinematics%p_real_cms%phs_point(i_phs) &
      = p_real
  end if
end associate
end subroutine phs_fks_generate_isr

```

The real phase space for an initial-state emission involved in a decay process is generated by first setting the gluon momentum like in the scattering case by using its angular coordinates y and ϕ and then adjusting the gluon energy with ξ . The emitter momentum is kept identical to the Born case, i.e. $p_{\text{in}} = \bar{p}_{\text{in}}$, so that after the emission it has momentum $p_{\text{virt}} = p_{\text{in}} - p_g$ and invariant mass $m^2 = p_{\text{virt}}^2$. Note that the final state momenta have to remain on-shell, so that $p_1^2 = \bar{p}_1^2 = m_1^2$ and $p_2^2 = \bar{p}_2^2 = m_2^2$. Let Λ be the boost from into the rest frame of the emitter after emission, i.e. $\Lambda p_{\text{virt}} = (m, 0, 0, 0)$. In this reference frame, the spatial components of the final-state momenta sum up to zero, and their magnitude is

$$p = \frac{\sqrt{\lambda(m^2, m_1^2, m_2^2)}}{2m},$$

a fact already used in the evaluation of the phase space trees of `phs_forest`.

Obviously, from this, the final-state energies can be deferred via $E_i^2 = m_i^2 - p^2$. In the next step, the $p_{1,2}$ are set up as vectors $(E, 0, 0, \pm p)$ along the z-axis and then rotated about the same azimuthal and polar angles as in the Born system. Finally, the momenta are boosted out of the rest frame by multiplying with Λ .

```

<phs fks: phs fks generator: TBP>+≡
  procedure :: generate_isr_fixed_beam_energy => &
    phs_fks_generator_generate_isr_fixed_beam_energy

<phs fks: procedures>+≡
  subroutine phs_fks_generator_generate_isr_fixed_beam_energy &
    (generator, i_phs, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(inout), dimension(:) :: p_real
    real(default) :: xi_max, xi, y, phi
    integer :: nlegborn, nlegreal, i
    real(default) :: k0_np1
    real(default) :: msq_in
    type(vector4_t) :: p_virt
    real(default) :: jac_real

    associate (rad_var => generator%real_kinematics)
      xi_max = rad_var%xi_max(i_phs)
      xi = rad_var%xi_tilde * xi_max
      y = rad_var%y(i_phs)
      phi = rad_var%phi
      rad_var%y_soft(i_phs) = y
    end associate

    nlegborn = size (p_born)
    nlegreal = nlegborn + 1

    msq_in = sum (p_born(1:generator%n_in))**2
    generator%real_kinematics%jac(i_phs)%jac = one

    p_real(1) = p_born(1)
    if (generator%n_in > 1) p_real(2) = p_born(2)
    k0_np1 = zero
    do i = 1, generator%n_in
      k0_np1 = k0_np1 + p_real(i)%p(0) * xi / two
    end do
    p_real(nlegreal)%p(0) = k0_np1
    p_real(nlegreal)%p(1) = k0_np1 * sqrt(one - y**2) * sin(phi)
    p_real(nlegreal)%p(2) = k0_np1 * sqrt(one - y**2) * cos(phi)
    p_real(nlegreal)%p(3) = k0_np1 * y

    p_virt = sum (p_real(1:generator%n_in)) - p_real(nlegreal)

    jac_real = one
    call generate_on_shell_decay (p_virt, &
      p_born(generator%n_in + 1 : nlegborn), p_real(generator%n_in + 1 : nlegreal - 1), &
      1, msq_in, jac_real)

```

```

        associate (jac => generator%real_kinematics%jac(i_phs))
            jac%jac(1) = jac_real
            jac%jac(2) = one
        end associate

end subroutine phs_fks_generator_generate_isr_fixed_beam_energy

<phs fks: phs fks generator: TBP>+≡
    procedure :: generate_isr_factorized => phs_fks_generator_generate_isr_factorized

<phs fks: procedures>+≡
    subroutine phs_fks_generator_generate_isr_factorized (generator, i_phs, emitter, p_born, p_real)
        class(phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in) :: i_phs, emitter
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(inout), dimension(:) :: p_real
        type(vector4_t), dimension(3) :: p_tmp_born
        type(vector4_t), dimension(4) :: p_tmp_real
        type(vector4_t) :: p_top
        type(lorentz_transformation_t) :: boost_to_rest_frame
        integer, parameter :: nlegreal = 7 !!! Factorized phase space so far only required for ee -> b

        p_tmp_born = vector4_null; p_tmp_real = vector4_null
        p_real(1:2) = p_born(1:2)
        if (emitter == THR_POS_B) then
            p_top = p_born (THR_POS_WP) + p_born (THR_POS_B)
            p_tmp_born(2) = p_born (THR_POS_WP)
            p_tmp_born(3) = p_born (THR_POS_B)
        else if (emitter == THR_POS_BBAR) then
            p_top = p_born (THR_POS_WM) + p_born (THR_POS_BBAR)
            p_tmp_born(2) = p_born (THR_POS_WM)
            p_tmp_born(3) = p_born (THR_POS_BBAR)
        else
            call msg_fatal ("Threshold computation requires emitters to be at position 5 and 6 " // &
                "Please check if your process specification fulfills this requirement.")
        end if
        p_tmp_born (1) = p_top
        boost_to_rest_frame = inverse (boost (p_top, p_top**1))
        p_tmp_born = boost_to_rest_frame * p_tmp_born
        call generator%compute_xi_max_isr_factorized (i_phs, p_tmp_born)
        call generator%generate_isr_fixed_beam_energy (i_phs, p_tmp_born, p_tmp_real)
        p_tmp_real = inverse (boost_to_rest_frame) * p_tmp_real
        if (emitter == THR_POS_B) then
            p_real(THR_POS_WP) = p_tmp_real(2)
            p_real(THR_POS_B) = p_tmp_real(3)
            p_real(THR_POS_WM) = p_born(THR_POS_WM)
            p_real(THR_POS_BBAR) = p_born(THR_POS_BBAR)
        !!! Exception has been handled above
        else
            p_real(THR_POS_WM) = p_tmp_real(2)
            p_real(THR_POS_BBAR) = p_tmp_real(3)
            p_real(THR_POS_WP) = p_born(THR_POS_WP)
            p_real(THR_POS_B) = p_born(THR_POS_B)
        end if
    end if
end subroutine

```

```

    p_real(nlegreal) = p_tmp_real(4)
end subroutine phs_fks_generator_generate_isr_factorized

```

Construction of the real momenta `p_real` in case of ISR. Follows the discussion in [0709.2092] sec. 5.1. The sequence of Lorentz boosts required to construct `p_real` from `p_born` is as follows:

- We construct the IS momenta of `p_real` from the Born momenta via rescaling: $\mathbf{p_real}(1:2) = \frac{x}{x} \cdot \mathbf{p_born}(1:2)$. If the Born momenta are imported in the lab frame, these will define the real lab frame.
- We construct the momentum of the radiated particle in the real CMS: $k_{n+1} = \frac{s\xi}{2} \cdot (1, \sin(\theta) \sin(\phi), \sin(\theta) \cos(\phi), \cos(\theta))$
- 0. We first boost the momentum of the radiated particle from the real CMS to the real lab frame determined from `p_real(1:2)`.
- 1. We initialize the non-radiated real FS momenta by a longitudinal boost of `p_born` to a system with zero rapidity, i.e. zero longitudinal momentum. This is \mathbb{B}_L .
- 2. We boost these momenta in a transverse direction to compensate the transverse momentum of the radiation. This is \mathbb{B}_T . Note: we switched \mathbb{B}_T and \mathbb{B}_T^{-1} in Eq. (5.16) and their definition w.r.t. [0709.2092].
- 3. We restore longitudinal momentum conservation by applying the inverse boost of \mathbb{B}_L to all non-radiated real FS momenta.

This way, all components of `p_real` are constructed in the real Lab frame.

```

<phs fks: phs fks generator: TBP>+≡
  procedure :: generate_isr => phs_fks_generator_generate_isr

<phs fks: procedures>+≡
  subroutine phs_fks_generator_generate_isr (generator, i_phs, p_born, p_real)
    !!! Important: Import Born momenta in the lab frame
    class(phs_fks_generator_t), intent(inout) :: generator
    integer, intent(in) :: i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(inout), dimension(:) :: p_real
    real(default) :: xi_max, xi_tilde, xi, y, phi
    integer :: nlegborn, nlegreal
    real(default) :: sqrts_real
    real(default) :: k0_np1
    type(lorentz_transformation_t) :: lambda_transv, lambda_longit, lambda_longit_inv
    real(default) :: x_plus, x_minus, xb_plus, xb_minus
    real(default) :: onemy, onepy
    integer :: i
    real(default) :: xi_plus, xi_minus
    real(default) :: beta_gamma
    type(vector3_t) :: beta_vec

    associate (rad_var => generator%real_kinematics)
      xi_max = rad_var%xi_max(i_phs)
      xi_tilde = rad_var%xi_tilde
    end associate
  end subroutine

```

```

xi = xi_tilde * xi_max
y = rad_var%y(i_phs)
onemy = one - y; onepy = one + y
phi = rad_var%phi
rad_var%y_soft(i_phs) = y
end associate

nlegborn = size(p_born)
nlegreal = nlegborn + 1
generator%isr_kinematics%sqrts_born = (p_born(1) + p_born(2))*1

!!! Initial state real momenta
xb_plus = generator%isr_kinematics%x(I_PLUS)
xb_minus = generator%isr_kinematics%x(I_MINUS)
x_plus = xb_plus / sqrt(one - xi) * sqrt((two - xi * onemy) / (two - xi * onepy))
x_minus = xb_minus / sqrt(one - xi) * sqrt((two - xi * onemy) / (two - xi * onepy))
xi_plus = xi_tilde * (one - xb_plus)
xi_minus = xi_tilde * (one - xb_minus)
p_real(I_PLUS) = x_plus / xb_plus * p_born(I_PLUS)
p_real(I_MINUS) = x_minus / xb_minus * p_born(I_MINUS)

!!! Fraction of momentum fractions in a collinear splitting
generator%isr_kinematics%z(I_PLUS) = (one - xi_plus)
generator%isr_kinematics%z(I_MINUS) = (one - xi_minus)

!!! Create radiation momentum in the real CMS
sqrts_real = generator%isr_kinematics%sqrts_born / sqrt(one - xi)
k0_np1 = sqrts_real * xi / two
p_real(nlegreal)%p(0) = k0_np1
p_real(nlegreal)%p(1) = k0_np1 * sqrt(one - y**2) * sin(phi)
p_real(nlegreal)%p(2) = k0_np1 * sqrt(one - y**2) * cos(phi)
p_real(nlegreal)%p(3) = k0_np1 * y

!!! Boosts the radiation from real CMS to the real LAB frame
call get_boost_parameters(p_real, beta_gamma, beta_vec)
lambda_longit = create_longitudinal_boost(beta_gamma, beta_vec, inverse = .true.)
p_real(nlegreal) = lambda_longit * p_real(nlegreal)

call get_boost_parameters(p_born, beta_gamma, beta_vec)
lambda_longit = create_longitudinal_boost(beta_gamma, beta_vec, inverse = .false.)
forall(i = 3 : nlegborn) p_real(i) = lambda_longit * p_born(i)

lambda_transv = create_transversal_boost(p_real(nlegreal), xi, sqrts_real)
forall(i = 3 : nlegborn) p_real(i) = lambda_transv * p_real(i)

lambda_longit_inv = create_longitudinal_boost(beta_gamma, beta_vec, inverse = .true.)
forall(i = 3 : nlegborn) p_real(i) = lambda_longit_inv * p_real(i)

!!! Compute Jacobians
associate(jac => generator%real_kinematics%jac(i_phs))
!!! Additional 1 / (1 - xi) factor because in the real jacobian,
!!! there is s_real in the numerator
!!! We also have to adapt the flux factor, which is 1/2s_real for the real component
!!! The reweighting factor is s_born / s_real, cancelling the (1-x) factor from above

```

```

        jac%jac(1) = one / (one - xi)
        jac%jac(2) = one
        jac%jac(3) = one / (one - xi_plus)**2
        jac%jac(4) = one / (one - xi_minus)**2
    end associate
contains
    subroutine get_boost_parameters (p, beta_gamma, beta_vec)
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), intent(out) :: beta_gamma
        type(vector3_t), intent(out) :: beta_vec
        beta_vec = (p(1)%p(1:3) + p(2)%p(1:3)) / (p(1)%p(0) + p(2)%p(0))
        beta_gamma = beta_vec**1 / sqrt (one - beta_vec**2)
        beta_vec = beta_vec / beta_vec**1
    end subroutine get_boost_parameters

    function create_longitudinal_boost (beta_gamma, beta_vec, inverse) result (lambda)
        real(default), intent(in) :: beta_gamma
        type(vector3_t), intent(in) :: beta_vec
        logical, intent(in) :: inverse
        type(lorentz_transformation_t) :: lambda
        if (inverse) then
            lambda = boost (beta_gamma, beta_vec)
        else
            lambda = boost (-beta_gamma, beta_vec)
        end if
    end function create_longitudinal_boost

    function create_transversal_boost (p_rad, xi, sqrts_real) result (lambda)
        type(vector4_t), intent(in) :: p_rad
        real(default), intent(in) :: xi, sqrts_real
        type(lorentz_transformation_t) :: lambda
        type(vector3_t) :: vec_transverse
        real(default) :: pt2, beta, beta_gamma
        pt2 = transverse_part (p_rad)**2
        beta = one / sqrt (one + sqrts_real**2 * (one - xi) / pt2)
        beta_gamma = beta / sqrt (one - beta**2)
        vec_transverse%p(1:2) = p_rad%p(1:2)
        vec_transverse%p(3) = zero
        vec_transverse = normalize (vec_transverse)
        lambda = boost (-beta_gamma, vec_transverse)
    end function create_transversal_boost
end subroutine phs_fks_generator_generate_isr

```

```

<phs fks: phs fks generator: TBP>+≡
    procedure :: set_sqrts_hat => phs_fks_generator_set_sqrts_hat
<phs fks: procedures>+≡
    subroutine phs_fks_generator_set_sqrts_hat (generator, sqrts)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: sqrts
        generator%sqrts = sqrts
    end subroutine phs_fks_generator_set_sqrts_hat

```

```

<phs fks: phs fks generator: TBP>+≡

```

```

    procedure :: set_emitters => phs_fks_generator_set_emitters
<phs fks: procedures>+≡
    subroutine phs_fks_generator_set_emitters (generator, emitters)
        class(phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in), dimension(:), allocatable :: emitters
        allocate (generator%emitters (size (emitters)))
        generator%emitters = emitters
    end subroutine phs_fks_generator_set_emitters

<phs fks: phs fks generator: TBP>+≡
    procedure :: setup_masses => phs_fks_generator_setup_masses
<phs fks: procedures>+≡
    subroutine phs_fks_generator_setup_masses (generator, n_tot)
        class (phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in) :: n_tot
        if (.not. allocated (generator%m2)) then
            allocate (generator%is_massive (n_tot))
            allocate (generator%m2 (n_tot))
            generator%is_massive = .false.
            generator%m2 = zero
        end if
    end subroutine phs_fks_generator_setup_masses

<phs fks: phs fks generator: TBP>+≡
    procedure :: set_xi_and_y_bounds => phs_fks_generator_set_xi_and_y_bounds
<phs fks: procedures>+≡
    subroutine phs_fks_generator_set_xi_and_y_bounds (generator, fks_xi_min, fks_y_max)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in), optional :: fks_xi_min, fks_y_max
        real(default) :: xi_min, y_max
        xi_min = zero; y_max = one
        if (present (fks_xi_min)) xi_min = fks_xi_min
        if (present (fks_y_max)) y_max = fks_y_max
        generator%xi_min = min (one, max (xi_min, tiny_07))
        generator%y_max = min (abs (y_max), one)
    end subroutine phs_fks_generator_set_xi_and_y_bounds

```

Sets x in the isr_kinematics of the generator.

```

<phs fks: phs fks generator: TBP>+≡
    procedure :: set_isr_kinematics => phs_fks_generator_set_isr_kinematics
<phs fks: procedures>+≡
    subroutine phs_fks_generator_set_isr_kinematics (generator, p)
        class(phs_fks_generator_t), intent(inout) :: generator
        type(vector4_t), dimension(2), intent(in) :: p
        if (allocated (generator%isr_kinematics%beam_energy)) then
            select case (size (generator%isr_kinematics%beam_energy))
            case (1)
                generator%isr_kinematics%x = p%p(0) / &
                    generator%isr_kinematics%beam_energy(1)
            case (2)

```



```

        generator%isr_kinematics%x = p%p(0) / &
        generator%isr_kinematics%beam_energy
    end select
else
    generator%isr_kinematics%x = 0
end if
end subroutine phs_fks_generator_set_isr_kinematics

```

(phs fks: phs fks generator: TBP)+≡

```

procedure :: generate_radiation_variables => &
    phs_fks_generator_generate_radiation_variables

```

(phs fks: procedures)+≡

```

subroutine phs_fks_generator_generate_radiation_variables &
    (generator, r_in, p_born, phs_identifiers, threshold)
class(phs_fks_generator_t), intent(inout) :: generator
real(default), intent(in), dimension(:) :: r_in
type(vector4_t), intent(in), dimension(:) :: p_born
type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
logical, intent(in), optional :: threshold

associate (rad_var => generator%real_kinematics)
    rad_var%phi = r_in (I_PHI) * twopi
    select case (generator%mode)
    case (GEN_REAL_PHASE_SPACE)
        rad_var%jac_rand = twopi
        call generator%compute_y_real_phs (r_in(I_Y), p_born, phs_identifiers, &
            rad_var%jac_rand, rad_var%y, threshold)
    case (GEN_SOFT_MISMATCH)
        rad_var%jac_mismatch = twopi
        call generator%compute_y_mismatch (r_in(I_Y), rad_var%jac_mismatch, &
            rad_var%y_mismatch, rad_var%y_soft)
    case default
        call generator%compute_y_test (rad_var%y)
    end select
    call generator%compute_xi_tilde (r_in(I_XI))
    call generator%set_masses (p_born, phs_identifiers)
end associate
end subroutine phs_fks_generator_generate_radiation_variables

```

(phs fks: phs fks generator: TBP)+≡

```

procedure :: compute_xi_ref_momenta => phs_fks_generator_compute_xi_ref_momenta

```

(phs fks: procedures)+≡

```

subroutine phs_fks_generator_compute_xi_ref_momenta &
    (generator, p_born, resonance_contributors)
class(phs_fks_generator_t), intent(inout) :: generator
type(vector4_t), intent(in), dimension(:) :: p_born
type(resonance_contributors_t), intent(in), dimension(:), optional &
    :: resonance_contributors
integer :: i_con, n_contributors
if (present (resonance_contributors)) then
    n_contributors = size (resonance_contributors)
    if (.not. allocated (generator%resonance_contributors)) &

```

```

        allocate (generator%resonance_contributors (n_contributors))
    do i_con = 1, n_contributors
        generator%real_kinematics%xi_ref_momenta(i_con) = &
            get_resonance_momentum (p_born, resonance_contributors(i_con)%c)
        generator%resonance_contributors(i_con) = resonance_contributors(i_con)
    end do
else
    generator%real_kinematics%xi_ref_momenta(1) = sum (p_born(1:generator%n_in))
end if
end subroutine phs_fks_generator_compute_xi_ref_momenta

<phs fks: phs fks generator: TBP>+≡
    procedure :: compute_xi_ref_momenta_threshold &
        => phs_fks_generator_compute_xi_ref_momenta_threshold

<phs fks: procedures>+≡
    subroutine phs_fks_generator_compute_xi_ref_momenta_threshold (generator, p_born)
        class(phs_fks_generator_t), intent(inout) :: generator
        type(vector4_t), intent(in), dimension(:) :: p_born
        generator%real_kinematics%xi_ref_momenta(1) = p_born(THR_POS_WP) + p_born(THR_POS_B)
        generator%real_kinematics%xi_ref_momenta(2) = p_born(THR_POS_WM) + p_born(THR_POS_BBAR)
    end subroutine phs_fks_generator_compute_xi_ref_momenta_threshold

<phs fks: phs fks generator: TBP>+≡
    procedure :: compute_cms_energy => phs_fks_generator_compute_cms_energy

<phs fks: procedures>+≡
    subroutine phs_fks_generator_compute_cms_energy (generator, p_born)
        class(phs_fks_generator_t), intent(inout) :: generator
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t) :: p_sum
        p_sum = sum (p_born (1 : generator%n_in))
        generator%real_kinematics%cms_energy2 = p_sum**2
    end subroutine phs_fks_generator_compute_cms_energy

<phs fks: phs fks generator: TBP>+≡
    procedure :: compute_xi_max => phs_fks_generator_compute_xi_max

<phs fks: procedures>+≡
    subroutine phs_fks_generator_compute_xi_max (generator, emitter, &
        i_phs, p, xi_max, i_con, y_in)
        class(phs_fks_generator_t), intent(inout) :: generator
        integer, intent(in) :: i_phs, emitter
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), intent(out) :: xi_max
        integer, intent(in), optional :: i_con
        real(default), intent(in), optional :: y_in
        real(default) :: q0
        type(vector4_t), dimension(:), allocatable :: pp, pp_decay
        type(vector4_t) :: p_res
        type(lorentz_transformation_t) :: L_to_resonance
        real(default) :: y
        if (.not. any (generator%emitters == emitter)) return
        allocate (pp (size (p)))

```

```

associate (rad_var => generator%real_kinematics)
  if (present (i_con)) then
    q0 = rad_var%xi_ref_momenta(i_con)**1
  else
    q0 = energy (sum (p(1:generator%n_in)))
  end if
  if (present (y_in)) then
    y = y_in
  else
    y = rad_var%y(i_phs)
  end if
  if (present (i_con)) then
    p_res = rad_var%xi_ref_momenta(i_con)
    L_to_resonance = inverse (boost (p_res, q0))
    pp = L_to_resonance * p
  else
    pp = p
  end if
  if (emitter <= generator%n_in) then
    select case (generator%isr_kinematics%isr_mode)
    case (SQRTS_FIXED)
      if (generator%n_in > 1) then
        allocate (pp_decay (size (pp) - 1))
      else
        allocate (pp_decay (size (pp)))
      end if
      pp_decay (1) = sum (pp(1:generator%n_in))
      pp_decay (2 : ) = pp (generator%n_in + 1 : )
      xi_max = get_xi_max_isr_decay (pp_decay)
      deallocate (pp_decay)
    case (SQRTS_VAR)
      xi_max = get_xi_max_isr (generator%isr_kinematics%x, y)
    end select
  else
    if (generator%is_massive(emitter)) then
      xi_max = get_xi_max_fsr (pp, q0, emitter, generator%m2(emitter), y)
    else
      xi_max = get_xi_max_fsr (pp, q0, emitter)
    end if
  end if
  deallocate (pp)
end associate
end subroutine phs_fks_generator_compute_xi_max

```

(phs fks: phs fks generator: TBP)+≡

```

procedure :: compute_xi_max_isr_factorized &
=> phs_fks_generator_compute_xi_max_isr_factorized

```

(phs fks: procedures)+≡

```

subroutine phs_fks_generator_compute_xi_max_isr_factorized &
(generator, i_phs, p)
class(phs_fks_generator_t), intent(inout) :: generator
integer, intent(in) :: i_phs
type(vector4_t), intent(in), dimension(:) :: p

```

```

        generator%real_kinematics%xi_max(i_phs) = get_xi_max_isr_decay (p)
    end subroutine phs_fks_generator_compute_xi_max_isr_factorized

<phs fks: phs fks generator: TBP>+≡
    procedure :: set_masses => phs_fks_generator_set_masses

<phs fks: procedures>+≡
    subroutine phs_fks_generator_set_masses (generator, p, phs_identifiers)
        class(phs_fks_generator_t), intent(inout) :: generator
        type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
        type(vector4_t), intent(in), dimension(:) :: p
        integer :: emitter, i_phs
        do i_phs = 1, size (phs_identifiers)
            emitter = phs_identifiers(i_phs)%emitter
            if (any (generator%emitters == emitter) .and. emitter > 0) then
                if (generator%is_massive (emitter) .and. emitter > generator%n_in) &
                    generator%m2(emitter) = p(emitter)**2
            end if
        end do
    end subroutine phs_fks_generator_set_masses

<phs fks: public>+≡
    public :: compute_y_from_emitter

<phs fks: procedures>+≡
    subroutine compute_y_from_emitter (r_y, p, n_in, emitter, massive, &
        y_max, jac_rand, y, contributors, threshold)
        real(default), intent(in) :: r_y
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in) :: n_in
        integer, intent(in) :: emitter
        logical, intent(in) :: massive
        real(default), intent(in) :: y_max
        real(default), intent(inout) :: jac_rand
        real(default), intent(out) :: y
        integer, intent(in), dimension(:), allocatable, optional :: contributors
        logical, intent(in), optional :: threshold
        logical :: thr, resonance
        type(vector4_t) :: p_res, p_em
        real(default) :: q0
        type(lorentz_transformation_t) :: boost_to_resonance
        integer :: i
        real(default) :: beta, one_m_beta, one_p_beta
        thr = .false.; if (present (threshold)) thr = threshold
        p_res = vector4_null
        if (present (contributors)) then
            resonance = allocated (contributors)
        else
            resonance = .false.
        end if
        if (massive) then
            if (resonance) then
                do i = 1, size (contributors)
                    p_res = p_res + p(contributors(i))
                end do
            end if
        end if
    end subroutine

```

```

        end do
    else if (thr) then
        p_res = p(ass_boson(thr_leg(emitter))) + p(ass_quark(thr_leg(emitter)))
    else
        p_res = sum (p(1:n_in))
    end if
    q0 = p_res**1
    boost_to_resonance = inverse (boost (p_res, q0))
    p_em = boost_to_resonance * p(emitter)
    beta = beta_emitter (q0, p_em)
    one_m_beta = one - beta
    one_p_beta = one + beta
    y = one / beta * (one - one_p_beta * &
        exp ( - r_y * log(one_p_beta / one_m_beta)))
    jac_rand = jac_rand * &
        (one - beta * y) * log(one_p_beta / one_m_beta) / beta
    else
        y = (one - two * r_y) * y_max
        jac_rand = jac_rand * 3 * (one - y**2) * y_max
        y = 1.5_default * (y - y**3 / 3)
    end if
end subroutine compute_y_from_emitter

```

<phs fks: phs fks generator: TBP>+≡

```

    procedure :: compute_y_real_phs => phs_fks_generator_compute_y_real_phs

```

<phs fks: procedures>+≡

```

    subroutine phs_fks_generator_compute_y_real_phs (generator, r_y, p, phs_identifiers, &
        jac_rand, y, threshold)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: r_y
        type(vector4_t), intent(in), dimension(:) :: p
        type(phs_identifier_t), intent(in), dimension(:) :: phs_identifiers
        real(default), intent(inout), dimension(:) :: jac_rand
        real(default), intent(out), dimension(:) :: y
        logical, intent(in), optional :: threshold
        real(default) :: beta, one_p_beta, one_m_beta
        type(lorentz_transformation_t) :: boost_to_resonance
        real(default) :: q0
        type(vector4_t) :: p_res, p_em
        integer :: i, i_phs, emitter
        logical :: thr
        logical :: construct_massive_fsr
        construct_massive_fsr = .false.
        thr = .false.; if (present (threshold)) thr = threshold
        do i_phs = 1, size (phs_identifiers)
            emitter = phs_identifiers(i_phs)%emitter
            !!! We need this additional check because of decay phase spaces
            !!! t -> bW has a massive emitter at position 1, which should
            !!! not be treated here.
            construct_massive_fsr = emitter > generator%n_in
            if (construct_massive_fsr) construct_massive_fsr = &
                construct_massive_fsr .and. generator%is_massive (emitter)
            call compute_y_from_emitter (r_y, p, generator%n_in, emitter, construct_massive_fsr, &

```

```

        generator%y_max, jac_rand(i_phs), y(i_phs), &
        phs_identifiers(i_phs)%contributors, threshold)
    end do
end subroutine phs_fks_generator_compute_y_real_phs

<phs fks: phs fks generator: TBP>+≡
    procedure :: compute_y_mismatch => phs_fks_generator_compute_y_mismatch

<phs fks: procedures>+≡
    subroutine phs_fks_generator_compute_y_mismatch (generator, r_y, jac_rand, y, y_soft)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: r_y
        real(default), intent(inout) :: jac_rand
        real(default), intent(out) :: y
        real(default), intent(out), dimension(:) :: y_soft
        y = (one - two * r_y) * generator%y_max
        jac_rand = jac_rand * 3 * (one - y**2) * generator%y_max
        y = 1.5_default * (y - y**3 / 3)
        y_soft = y
    end subroutine phs_fks_generator_compute_y_mismatch

<phs fks: phs fks generator: TBP>+≡
    procedure :: compute_y_test => phs_fks_generator_compute_y_test

<phs fks: procedures>+≡
    subroutine phs_fks_generator_compute_y_test (generator, y)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(out), dimension(:) :: y
        select case (generator%mode)
        case (GEN_SOFT_LIMIT_TEST)
            y = y_test_soft
        case (GEN_COLL_LIMIT_TEST)
            y = y_test_coll
        case (GEN_ANTI_COLL_LIMIT_TEST)
            y = - y_test_coll
        case (GEN_SOFT_COLL_LIMIT_TEST)
            y = y_test_coll
        case (GEN_SOFT_ANTI_COLL_LIMIT_TEST)
            y = - y_test_coll
        end select
    end subroutine phs_fks_generator_compute_y_test

<phs fks: public>+≡
    public :: beta_emitter

<phs fks: procedures>+≡
    pure function beta_emitter (q0, p) result (beta)
        real(default), intent(in) :: q0
        type(vector4_t), intent(in) :: p
        real(default) :: beta
        real(default) :: m2, mrec2, k0_max
        m2 = p**2
        mrec2 = (q0 - p%p(0))**2 - p%p(1)**2 - p%p(2)**2 - p%p(3)**2
        k0_max = (q0**2 - mrec2 + m2) / (two * q0)

```

```

        beta = sqrt(one - m2 / k0_max**2)
    end function beta_emitter

<phs fks: phs fks generator: TBP>+≡
    procedure :: compute_xi_tilde => phs_fks_generator_compute_xi_tilde

<phs fks: procedures>+≡
    pure subroutine phs_fks_generator_compute_xi_tilde (generator, r)
        class(phs_fks_generator_t), intent(inout) :: generator
        real(default), intent(in) :: r
        real(default) :: deno
        associate (rad_var => generator%real_kinematics)
            select case (generator%mode)
            case (GEN_REAL_PHASE_SPACE)
                if (generator%singular_jacobian) then
                    rad_var%xi_tilde = (one - generator%xi_min) - (one - r)**2 * &
                        (one - two * generator%xi_min)
                    rad_var%jac_rand = rad_var%jac_rand * two * (one - r) * &
                        (one - two * generator%xi_min)
                else
                    rad_var%xi_tilde = generator%xi_min + r * (one - generator%xi_min)
                    rad_var%jac_rand = rad_var%jac_rand * (one - generator%xi_min)
                end if
            case (GEN_SOFT_MISMATCH)
                deno = one - r
                if (deno < tiny_13) deno = tiny_13
                rad_var%xi_mismatch = generator%xi_min + r / deno
                rad_var%jac_mismatch = rad_var%jac_mismatch / deno**2
            case (GEN_SOFT_LIMIT_TEST)
                rad_var%xi_tilde = r * two * xi_tilde_test_soft
                rad_var%jac_rand = two * xi_tilde_test_soft
            case (GEN_COLL_LIMIT_TEST)
                rad_var%xi_tilde = xi_tilde_test_coll
                rad_var%jac_rand = xi_tilde_test_coll
            case (GEN_ANTI_COLL_LIMIT_TEST)
                rad_var%xi_tilde = xi_tilde_test_coll
                rad_var%jac_rand = xi_tilde_test_coll
            case (GEN_SOFT_COLL_LIMIT_TEST)
                rad_var%xi_tilde = r * two * xi_tilde_test_soft
                rad_var%jac_rand = two * xi_tilde_test_soft
            case (GEN_SOFT_ANTI_COLL_LIMIT_TEST)
                rad_var%xi_tilde = r * two * xi_tilde_test_soft
                rad_var%jac_rand = two * xi_tilde_test_soft
            end select
        end associate
    end subroutine phs_fks_generator_compute_xi_tilde

<phs fks: phs fks generator: TBP>+≡
    procedure :: prepare_generation => phs_fks_generator_prepare_generation

<phs fks: procedures>+≡
    subroutine phs_fks_generator_prepare_generation (generator, r_in, i_phs, &
        emitter, p_born, phs_identifiers, contributors, i_con)
        class(phs_fks_generator_t), intent(inout) :: generator

```

```

real(default), dimension(3), intent(in) :: r_in
integer, intent(in) :: i_phs, emitter
type(vector4_t), intent(in), dimension(:) :: p_born
type(phs_identifer_t), intent(in), dimension(:) :: phs_identifiers
type(resonance_contributors_t), intent(in), dimension(:), optional :: contributors
integer, intent(in), optional :: i_con
call generator%generate_radiation_variables (r_in, p_born, phs_identifiers)
call generator%compute_xi_ref_momenta &
    (generator%real_kinematics%p_born_lab%phs_point(1)%get (), contributors)
call generator%compute_xi_max (emitter, i_phs, p_born, &
    generator%real_kinematics%xi_max(i_phs), i_con = i_con)
end subroutine phs_fks_generator_prepare_generation

```

Get xi and y from an external routine (e.g. powheg) and generate an FSR phase space. Note that the flag `supply_xi_max` is set to `.false.` because it is assumed that the upper bound on xi has already been taken into account during its generation.

```

<phs fks: phs fks generator: TBP>+≡
  procedure :: generate_fsr_from_xi_and_y => &
    phs_fks_generator_generate_fsr_from_xi_and_y

<phs fks: procedures>+≡
  subroutine phs_fks_generator_generate_fsr_from_xi_and_y (generator, xi, y, &
    phi, emitter, i_phs, p_born, p_real)
    class(phs_fks_generator_t), intent(inout) :: generator
    real(default), intent(in) :: xi, y, phi
    integer, intent(in) :: emitter, i_phs
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(inout), dimension(:) :: p_real
    associate (rad_var => generator%real_kinematics)
      rad_var%supply_xi_max = .false.
      rad_var%xi_tilde = xi
      rad_var%y(i_phs) = y
      rad_var%phi = phi
    end associate
    call generator%set_sqrts_hat (p_born(1)%p(0) + p_born(2)%p(0))
    call generator%generate_fsr (emitter, i_phs, p_born, p_real)
  end subroutine phs_fks_generator_generate_fsr_from_xi_and_y

```

```

<phs fks: phs fks generator: TBP>+≡
  procedure :: get_radiation_variables => &
    phs_fks_generator_get_radiation_variables

<phs fks: procedures>+≡
  pure subroutine phs_fks_generator_get_radiation_variables (generator, &
    i_phs, xi, y, phi)
    class(phs_fks_generator_t), intent(in) :: generator
    integer, intent(in) :: i_phs
    real(default), intent(out) :: xi, y
    real(default), intent(out), optional :: phi
    associate (rad_var => generator%real_kinematics)
      xi = rad_var%xi_max(i_phs) * rad_var%xi_tilde
      y = rad_var%y(i_phs)
      if (present (phi)) phi = rad_var%phi
    end associate
  end subroutine

```



```

        end associate
    end subroutine phs_fks_generator_get_radiation_variables

<phs fks: phs fks generator: TBP>+≡
    procedure :: write => phs_fks_generator_write

<phs fks: procedures>+≡
    subroutine phs_fks_generator_write (generator, unit)
        class(phs_fks_generator_t), intent(in) :: generator
        integer, intent(in), optional :: unit
        integer :: u
        type(string_t) :: massive_phsp
        u = given_output_unit (unit); if (u < 0) return
        if (generator%massive_phsp) then
            massive_phsp = " massive "
        else
            massive_phsp = " massless "
        end if
        write (u, "(A)") char ("This is a generator for a" &
            // massive_phsp // "phase space")
        if (associated (generator%real_kinematics)) then
            call generator%real_kinematics%write ()
        else
            write (u, "(A)") "Warning: There are no real " // &
                "kinematics associated with this generator"
        end if
        call write_separator (u)
        write (u, "(A," // FMT_17 // ",1X)") "sqrts      : ", generator%sqrts
        write (u, "(A," // FMT_17 // ",1X)") "E_gluon      : ", generator%E_gluon
        write (u, "(A," // FMT_17 // ",1X)") "mrec2        : ", generator%mrec2
    end subroutine phs_fks_generator_write

<phs fks: phs fks: TBP>+≡
    procedure :: compute_isr_kinematics => phs_fks_compute_isr_kinematics

<phs fks: procedures>+≡
    subroutine phs_fks_compute_isr_kinematics (phs, r)
        class(phs_fks_t), intent(inout) :: phs
        real(default), intent(in) :: r
        if (.not. phs%config%lab_is_cm) then
            call phs%generator%compute_isr_kinematics (r, phs%lt_cm_to_lab * phs%phs_wood_t%p)
        else
            call phs%generator%compute_isr_kinematics (r, phs%phs_wood_t%p)
        end if
    end subroutine phs_fks_compute_isr_kinematics

<phs fks: phs fks: TBP>+≡
    procedure :: final => phs_fks_final

<phs fks: procedures>+≡
    subroutine phs_fks_final (object)
        class(phs_fks_t), intent(inout) :: object
        call phs_forest_final (object%forest)
        call object%generator%final ()

```

```

end subroutine phs_fks_final

<phs fks: public>+≡
public :: get_filtered_resonance_histories

<phs fks: procedures>+≡
subroutine filter_particles_from_resonances (res_hist, exclusion_list, &
model, res_hist_filtered)
type(resonance_history_t), intent(in), dimension(:) :: res_hist
type(string_t), intent(in), dimension(:) :: exclusion_list
type(model_t), intent(in) :: model
type(resonance_history_t), intent(out), dimension(:), allocatable :: res_hist_filtered
integer :: i_hist, i_flv, i_new, n_orig
logical, dimension(size (res_hist)) :: to_filter
type(flavor_t) :: flv
to_filter = .false.
n_orig = size (res_hist)
do i_flv = 1, size (exclusion_list)
call flv%init (exclusion_list (i_flv), model)
do i_hist = 1, size (res_hist)
if (res_hist(i_hist)%has_flavor (flv)) to_filter (i_hist) = .true.
end do
end do
allocate (res_hist_filtered (n_orig - count (to_filter)))
i_new = 1
do i_hist = 1, size (res_hist)
if (.not. to_filter (i_hist)) then
res_hist_filtered (i_new) = res_hist (i_hist)
i_new = i_new + 1
end if
end do
end subroutine filter_particles_from_resonances

<phs fks: procedures>+≡
subroutine clean_resonance_histories (res_hist, n_in, flv, res_hist_clean, success)
type(resonance_history_t), intent(in), dimension(:) :: res_hist
integer, intent(in) :: n_in
integer, intent(in), dimension(:) :: flv
type(resonance_history_t), intent(out), dimension(:), allocatable :: res_hist_clean
logical, intent(out) :: success
integer :: i_hist
type(resonance_history_t), dimension(:), allocatable :: res_hist_colored, res_hist_contracted

if (debug_on) call msg_debug (D_SUBTRACTION, "resonance_mapping_init")
if (debug_active (D_SUBTRACTION)) then
call msg_debug (D_SUBTRACTION, "Original resonances:")
do i_hist = 1, size(res_hist)
call res_hist(i_hist)%write ()
end do
end if

call remove_uncolored_resonances ()
call contract_resonances (res_hist_colored, res_hist_contracted)

```

```

call remove_subresonances (res_hist_contracted, res_hist_clean)
!!! Here, we are still not sure whether we actually would rather use
!!! call remove_multiple_resonances (res_hist_contracted, res_hist_clean)
if (debug_active (D_SUBTRACTION)) then
    call msg_debug (D_SUBTRACTION, "Resonances after removing uncolored and duplicates: ")
    do i_hist = 1, size (res_hist_clean)
        call res_hist_clean(i_hist)%write ()
    end do
end if
if (size (res_hist_clean) == 0) then
    call msg_warning ("No resonances found. Proceed in usual FKS mode.")
    success = .false.
else
    success = .true.
end if

contains

subroutine remove_uncolored_resonances ()
    type(resonance_history_t), dimension(:), allocatable :: res_hist_tmp
    integer :: n_hist, nleg_out, n_removed
    integer :: i_res, i_hist
    n_hist = size (res_hist)
    nleg_out = size (flv) - n_in
    allocate (res_hist_tmp (n_hist))
    allocate (res_hist_colored (n_hist))
    do i_hist = 1, n_hist
        res_hist_tmp(i_hist) = res_hist(i_hist)
        call res_hist_tmp(i_hist)%add_offset (n_in)
        n_removed = 0
        do i_res = 1, res_hist_tmp(i_hist)%n_resonances
            associate (resonance => res_hist_tmp(i_hist)%resonances(i_res - n_removed))
                if (.not. any (is_colored (flv (resonance%contributors%c))) &
                    .or. size (resonance%contributors%c) == nleg_out) then
                    call res_hist_tmp(i_hist)%remove_resonance (i_res - n_removed)
                    n_removed = n_removed + 1
                end if
            end associate
        end do
        if (allocated (res_hist_tmp(i_hist)%resonances)) then
            if (any (res_hist_colored == res_hist_tmp(i_hist))) then
                cycle
            else
                do i_res = 1, res_hist_tmp(i_hist)%n_resonances
                    associate (resonance => res_hist_tmp(i_hist)%resonances(i_res))
                        call res_hist_colored(i_hist)%add_resonance (resonance)
                    end associate
                end do
            end if
        end if
    end do
end subroutine remove_uncolored_resonances

subroutine contract_resonances (res_history_in, res_history_out)
    type(resonance_history_t), intent(in), dimension(:) :: res_history_in

```

```

type(resonance_history_t), intent(out), dimension(:), allocatable :: res_history_out
logical, dimension(:), allocatable :: i_non_zero
integer :: n_hist_non_zero, n_hist
integer :: i_hist_new
n_hist = size (res_history_in); n_hist_non_zero = 0
allocate (i_non_zero (n_hist))
i_non_zero = .false.
do i_hist = 1, n_hist
    if (res_history_in(i_hist)%n_resonances /= 0) then
        n_hist_non_zero = n_hist_non_zero + 1
        i_non_zero(i_hist) = .true.
    end if
end do
allocate (res_history_out (n_hist_non_zero))
i_hist_new = 1
do i_hist = 1, n_hist
    if (i_non_zero (i_hist)) then
        res_history_out (i_hist_new) = res_history_in (i_hist)
        i_hist_new = i_hist_new + 1
    end if
end do
end subroutine contract_resonances

subroutine remove_subresonances (res_history_in, res_history_out)
type(resonance_history_t), intent(in), dimension(:) :: res_history_in
type(resonance_history_t), intent(out), dimension(:), allocatable :: res_history_out
logical, dimension(:), allocatable :: i_non_sub_res
integer :: n_hist, n_hist_non_sub_res
integer :: i_hist1, i_hist2
logical :: is_not_subres
n_hist = size (res_history_in); n_hist_non_sub_res = 0
allocate (i_non_sub_res (n_hist)); i_non_sub_res = .false.
do i_hist1 = 1, n_hist
    is_not_subres = .true.
    do i_hist2 = 1, n_hist
        if (i_hist1 == i_hist2) cycle
        is_not_subres = is_not_subres .and. &
            .not.(res_history_in(i_hist2) .contains. res_history_in(i_hist1))
    end do
    if (is_not_subres) then
        n_hist_non_sub_res = n_hist_non_sub_res + 1
        i_non_sub_res (i_hist1) = .true.
    end if
end do

allocate (res_history_out (n_hist_non_sub_res))
i_hist2 = 1
do i_hist1 = 1, n_hist
    if (i_non_sub_res (i_hist1)) then
        res_history_out (i_hist2) = res_history_in (i_hist1)
        i_hist2 = i_hist2 + 1
    end if
end do
end subroutine remove_subresonances

```

```

subroutine remove_multiple_resonances (res_history_in, res_history_out)
  type(resonance_history_t), intent(in), dimension(:) :: res_history_in
  type(resonance_history_t), intent(out), dimension(:), allocatable :: res_history_out
  integer :: n_hist, n_hist_single
  logical, dimension(:), allocatable :: i_hist_single
  integer :: i_hist, j
  n_hist = size (res_history_in)
  n_hist_single = 0
  allocate (i_hist_single (n_hist)); i_hist_single = .false.
  do i_hist = 1, n_hist
    if (res_history_in(i_hist)%n_resonances == 1) then
      n_hist_single = n_hist_single + 1
      i_hist_single(i_hist) = .true.
    end if
  end do

  allocate (res_history_out (n_hist_single))
  j = 1
  do i_hist = 1, n_hist
    if (i_hist_single(i_hist)) then
      res_history_out(j) = res_history_in(i_hist)
      j = j + 1
    end if
  end do
end subroutine remove_multiple_resonances
end subroutine clean_resonance_histories

```

(phs fks: procedures)+≡

```

subroutine get_filtered_resonance_histories (phs_config, n_in, flv_state, model, &
  excluded_resonances, resonance_histories_filtered, success)
  type(phs_fks_config_t), intent(inout) :: phs_config
  integer, intent(in) :: n_in
  integer, intent(in), dimension(:,:), allocatable :: flv_state
  type(model_t), intent(in) :: model
  type(string_t), intent(in), dimension(:), allocatable :: excluded_resonances
  type(resonance_history_t), intent(out), dimension(:), &
    allocatable :: resonance_histories_filtered
  logical, intent(out) :: success
  type(resonance_history_t), dimension(:), allocatable :: resonance_histories
  type(resonance_history_t), dimension(:), allocatable :: &
    resonance_histories_clean!, resonance_histories_filtered
  allocate (resonance_histories (size (phs_config%get_resonance_histories ())))
  resonance_histories = phs_config%get_resonance_histories ()
  call clean_resonance_histories (resonance_histories, &
    n_in, flv_state (:,1), resonance_histories_clean, success)
  if (success .and. allocated (excluded_resonances)) then
    call filter_particles_from_resonances (resonance_histories_clean, &
      excluded_resonances, model, resonance_histories_filtered)
  else
    allocate (resonance_histories_filtered (size (resonance_histories_clean)))
    resonance_histories_filtered = resonance_histories_clean
  end if
end subroutine get_filtered_resonance_histories

```


19.11.3 Unit tests

Test module for FKS phase space, followed by the corresponding implementation module.

```
<phs_fks_ut.f90>≡
  <File header>

  module phs_fks_ut
    use unit_tests
    use phs_fks_uti

  <Standard module head>

  <phs fks: public test>

  contains

  <phs fks: test driver>

  end module phs_fks_ut
<phs_fks_uti.f90>≡
  <File header>

  module phs_fks_uti

  <Use kinds>
    use format_utils, only: write_separator, pac_fmt
    use format_defs, only: FMT_15, FMT_19
    use numeric_utils, only: nearly_equal
    use constants, only: tiny_07, zero, one, two
    use lorentz
    use phs_points, only: assignment(=)

    use physics_defs, only: THR_POS_B, THR_POS_BBAR, THR_POS_WP, THR_POS_WM, THR_POS_GLUON
    use physics_defs, only: thr_leg

    use resonances, only: resonance_contributors_t
    use phs_fks

  <Standard module head>

  <phs fks: test declarations>

  contains

  <phs fks: tests>

  end module phs_fks_uti
API: driver for the unit tests below.
<phs fks: public test>≡
  public :: phs_fks_generator_test
<phs fks: test driver>≡
  subroutine phs_fks_generator_test (u, results)
```

```

integer, intent(in) :: u
type(test_results_t), intent(inout) :: results
call test(phs_fks_generator_1, "phs_fks_generator_1", &
  "Test the generation of FKS phase spaces", u, results)
call test(phs_fks_generator_2, "phs_fks_generator_2", &
  "Test the generation of an ISR FKS phase space", u, results)
call test(phs_fks_generator_3, "phs_fks_generator_3", &
  "Test the generation of a real phase space for decays", &
  u, results)
call test(phs_fks_generator_4, "phs_fks_generator_4", &
  "Test the generation of an FSR phase space with "&
  &"conserved invariant resonance masses", u, results)
call test(phs_fks_generator_5, "phs_fks_generator_5", &
  "Test on-shell projection of a Born phase space and the generation"&
  &" of a real phase-space from that", u, results)
call test(phs_fks_generator_6, "phs_fks_generator_6", &
  "Test the generation of a real phase space for 1 -> 3 decays", &
  u, results)
call test(phs_fks_generator_7, "phs_fks_generator_7", &
  "Test the generation of an ISR FKS phase space for fixed beam energy", &
  u, results)
end subroutine phs_fks_generator_test

```

```

<phs fks: test declarations>≡
public :: phs_fks_generator_1

```

```

<phs fks: tests>≡
subroutine phs_fks_generator_1 (u)
  integer, intent(in) :: u
  type(phs_fks_generator_t) :: generator
  type(vector4_t), dimension(:), allocatable :: p_born
  type(vector4_t), dimension(:), allocatable :: p_real
  integer :: emitter, i_phs
  real(default) :: x1, x2, x3
  real(default), parameter :: sqrts = 250.0_default
  type(phs_identifier_t), dimension(2) :: phs_identifiers
  write (u, "(A)") "* Test output: phs_fks_generator_1"
  write (u, "(A)") "* Purpose: Create massless fsr phase space"
  write (u, "(A)")

  allocate (p_born (4))
  p_born(1)%p(0) = 125.0_default
  p_born(1)%p(1:2) = 0.0_default
  p_born(1)%p(3) = 125.0_default
  p_born(2)%p(0) = 125.0_default
  p_born(2)%p(1:2) = 0.0_default
  p_born(2)%p(3) = -125.0_default
  p_born(3)%p(0) = 125.0_default
  p_born(3)%p(1) = -39.5618_default
  p_born(3)%p(2) = -20.0791_default
  p_born(3)%p(3) = -114.6957_default
  p_born(4)%p(0) = 125.0_default
  p_born(4)%p(1:3) = -p_born(3)%p(1:3)

```



```

allocate (generator%isr_kinematics)
generator%n_in = 2
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

call generator%set_sqrts_hat (sqrts)

write (u, "(A)") "* Use four-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.75_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,1X,A,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (4, 2, 2, 1)

allocate (generator%emitters (2))
generator%emitters(1) = 3; generator%emitters(2) = 4
allocate (generator%m2 (4))
generator%m2 = zero
allocate (generator%is_massive (4))
generator%is_massive(1:2) = .false.
generator%is_massive(3:4) = .true.
phs_identifiers(1)%emitter = 3
phs_identifiers(2)%emitter = 4
call generator%compute_xi_ref_momenta (p_born)
call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do
write (u, "(A)") &
    "* With these, the following radiation variables have been produced:"
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F3.2)") "xi_tilde: ", rad_var%xi_tilde
    write (u, "(A,F3.2)") "y: " , rad_var%y(1)
    write (u, "(A,F3.2)") "phi: ", rad_var%phi
end associate
call write_separator (u)
write (u, "(A)") "Produce real momenta: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter

allocate (p_real (5))
call generator%generate_fsr (emitter, i_phs, p_born, p_real)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator (u)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_1"

```

```

end subroutine phs_fks_generator_1

<phs fks: test declarations>+≡
public :: phs_fks_generator_2

<phs fks: tests>+≡
subroutine phs_fks_generator_2 (u)
  integer, intent(in) :: u
  type(phs_fks_generator_t) :: generator
  type(vector4_t), dimension(:), allocatable :: p_born
  type(vector4_t), dimension(:), allocatable :: p_real
  integer :: emitter, i_phs
  real(default) :: x1, x2, x3
  real(default), parameter :: sqrts_hadronic = 250.0_default
  type(phs_identifier_t), dimension(2) :: phs_identifiers
  write (u, "(A)") "* Test output: phs_fks_generator_2"
  write (u, "(A)") "* Purpose: Create massless ISR phase space"
  write (u, "(A)")

  allocate (p_born (4))
  p_born(1)%p(0) = 114.661_default
  p_born(1)%p(1:2) = 0.0_default
  p_born(1)%p(3) = 114.661_default
  p_born(2)%p(0) = 121.784_default
  p_born(2)%p(1:2) = 0.0_default
  p_born(2)%p(3) = -121.784_default
  p_born(3)%p(0) = 115.148_default
  p_born(3)%p(1) = -46.250_default
  p_born(3)%p(2) = -37.711_default
  p_born(3)%p(3) = 98.478_default
  p_born(4)%p(0) = 121.296_default
  p_born(4)%p(1:2) = -p_born(3)%p(1:2)
  p_born(4)%p(3) = -105.601_default

  phs_identifiers(1)%emitter = 1
  phs_identifiers(2)%emitter = 2

  allocate (generator%emitters (2))
  allocate (generator%isr_kinematics)
  generator%emitters(1) = 1; generator%emitters(2) = 2
  generator%sqrts = sqrts_hadronic
  allocate (generator%isr_kinematics%beam_energy(2))
  generator%isr_kinematics%beam_energy = sqrts_hadronic / two
  call generator%set_sqrts_hat (sqrts_hadronic)
  call generator%set_isr_kinematics (p_born)
  generator%n_in = 2
  generator%isr_kinematics%isr_mode = SQRTS_VAR
  call generator%set_xi_and_y_bounds ()
  write (u, "(A)") "* Use four-particle phase space containing: "
  call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
  write (u, "(A)") "*****"
  write (u, "(A)")

```

```

x1=0.5_default; x2=0.25_default; x3=0.65_default
write (u, "(A)" ) "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,1X,A,F3.2)" ) &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (4, 2, 2, 1)
call generator%real_kinematics%p_born_lab%set_momenta (1, p_born)

allocate (generator%m2 (2))
generator%m2(1) = 0._default; generator%m2(2) = 0._default
allocate (generator%is_massive (4))
generator%is_massive = .false.
call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
call generator%compute_xi_ref_momenta (p_born)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do
write (u, "(A)" ) &
    "* With these, the following radiation variables have been produced:"
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F3.2)" ) "xi_tilde: ", rad_var%xi_tilde
    write (u, "(A,F3.2)" ) "y: " , rad_var%y(1)
    write (u, "(A,F3.2)" ) "phi: ", rad_var%phi
end associate
write (u, "(A)" ) "Initial-state momentum fractions: "
associate (xb => generator%isr_kinematics%x)
    write (u, "(A,F3.2)" ) "x_born_plus: ", xb(1)
    write (u, "(A,F3.2)" ) "x_born_minus: ", xb(2)
end associate
call write_separator (u)
write (u, "(A)" ) "Produce real momenta: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)" ) "emitter: ", emitter
allocate (p_real(5))
call generator%generate_isr (i_phs, p_born, p_real)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator (u)
write (u, "(A)" )
write (u, "(A)" ) "* Test output end: phs_fks_generator_2"

end subroutine phs_fks_generator_2

<phs fks: test declarations>+≡
public :: phs_fks_generator_3

<phs fks: tests>+≡
subroutine phs_fks_generator_3 (u)
    integer, intent(in) :: u
    type(phs_fks_generator_t) :: generator
    type(vector4_t), dimension(:), allocatable :: p_born

```

```

type(vector4_t), dimension(:), allocatable :: p_real
real(default) :: x1, x2, x3
real(default) :: mB, mW, mT
integer :: i, emitter, i_phs
type(phs_identfier_t), dimension(2) :: phs_identifiers

write (u, "(A)") "* Test output: phs_fks_generator_3"
write (u, "(A)") "* Puropse: Create real phase space for particle decays"
write (u, "(A)")

allocate (p_born(3))
p_born(1)%p(0) = 172._default
p_born(1)%p(1) = 0._default
p_born(1)%p(2) = 0._default
p_born(1)%p(3) = 0._default
p_born(2)%p(0) = 104.72866679_default
p_born(2)%p(1) = 45.028053213_default
p_born(2)%p(2) = 29.450337581_default
p_born(2)%p(3) = -5.910229156_default
p_born(3)%p(0) = 67.271333209_default
p_born(3)%p(1:3) = -p_born(2)%p(1:3)

generator%n_in = 1
allocate (generator%isr_kinematics)
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

mB = 4.2_default
mW = 80.376_default
mT = 172._default

generator%sqrts = mT

write (u, "(A)") "* Use three-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.6_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,A,1X,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (3, 2, 2, 1)
call generator%real_kinematics%p_born_lab%set_momenta (1, p_born)

allocate (generator%emitters(2))
generator%emitters(1) = 1
generator%emitters(2) = 3
allocate (generator%m2 (3), generator%is_massive(3))
generator%m2(1) = mT**2
generator%m2(2) = mW**2
generator%m2(3) = mB**2

```

```

generator%is_massive = .true.
phs_identifiers(1)%emitter = 1
phs_identifiers(2)%emitter = 3

call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
call generator%compute_xi_ref_momenta (p_born)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do

write (u, "(A)") &
    "* With these, the following radiation variables have been produced: "
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F4.2)") "xi_tilde: ", rad_var%xi_tilde
    do i = 1, 2
        write (u, "(A,I1,A,F5.2)") "i: ", i, "y: " , rad_var%y(i)
    end do
    write (u, "(A,F4.2)") "phi: ", rad_var%phi
end associate

call write_separator (u)
write (u, "(A)") "Produce real momenta via initial-state emission: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
allocate (p_real (4))
call generator%generate_isr_fixed_beam_energy (i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator(u)
write (u, "(A)") "Produce real momenta via final-state emission: "
i_phs = 2; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
call generator%generate_fsr (emitter, i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_3"

end subroutine phs_fks_generator_3

```

<phs fks: test declarations>+≡

public :: phs_fks_generator_4

<phs fks: tests>+≡

```

subroutine phs_fks_generator_4 (u)
    integer, intent(in) :: u
    type(phs_fks_generator_t) :: generator
    type(vector4_t), dimension(:), allocatable :: p_born
    type(vector4_t), dimension(:), allocatable :: p_real
    integer, dimension(:), allocatable :: emitters
    integer, dimension(:,:), allocatable :: resonance_lists
    type(resonance_contributors_t), dimension(2) :: alr_contributors

```

```

real(default) :: x1, x2, x3
real(default), parameter :: sqrts = 250.0_default
integer, parameter :: nlegborn = 6
integer :: i_phs, i_con, emitter
real(default) :: m_inv_born, m_inv_real
character(len=7) :: fmt
type(phs_identifier_t), dimension(2) :: phs_identifiers

call pac_fmt (fmt, FMT_19, FMT_15, .true.)

write (u, "(A)") "* Test output: phs_fks_generator_4"
write (u, "(A)") "* Purpose: Create FSR phase space with fixed resonances"
write (u, "(A)")

allocate (p_born (nlegborn))
p_born(1)%p(0) = 250._default
p_born(1)%p(1) = 0._default
p_born(1)%p(2) = 0._default
p_born(1)%p(3) = 250._default
p_born(2)%p(0) = 250._default
p_born(2)%p(1) = 0._default
p_born(2)%p(2) = 0._default
p_born(2)%p(3) = -250._default
p_born(3)%p(0) = 145.91184486_default
p_born(3)%p(1) = 50.39727589_default
p_born(3)%p(2) = 86.74156041_default
p_born(3)%p(3) = -69.03608748_default
p_born(4)%p(0) = 208.1064784_default
p_born(4)%p(1) = -44.07610020_default
p_born(4)%p(2) = -186.34264578_default
p_born(4)%p(3) = 13.48038407_default
p_born(5)%p(0) = 26.25614471_default
p_born(5)%p(1) = -25.12258068_default
p_born(5)%p(2) = -1.09540228_default
p_born(5)%p(3) = -6.27703505_default
p_born(6)%p(0) = 119.72553196_default
p_born(6)%p(1) = 18.80140499_default
p_born(6)%p(2) = 100.69648766_default
p_born(6)%p(3) = 61.83273846_default

allocate (generator%isr_kinematics)
generator%n_in = 2
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

call generator%set_sqrts_hat (sqrts)

write (u, "(A)") "* Test process: e+ e- -> W+ W- b b~"
write (u, "(A)") "* Resonance pairs: (3,5) and (4,6)"
write (u, "(A)") "* Use four-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

```

```

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.75_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,1X,A,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (nlegborn, 2, 2, 2)

allocate (generator%emitters (2))
generator%emitters(1) = 5; generator%emitters(2) = 6
allocate (generator%m2 (nlegborn))
generator%m2 = p_born**2
allocate (generator%is_massive (nlegborn))
generator%is_massive (1:2) = .false.
generator%is_massive (3:6) = .true.

phs_identifiers(1)%emitter = 5
phs_identifiers(2)%emitter = 6
do i_phs = 1, 2
    allocate (phs_identifiers(i_phs)%contributors (2))
end do
allocate (resonance_lists (2, 2))
resonance_lists (1,:) = [3,5]
resonance_lists (2,:) = [4,6]
!!! Here is obviously some redundancy. Surely we can improve on this.
do i_phs = 1, 2
    phs_identifiers(i_phs)%contributors = resonance_lists(i_phs,:)
end do
do i_con = 1, 2
    allocate (alr_contributors(i_con)%c (size (resonance_lists(i_con,:))))
    alr_contributors(i_con)%c = resonance_lists(i_con,:)
end do
call generator%generate_radiation_variables &
    ([x1, x2, x3], p_born, phs_identifiers)

allocate (p_real(nlegborn + 1))
call generator%compute_xi_ref_momenta (p_born, alr_contributors)
!!! Keep the distinction between i_phs and i_con because in general,
!!! they are not the same.
do i_phs = 1, 2
    i_con = i_phs
    emitter = phs_identifiers(i_phs)%emitter
    write (u, "(A,I1,1X,A,I1,A,I1,A)") &
        "* Generate FSR phase space for emitter ", emitter, &
        "and resonance pair (" , resonance_lists (i_con, 1), ",", &
        resonance_lists (i_con, 2), ")"
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs), i_con = i_con)
    call generator%generate_fsr (emitter, i_phs, i_con, p_born, p_real)
    call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
    call write_separator(u)
    write (u, "(A)") "* Check if resonance masses are conserved: "
    m_inv_born = compute_resonance_mass (p_born, resonance_lists (i_con,:))
    m_inv_real = compute_resonance_mass (p_real, resonance_lists (i_con,:), 7)

```

```

write (u, "(A,1X, " // fmt // ")") "m_inv_born = ", m_inv_born
write (u, "(A,1X, " // fmt // ")") "m_inv_real = ", m_inv_real
if (abs (m_inv_born - m_inv_real) < tiny_07) then
  write (u, "(A)") " Success! "
else
  write (u, "(A)") " Failure! "
end if
call write_separator(u)
call write_separator(u)
end do
deallocate (p_real)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_4"
end subroutine phs_fks_generator_4

```

<phs fks: test declarations>+≡

```
public :: phs_fks_generator_5
```

<phs fks: tests>+≡

```

subroutine phs_fks_generator_5 (u)
  use ttv_formfactors, only: init_parameters
  integer, intent(in) :: u
  type(phs_fks_generator_t) :: generator
  type(vector4_t), dimension(:), allocatable :: p_born, pb1
  type(vector4_t), dimension(:), allocatable :: p_born_onshell, pb1_os
  type(vector4_t), dimension(:), allocatable :: p_real
  real(default) :: x1, x2, x3
  real(default) :: mB, mW, mtop, mcheck
  integer :: i, emitter, i_phs
  type(phs_identifier_t), dimension(2) :: phs_identifiers
  type(lorentz_transformation_t) :: L_to_cms
  real(default), parameter :: sqrts = 360._default
  real(default), parameter :: momentum_tolerance = 1E-10_default
  real(default) :: mpole, gam_out

  write (u, "(A)") "* Test output: phs_fks_generator_5"
  write (u, "(A)") "* Puropse: Perform threshold on-shell projection of "
  write (u, "(A)") "*           Born momenta and create a real phase-space "
  write (u, "(A)") "*           point from those. "
  write (u, "(A)")

  allocate (p_born(6), p_born_onshell(6))
  p_born(1)%p(0) = sqrts / two
  p_born(1)%p(1:2) = zero
  p_born(1)%p(3) = sqrts / two
  p_born(2)%p(0) = sqrts / two
  p_born(2)%p(1:2) = zero
  p_born(2)%p(3) = -sqrts / two
  p_born(3)%p(0) = 117.1179139230_default
  p_born(3)%p(1) = 56.91215483880_default
  p_born(3)%p(2) = -40.02386013017_default
  p_born(3)%p(3) = -49.07634310496_default
  p_born(4)%p(0) = 98.91904548743_default
  p_born(4)%p(1) = 56.02241403836_default

```



```

p_born(4)%p(2) = -8.302977504723_default
p_born(4)%p(3) = -10.50293716131_default
p_born(5)%p(0) = 62.25884689208_default
p_born(5)%p(1) = -60.00786540278_default
p_born(5)%p(2) = 4.753602375910_default
p_born(5)%p(3) = 15.32916731546_default
p_born(6)%p(0) = 81.70419369751_default
p_born(6)%p(1) = -52.92670347439_default
p_born(6)%p(2) = 43.57323525898_default
p_born(6)%p(3) = 44.25011295081_default

generator%n_in = 2
allocate (generator%isr_kinematics)
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

mB = 4.2_default
mW = 80.376_default
mtop = 172._default

generator%sqrts = sqrts

!!! Dummy-initialization of the threshold model because generate_fsr_threshold
!!! uses mis_to_mpole to determine if it is above or below threshold.
call init_parameters (mpole, gam_out, mtop, one, one / 1.5_default, 125._default, &
    0.47_default, 0.118_default, 91._default, 80._default, 4.2_default, &
    one, one, one, one, zero, zero, zero, zero, zero, zero, .false., zero)

write (u, "(A)") "* Use four-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
call vector4_check_momentum_conservation &
    (p_born, 2, unit = u, abs_smallness = momentum_tolerance, verbose = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

allocate (generator%real_kinematics)
call generator%real_kinematics%init (7, 2, 2, 2)
call generator%real_kinematics%init_onshell (7, 2)
generator%real_kinematics%p_born_cms%phs_point(1) = p_born

write (u, "(A)") "Get boost projection system -> CMS: "
L_to_cms = get_boost_for_threshold_projection (p_born, sqrts, mtop)
call L_to_cms%write (u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

write (u, "(A)") "* Perform onshell-projection:"
pb1 = generator%real_kinematics%p_born_cms%phs_point(1)
call threshold_projection_born (mtop, L_to_cms, pb1, p_born_onshell)
generator%real_kinematics%p_born_onshell%phs_point(1) = p_born_onshell

call generator%real_kinematics%p_born_onshell%write &
    (1, unit = u, testflag = .true., ultra = .true.)

```

```

pb1_os = generator%real_kinematics%p_born_onshell%phs_point(1)
call check_phsp (pb1_os, 0)

allocate (generator%emitters (2))
generator%emitters(1) = THR_POS_B; generator%emitters(2) = THR_POS_BBAR

allocate (generator%m2 (6), generator%is_massive(6))
generator%m2 = p_born**2
generator%is_massive (1:2) = .false.
generator%is_massive (3:6) = .true.

phs_identifiers(1)%emitter = THR_POS_B
phs_identifiers(2)%emitter = THR_POS_BBAR

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.6_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,A,1X,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

call generator%generate_radiation_variables ([x1,x2,x3], p_born_onshell, phs_identifiers)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_ref_momenta_threshold (p_born_onshell)
    call generator%compute_xi_max (emitter, i_phs, p_born_onshell, &
        generator%real_kinematics%xi_max(i_phs), i_con = thr_leg(emitter))
end do
write (u, "(A)") &
    "* With these, the following radiation variables have been produced: "
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F4.2)") "xi_tilde: ", rad_var%xi_tilde
    write (u, "(A)") "xi_max: "
    write (u, "(2F5.2)") rad_var%xi_max(1), rad_var%xi_max(2)
    write (u, "(A)") "y: "
    write (u, "(2F5.2)") rad_var%y(1), rad_var%y(2)
    write (u, "(A,F4.2)") "phi: ", rad_var%phi
end associate

call write_separator (u)
write (u, "(A)") "* Produce real momenta from on-shell phase space: "
allocate (p_real(7))
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    write (u, "(A,I1)") "emitter: ", emitter
    call generator%generate_fsr_threshold (emitter, i_phs, p_born_onshell, p_real)
    call check_phsp (p_real, emitter)
end do

call write_separator(u)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_5"

contains
subroutine check_phsp (p, emitter)

```

```

type(vector4_t), intent(inout), dimension(:) :: p
integer, intent(in) :: emitter
type(vector4_t) :: pp
real(default) :: E_tot
logical :: check
write (u, "(A)") "* Check momentum conservation: "
call vector4_check_momentum_conservation &
    (p, 2, unit = u, abs_smallness = momentum_tolerance, verbose = .true.)
write (u, "(A)") "* Check invariant masses: "
write (u, "(A)", advance = "no") "inv(W+, b, gl): "
pp = p(THR_POS_WP) + p(THR_POS_B)
if (emitter == THR_POS_B) pp = pp + p(THR_POS_GLUON)
if (nearly_equal (pp**1, mtop)) then
    write (u, "(A)") "CHECK"
else
    write (u, "(A,F7.3)") "FAIL: ", pp**1
end if
write (u, "(A)", advance = "no") "inv(W-, bbar): "
pp = p(THR_POS_WM) + p(THR_POS_BBAR)
if (emitter == THR_POS_BBAR) pp = pp + p(THR_POS_GLUON)
if (nearly_equal (pp**1, mtop)) then
    write (u, "(A)") "CHECK"
else
    write (u, "(A,F7.3)") "FAIL: ", pp**1
end if
write (u, "(A)") "* Sum of energies equal to sqrts?"
E_tot = sum(p(1:2)%p(0)); check = nearly_equal (E_tot, sqrts)
write (u, "(A,L1)") "Initial state: ", check
if (.not. check) write (u, "(A,F7.3)") "E_tot: ", E_tot
if (emitter > 0) then
    E_tot = sum(p(3:7)%p(0))
else
    E_tot = sum(p(3:6)%p(0))
end if
check = nearly_equal (E_tot, sqrts)
write (u, "(A,L1)") "Final state : ", check
if (.not. check) write (u, "(A,F7.3)") "E_tot: ", E_tot
call pacify (p, 1E-6_default)
call vector4_write_set (p, u, testflag = .true., ultra = .true.)

end subroutine check_phsp
end subroutine phs_fks_generator_5

```

<phs fks: test declarations>+≡

public :: phs_fks_generator_6

<phs fks: tests>+≡

```

subroutine phs_fks_generator_6 (u)
integer, intent(in) :: u
type(phs_fks_generator_t) :: generator
type(vector4_t), dimension(:), allocatable :: p_born
type(vector4_t), dimension(:), allocatable :: p_real
real(default) :: x1, x2, x3
real(default) :: mB, mW, mT

```

```

integer :: i, emitter, i_phs
type(phs_identifer_t), dimension(2) :: phs_identifiers

write (u, "(A)") "* Test output: phs_fks_generator_6"
write (u, "(A)") "* Puropse: Create real phase space for particle decays"
write (u, "(A)")

allocate (p_born(4))
p_born(1)%p(0) = 173.1_default
p_born(1)%p(1) = zero
p_born(1)%p(2) = zero
p_born(1)%p(3) = zero
p_born(2)%p(0) = 68.17074462929_default
p_born(2)%p(1) = -37.32578717617_default
p_born(2)%p(2) = 30.99675959336_default
p_born(2)%p(3) = -47.70321718398_default
p_born(3)%p(0) = 65.26639312326_default
p_born(3)%p(1) = -1.362927648502_default
p_born(3)%p(2) = -33.25327150840_default
p_born(3)%p(3) = 56.14324922494_default
p_born(4)%p(0) = 39.66286224745_default
p_born(4)%p(1) = 38.68871482467_default
p_born(4)%p(2) = 2.256511915049_default
p_born(4)%p(3) = -8.440032040958_default

generator%n_in = 1
allocate (generator%isr_kinematics)
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()

mB = 4.2_default
mW = 80.376_default
mT = 173.1_default

generator%sqrts = mT

write (u, "(A)") "* Use four-particle phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

x1=0.5_default; x2=0.25_default; x3=0.6_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,A,1X,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (3, 2, 2, 1)
call generator%real_kinematics%p_born_lab%set_momenta (1, p_born)

allocate (generator%emitters(2))
generator%emitters(1) = 1
generator%emitters(2) = 2
allocate (generator%m2 (4), generator%is_massive(4))

```

```

generator%m2(1) = mT**2
generator%m2(2) = mB**2
generator%m2(3) = zero
generator%m2(4) = zero
generator%is_massive(1:2) = .true.
generator%is_massive(3:4) = .false.
phs_identifiers(1)%emitter = 1
phs_identifiers(2)%emitter = 2

call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
call generator%compute_xi_ref_momenta (p_born)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do

write (u, "(A)") &
    "* With these, the following radiation variables have been produced: "
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F4.2)") "xi_tilde: ", rad_var%xi_tilde
    do i = 1, 2
        write (u, "(A,I1,A,F5.2)") "i: ", i, "y: " , rad_var%y(i)
    end do
    write (u, "(A,F4.2)") "phi: ", rad_var%phi
end associate

call write_separator (u)
write (u, "(A)") "Produce real momenta via initial-state emission: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
allocate (p_real(5))
call generator%generate_isr_fixed_beam_energy (i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator(u)
write (u, "(A)") "Produce real momenta via final-state emission: "
i_phs = 2; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
call generator%generate_fsr (emitter, i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_6"

end subroutine phs_fks_generator_6

```

```

<phs fks: test declarations>+≡
public :: phs_fks_generator_7

<phs fks: tests>+≡
subroutine phs_fks_generator_7 (u)
    integer, intent(in) :: u
    type(phs_fks_generator_t) :: generator

```

```

type(vector4_t), dimension(:), allocatable :: p_born
type(vector4_t), dimension(:), allocatable :: p_real
real(default) :: x1, x2, x3
integer :: i, emitter, i_phs
type(phs_identifier_t), dimension(2) :: phs_identifiers
real(default), parameter :: sqrts = 1000.0_default

write (u, "(A)") "* Test output: phs_fks_generator_7"
write (u, "(A)") "* Puropse: Create real phase space for scattering ISR"
write (u, "(A)") "*           keeping the beam energy fixed."
write (u, "(A)")

allocate (p_born(4))
p_born(1)%p(0) = 500._default
p_born(1)%p(1) = 0._default
p_born(1)%p(2) = 0._default
p_born(1)%p(3) = 500._default
p_born(2)%p(0) = 500._default
p_born(2)%p(1) = 0._default
p_born(2)%p(2) = 0._default
p_born(2)%p(3) = -500._default
p_born(3)%p(0) = 500._default
p_born(3)%p(1) = 11.275563070_default
p_born(3)%p(2) = -13.588797663_default
p_born(3)%p(3) = 486.93070588_default
p_born(4)%p(0) = 500._default
p_born(4)%p(1:3) = -p_born(3)%p(1:3)

phs_identifiers(1)%emitter = 1
phs_identifiers(2)%emitter = 2

allocate (generator%emitters(2))
generator%n_in = 2
allocate (generator%isr_kinematics)
generator%isr_kinematics%isr_mode = SQRTS_FIXED
call generator%set_xi_and_y_bounds ()
generator%emitters(1) = 1; generator%emitters(2) = 2
generator%sqrts = sqrts

write (u, "(A)") "* Use 2 -> 2 phase space containing: "
call vector4_write_set (p_born, u, testflag = .true., ultra = .true.)
write (u, "(A)") "*****"
write (u, "(A)")

x1 = 0.5_default; x2 = 0.25_default; x3 = 0.6_default
write (u, "(A)") "* Use random numbers: "
write (u, "(A,F3.2,1X,A,F3.2,A,1X,F3.2)") &
    "x1: ", x1, "x2: ", x2, "x3: ", x3

allocate (generator%real_kinematics)
call generator%real_kinematics%init (4, 2, 2, 1)
call generator%real_kinematics%p_born_lab%set_momenta (1, p_born)

allocate (generator%m2 (4))

```

```

generator%m2 = 0._default
allocate (generator%is_massive(4))
generator%is_massive = .false.
call generator%generate_radiation_variables ([x1,x2,x3], p_born, phs_identifiers)
call generator%compute_xi_ref_momenta (p_born)
do i_phs = 1, 2
    emitter = phs_identifiers(i_phs)%emitter
    call generator%compute_xi_max (emitter, i_phs, p_born, &
        generator%real_kinematics%xi_max(i_phs))
end do

write (u, "(A)") &
    "* With these, the following radiation variables have been produced: "
associate (rad_var => generator%real_kinematics)
    write (u, "(A,F4.2)") "xi_tilde: ", rad_var%xi_tilde
    do i = 1, 2
        write (u, "(A,I1,A,F5.2)") "i: ", i, "y: " , rad_var%y(i)
    end do
    write (u, "(A,F4.2)") "phi: ", rad_var%phi
end associate

call write_separator (u)
write (u, "(A)") "Produce real momenta via initial-state emission: "
i_phs = 1; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
allocate (p_real(5))
call generator%generate_isr_fixed_beam_energy (i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
call write_separator(u)
i_phs = 2; emitter = phs_identifiers(i_phs)%emitter
write (u, "(A,I1)") "emitter: ", emitter
call generator%generate_isr_fixed_beam_energy (i_phs, p_born, p_real)
call pacify (p_real, 1E-6_default)
call vector4_write_set (p_real, u, testflag = .true., ultra = .true.)
write (u, "(A)")
write (u, "(A)") "* Test output end: phs_fks_generator_7"

end subroutine phs_fks_generator_7

```

19.12 Dispatch

⟨dispatch_phase_space.f90⟩≡
 ⟨File header⟩

module dispatch_phase_space

⟨Use kinds⟩

⟨Use strings⟩

use io_units, only: free_unit

use variables, only: var_list_t

use os_interface, only: os_data_t

```

use diagnostics

use sf_mappings, only: sf_channel_t
use beam_structures, only: beam_structure_t
use dispatch_beams, only: sf_prop_t, strfun_mode

use mappings
use phs_forests, only: phs_parameters_t
use phs_base
use phs_none
use phs_single
use phs_rambo
use phs_wood
use phs_fks

<Standard module head>

<Dispatch phs: public>

contains

<Dispatch phs: procedures>

end module dispatch_phase_space

```

Allocate a phase-space object according to the variable \$phs_method.

```

<Dispatch phs: public>≡
    public :: dispatch_phs

<Dispatch phs: procedures>≡
    subroutine dispatch_phs (phs, var_list, os_data, process_id, &
        mapping_defaults, phs_par, phs_method_in)
        class(phs_config_t), allocatable, intent(inout) :: phs
        type(var_list_t), intent(in) :: var_list
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: process_id
        type(mapping_defaults_t), intent(in), optional :: mapping_defaults
        type(phs_parameters_t), intent(in), optional :: phs_par
        type(string_t), intent(in), optional :: phs_method_in
        type(string_t) :: phs_method, phs_file, run_id
        logical :: use_equivalences, vis_channels, fatal_beam_decay
        integer :: u_phs
        logical :: exist
        if (present (phs_method_in)) then
            phs_method = phs_method_in
        else
            phs_method = &
                var_list%get_sval (var_str ("phs_method"))
        end if
        phs_file = &
            var_list%get_sval (var_str ("phs_file"))
        use_equivalences = &
            var_list%get_lval (var_str ("?use_vamp_equivalences"))
        vis_channels = &
            var_list%get_lval (var_str ("?vis_channels"))
    end subroutine

```



```

fatal_beam_decay = &
    var_list%get_lval (var_str ("?fatal_beam_decay"))
run_id = &
    var_list%get_sval (var_str ("$run_id"))
select case (char (phs_method))
case ("none")
    allocate (phs_none_config_t :: phs)
case ("single")
    allocate (phs_single_config_t :: phs)
    if (vis_channels) then
        call msg_warning ("Visualizing phase space channels not " // &
            "available for method 'single'.")
    end if
case ("rambo")
    allocate (phs_rambo_config_t :: phs)
    if (vis_channels) &
        call msg_warning ("Visualizing phase space channels not " // &
            "available for method 'rambo'.")
case ("fks")
    allocate (phs_fks_config_t :: phs)
    if (use_equivalences) then
        select type (phs)
        type is (phs_fks_config_t)
            call phs%enable_equivalences ()
        end select
    end if
case ("wood", "default", "fast_wood")
    call dispatch_wood ()
case default
    call msg_fatal ("Phase space: parameterization method '" &
        // char (phs_method) // "' not implemented")
end select
contains
<Dispatch phs: dispatch phs: procedures>
end subroutine dispatch_phs

```

```

<Dispatch phs: dispatch phs: procedures>≡
subroutine dispatch_wood ()
    allocate (phs_wood_config_t :: phs)
    select type (phs)
    type is (phs_wood_config_t)
        if (phs_file /= "") then
            inquire (file = char (phs_file), exist = exist)
            if (exist) then
                call msg_message ("Phase space: reading configuration from '" &
                    // char (phs_file) // "'")
                u_phs = free_unit ()
                open (u_phs, file = char (phs_file), &
                    action = "read", status = "old")
                call phs%set_input (u_phs)
            else
                call msg_fatal ("Phase space: configuration file '" &
                    // char (phs_file) // "' not found")
            end if
        end if
    end select
end subroutine dispatch_wood

```

```

end if
if (present (phs_par)) &
    call phs%set_parameters (phs_par)
if (use_equivalences) &
    call phs%enable_equivalences ()
if (present (mapping_defaults)) &
    call phs%set_mapping_defaults (mapping_defaults)
if (phs_method == "fast_wood") phs%use_cascades2 = .true.
phs%vis_channels = vis_channels
phs%fatal_beam_decay = fatal_beam_decay
phs%os_data = os_data
phs%run_id = run_id
end select
end subroutine dispatch_wood

```

Configure channel mappings, using some conditions from the phase space configuration. If there are no structure functions, we enable a default setup with a single (dummy) structure-function channel. Otherwise, we look at the channel collection that we got from the phase-space configuration step. Each entry should be translated into an independent structure-function channel, where typically there is one default entry, which could be mapped using a standard s-channel mapping if the structure function setup recommends this, and other entries with s-channel resonances. The latter need to be translated into global mappings from the structure-function chain.

```

<Dispatch phs: public>+≡
    public :: dispatch_sf_channels

<Dispatch phs: procedures>+≡
    subroutine dispatch_sf_channels (sf_channel, sf_string, sf_prop, coll, &
        var_list, sqrts, beam_structure)
        type(sf_channel_t), dimension(:), allocatable, intent(out) :: sf_channel
        type(string_t), intent(out) :: sf_string
        type(sf_prop_t), intent(in) :: sf_prop
        type(phs_channel_collection_t), intent(in) :: coll
        type(var_list_t), intent(in) :: var_list
        real(default), intent(in) :: sqrts
        type(beam_structure_t), intent(in) :: beam_structure
        type(beam_structure_t) :: beam_structure_tmp
        class(channel_prop_t), allocatable :: prop
        integer :: n_strfun, n_sf_channel, i
        logical :: sf_allow_s_mapping, circe1_map, circe1_generate
        logical :: s_mapping_enable, endpoint_mapping, power_mapping
        logical :: single_parameter
        integer, dimension(:), allocatable :: s_mapping, single_mapping
        real(default) :: s_mapping_power
        real(default) :: circe1_mapping_slope, endpoint_mapping_slope
        real(default) :: power_mapping_eps
        beam_structure_tmp = beam_structure
        call beam_structure_tmp%expand (strfun_mode)
        n_strfun = beam_structure_tmp%get_n_record ()
        sf_string = beam_structure_tmp%to_string (sf_only = .true.)
        sf_allow_s_mapping = &
            var_list%get_lval (var_str ("?sf_allow_s_mapping"))
    end subroutine

```

```

circe1_generate = &
    var_list%get_lval (var_str ("?circe1_generate"))
circe1_map = &
    var_list%get_lval (var_str ("?circe1_map"))
circe1_mapping_slope = &
    var_list%get_rval (var_str ("circe1_mapping_slope"))
s_mapping_enable = .false.
s_mapping_power = 1
endpoint_mapping = .false.
endpoint_mapping_slope = 1
power_mapping = .false.
single_parameter = .false.
select case (char (sf_string))
case ("", "[any particles]")
case ("pdf_builtin, none", &
    "pdf_builtin_photon, none", &
    "none, pdf_builtin", &
    "none, pdf_builtin_photon", &
    "lhpdf, none", &
    "lhpdf_photon, none", &
    "none, lhpdf", &
    "none, lhpdf_photon")
    single_parameter = .true.
case ("pdf_builtin, none => none, pdf_builtin", &
    "pdf_builtin, none => none, pdf_builtin_photon", &
    "pdf_builtin_photon, none => none, pdf_builtin", &
    "pdf_builtin_photon, none => none, pdf_builtin_photon", &
    "lhpdf, none => none, lhpdf", &
    "lhpdf, none => none, lhpdf_photon", &
    "lhpdf_photon, none => none, lhpdf", &
    "lhpdf_photon, none => none, lhpdf_photon")
    allocate (s_mapping (2), source = [1, 2])
    s_mapping_enable = .true.
    s_mapping_power = 2
case ("pdf_builtin, none => none, pdf_builtin => epa, none => none, epa", &
    "pdf_builtin, none => none, pdf_builtin => ewa, none => none, ewa", &
    "pdf_builtin, none => none, pdf_builtin => ewa, none => none, epa", &
    "pdf_builtin, none => none, pdf_builtin => epa, none => none, ewa")
    allocate (s_mapping (2), source = [1, 2])
    s_mapping_enable = .true.
    s_mapping_power = 2
case ("isr, none", &
    "none, isr")
    allocate (single_mapping (1), source = [1])
    single_parameter = .true.
case ("isr, none => none, isr")
    allocate (s_mapping (2), source = [1, 2])
    power_mapping = .true.
    power_mapping_eps = minval (sf_prop%isr_eps)
case ("isr, none => none, isr => epa, none => none, epa", &
    "isr, none => none, isr => ewa, none => none, ewa", &
    "isr, none => none, isr => ewa, none => none, epa", &
    "isr, none => none, isr => epa, none => none, ewa")
    allocate (s_mapping (2), source = [1, 2])

```

```

power_mapping = .true.
power_mapping_eps = minval (sf_prop%isr_eps)
case ("circe1 => isr, none => none, isr => epa, none => none, epa", &
      "circe1 => isr, none => none, isr => ewa, none => none, ewa", &
      "circe1 => isr, none => none, isr => ewa, none => none, epa", &
      "circe1 => isr, none => none, isr => epa, none => none, ewa")
if (circe1_generate) then
  allocate (s_mapping (2), source = [2, 3])
else
  allocate (s_mapping (3), source = [1, 2, 3])
  endpoint_mapping = .true.
  endpoint_mapping_slope = circe1_mapping_slope
end if
power_mapping = .true.
power_mapping_eps = minval (sf_prop%isr_eps)
case ("pdf_builtin, none => none, isr", &
      "pdf_builtin_photon, none => none, isr", &
      "lhpdf, none => none, isr", &
      "lhpdf_photon, none => none, isr")
  allocate (single_mapping (1), source = [2])
case ("isr, none => none, pdf_builtin", &
      "isr, none => none, pdf_builtin_photon", &
      "isr, none => none, lhpdf", &
      "isr, none => none, lhpdf_photon")
  allocate (single_mapping (1), source = [1])
case ("epa, none", &
      "none, epa")
  allocate (single_mapping (1), source = [1])
  single_parameter = .true.
case ("epa, none => none, epa")
  allocate (single_mapping (2), source = [1, 2])
case ("epa, none => none, isr", &
      "isr, none => none, epa", &
      "ewa, none => none, isr", &
      "isr, none => none, ewa")
  allocate (single_mapping (2), source = [1, 2])
case ("pdf_builtin, none => none, epa", &
      "pdf_builtin_photon, none => none, epa", &
      "lhpdf, none => none, epa", &
      "lhpdf_photon, none => none, epa")
  allocate (single_mapping (1), source = [2])
case ("pdf_builtin, none => none, ewa", &
      "pdf_builtin_photon, none => none, ewa", &
      "lhpdf, none => none, ewa", &
      "lhpdf_photon, none => none, ewa")
  allocate (single_mapping (1), source = [2])
case ("epa, none => none, pdf_builtin", &
      "epa, none => none, pdf_builtin_photon", &
      "epa, none => none, lhpdf", &
      "epa, none => none, lhpdf_photon")
  allocate (single_mapping (1), source = [1])
case ("ewa, none => none, pdf_builtin", &
      "ewa, none => none, pdf_builtin_photon", &
      "ewa, none => none, lhpdf", &

```

```

        "ewa, none => none, lhpdf_photon")
        allocate (single_mapping (1), source = [1])
case ("ewa, none", &
      "none, ewa")
        allocate (single_mapping (1), source = [1])
        single_parameter = .true.
case ("ewa, none => none, ewa")
        allocate (single_mapping (2), source = [1, 2])
case ("energy_scan, none => none, energy_scan")
        allocate (s_mapping (2), source = [1, 2])
case ("sf_test_1, none => none, sf_test_1")
        allocate (s_mapping (2), source = [1, 2])
case ("circe1")
        if (circe1_generate) then
            !!! no mapping
        else if (circe1_map) then
            allocate (s_mapping (1), source = [1])
            endpoint_mapping = .true.
            endpoint_mapping_slope = circe1_mapping_slope
        else
            allocate (s_mapping (1), source = [1])
            s_mapping_enable = .true.
        end if
case ("circe1 => isr, none => none, isr")
        if (circe1_generate) then
            allocate (s_mapping (2), source = [2, 3])
        else
            allocate (s_mapping (3), source = [1, 2, 3])
            endpoint_mapping = .true.
            endpoint_mapping_slope = circe1_mapping_slope
        end if
        power_mapping = .true.
        power_mapping_eps = minval (sf_prop%isr_eps)
case ("circe1 => isr, none", &
      "circe1 => none, isr")
        allocate (single_mapping (1), source = [2])
case ("circe1 => epa, none => none, epa")
        if (circe1_generate) then
            allocate (single_mapping (2), source = [2, 3])
        else
            call msg_fatal ("CIRCE/EPA: supported with ?circe1_generate=true &
                           &only")
        end if
case ("circe1 => ewa, none => none, ewa")
        if (circe1_generate) then
            allocate (single_mapping (2), source = [2, 3])
        else
            call msg_fatal ("CIRCE/EWA: supported with ?circe1_generate=true &
                           &only")
        end if
case ("circe1 => epa, none", &
      "circe1 => none, epa")
        if (circe1_generate) then
            allocate (single_mapping (1), source = [2])

```

```

else
  call msg_fatal ("CIRCE/EPA: supported with ?circe1_generate=true &
    &only")
end if
case ("circe1 => epa, none => none, isr", &
  "circe1 => isr, none => none, epa", &
  "circe1 => ewa, none => none, isr", &
  "circe1 => isr, none => none, ewa")
if (circe1_generate) then
  allocate (single_mapping (2), source = [2, 3])
else
  call msg_fatal ("CIRCE/EPA: supported with ?circe1_generate=true &
    &only")
end if
case ("circe2", &
  "gaussian", &
  "beam_events")
  !!! no mapping
case ("circe2 => isr, none => none, isr", &
  "gaussian => isr, none => none, isr", &
  "beam_events => isr, none => none, isr")
  allocate (s_mapping (2), source = [2, 3])
  power_mapping = .true.
  power_mapping_eps = minval (sf_prop%isr_eps)
case ("circe2 => isr, none", &
  "circe2 => none, isr", &
  "gaussian => isr, none", &
  "gaussian => none, isr", &
  "beam_events => isr, none", &
  "beam_events => none, isr")
  allocate (single_mapping (1), source = [2])
case ("circe2 => epa, none => none, epa", &
  "gaussian => epa, none => none, epa", &
  "beam_events => epa, none => none, epa")
  allocate (single_mapping (2), source = [2, 3])
case ("circe2 => epa, none", &
  "circe2 => none, epa", &
  "circe2 => ewa, none", &
  "circe2 => none, ewa", &
  "gaussian => epa, none", &
  "gaussian => none, epa", &
  "gaussian => ewa, none", &
  "gaussian => none, ewa", &
  "beam_events => epa, none", &
  "beam_events => none, epa", &
  "beam_events => ewa, none", &
  "beam_events => none, ewa")
  allocate (single_mapping (1), source = [2])
case ("circe2 => epa, none => none, isr", &
  "circe2 => isr, none => none, epa", &
  "circe2 => ewa, none => none, isr", &
  "circe2 => isr, none => none, ewa", &
  "gaussian => epa, none => none, isr", &
  "gaussian => isr, none => none, epa", &

```

```

    "gaussian => ewa, none => none, isr", &
    "gaussian => isr, none => none, ewa", &
    "beam_events => epa, none => none, isr", &
    "beam_events => isr, none => none, epa", &
    "beam_events => ewa, none => none, isr", &
    "beam_events => isr, none => none, ewa")
    allocate (single_mapping (2), source = [2, 3])
case ("energy_scan")
case default
    call msg_fatal ("Beam structure: " &
        // char (sf_string) // " not supported")
end select
if (sf_allow_s_mapping .and. coll%n > 0) then
    n_sf_channel = coll%n
    allocate (sf_channel (n_sf_channel))
    do i = 1, n_sf_channel
        call sf_channel(i)%init (n_strfun)
        if (allocated (single_mapping)) then
            call sf_channel(i)%activate_mapping (single_mapping)
        end if
        if (allocated (prop)) deallocate (prop)
        call coll%get_entry (i, prop)
        if (allocated (prop)) then
            if (endpoint_mapping .and. power_mapping) then
                select type (prop)
                type is (resonance_t)
                    call sf_channel(i)%set_eir_mapping (s_mapping, &
                        a = endpoint_mapping_slope, eps = power_mapping_eps, &
                        m = prop%mass / sqrts, w = prop%width / sqrts)
                type is (on_shell_t)
                    call sf_channel(i)%set_eio_mapping (s_mapping, &
                        a = endpoint_mapping_slope, eps = power_mapping_eps, &
                        m = prop%mass / sqrts)
                end select
            else if (endpoint_mapping) then
                select type (prop)
                type is (resonance_t)
                    call sf_channel(i)%set_epr_mapping (s_mapping, &
                        a = endpoint_mapping_slope, &
                        m = prop%mass / sqrts, w = prop%width / sqrts)
                type is (on_shell_t)
                    call sf_channel(i)%set_epo_mapping (s_mapping, &
                        a = endpoint_mapping_slope, &
                        m = prop%mass / sqrts)
                end select
            else if (power_mapping) then
                select type (prop)
                type is (resonance_t)
                    call sf_channel(i)%set_ipr_mapping (s_mapping, &
                        eps = power_mapping_eps, &
                        m = prop%mass / sqrts, w = prop%width / sqrts)
                type is (on_shell_t)
                    call sf_channel(i)%set_ipo_mapping (s_mapping, &
                        eps = power_mapping_eps, &

```

```

        m = prop%mass / sqrts)
    end select
else if (allocated (s_mapping)) then
    select type (prop)
    type is (resonance_t)
        call sf_channel(i)%set_res_mapping (s_mapping, &
            m = prop%mass / sqrts, w = prop%width / sqrts, &
            single = single_parameter)
    type is (on_shell_t)
        call sf_channel(i)%set_os_mapping (s_mapping, &
            m = prop%mass / sqrts, &
            single = single_parameter)
    end select
else if (allocated (single_mapping)) then
    select type (prop)
    type is (resonance_t)
        call sf_channel(i)%set_res_mapping (single_mapping, &
            m = prop%mass / sqrts, w = prop%width / sqrts, &
            single = single_parameter)
    type is (on_shell_t)
        call sf_channel(i)%set_os_mapping (single_mapping, &
            m = prop%mass / sqrts, &
            single = single_parameter)
    end select
end if
else if (endpoint_mapping .and. power_mapping) then
    call sf_channel(i)%set_ei_mapping (s_mapping, &
        a = endpoint_mapping_slope, eps = power_mapping_eps)
else if (endpoint_mapping .and. .not. allocated (single_mapping)) then
    call sf_channel(i)%set_ep_mapping (s_mapping, &
        a = endpoint_mapping_slope)
else if (power_mapping .and. .not. allocated (single_mapping)) then
    call sf_channel(i)%set_ip_mapping (s_mapping, &
        eps = power_mapping_eps)
else if (s_mapping_enable .and. .not. allocated (single_mapping)) then
    call sf_channel(i)%set_s_mapping (s_mapping, &
        power = s_mapping_power)
end if
end do
else if (sf_allow_s_mapping) then
    allocate (sf_channel (1))
    call sf_channel(1)%init (n_strfun)
    if (allocated (single_mapping)) then
        call sf_channel(1)%activate_mapping (single_mapping)
    else if (endpoint_mapping .and. power_mapping) then
        call sf_channel(i)%set_ei_mapping (s_mapping, &
            a = endpoint_mapping_slope, eps = power_mapping_eps)
    else if (endpoint_mapping) then
        call sf_channel(1)%set_ep_mapping (s_mapping, &
            a = endpoint_mapping_slope)
    else if (power_mapping) then
        call sf_channel(1)%set_ip_mapping (s_mapping, &
            eps = power_mapping_eps)
    else if (s_mapping_enable) then

```



```

        call sf_channel(1)%set_s_mapping (s_mapping, &
            power = s_mapping_power)
    end if
else
    allocate (sf_channel (1))
    call sf_channel(1)%init (n_strfun)
    if (allocated (single_mapping)) then
        call sf_channel(1)%activate_mapping (single_mapping)
    end if
end if
end subroutine dispatch_sf_channels

```

19.12.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<dispatch_phs_ut.f90>≡
  <File header>

  module dispatch_phs_ut
    use unit_tests
    use dispatch_phs_uti

    <Standard module head>

    <Dispatch phs: public test>

    contains

    <Dispatch phs: test driver>

  end module dispatch_phs_ut

<dispatch_phs_uti.f90>≡
  <File header>

  module dispatch_phs_uti

    <Use kinds>
    <Use strings>
    use variables
    use io_units, only: free_unit
    use os_interface, only: os_data_t
    use process_constants
    use model_data
    use models
    use phs_base
    use phs_none
    use phs_forests
    use phs_wood
    use mappings
    use dispatch_phase_space

    <Standard module head>

```

<Dispatch phs: test declarations>

contains

<Dispatch phs: tests>

end module dispatch_phs_util

API: driver for the unit tests below.

<Dispatch phs: public test>≡

public :: dispatch_phs_test

<Dispatch phs: test driver>≡

subroutine dispatch_phs_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<Dispatch phs: execute tests>

end subroutine dispatch_phs_test

Select type: phase-space configuration object

<Dispatch phs: execute tests>≡

call test (dispatch_phs_1, "dispatch_phs_1", &
"phase-space configuration", &
u, results)

<Dispatch phs: test declarations>≡

public :: dispatch_phs_1

<Dispatch phs: tests>≡

subroutine dispatch_phs_1 (u)

integer, intent(in) :: u

type(var_list_t) :: var_list

class(phs_config_t), allocatable :: phs

type(phs_parameters_t) :: phs_par

type(os_data_t) :: os_data

type(mapping_defaults_t) :: mapping_defs

write (u, "(A)") " * Test output: dispatch_phs_1"

write (u, "(A)") " * Purpose: select phase-space configuration method"

write (u, "(A)")

call var_list%init_defaults (0)

write (u, "(A)") " * Allocate PHS as phs_none_t"

write (u, "(A)")

call var_list%set_string (&

var_str ("phs_method"), &

var_str ("none"), is_known = .true.)

call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_1"))

call phs%write (u)

```

call phs%final ()
deallocate (phs)

write (u, "(A)")
write (u, "(A)")  "* Allocate PHS as phs_single_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("phs_method"), &
    var_str ("single"), is_known = .true.)
call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_1"))
call phs%write (u)

call phs%final ()
deallocate (phs)

write (u, "(A)")
write (u, "(A)")  "* Allocate PHS as phs_wood_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("phs_method"), &
    var_str ("wood"), is_known = .true.)
call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_1"))
call phs%write (u)

call phs%final ()
deallocate (phs)

write (u, "(A)")
write (u, "(A)")  "* Setting parameters for phs_wood_t"
write (u, "(A)")

phs_par%m_threshold_s = 123
phs_par%m_threshold_t = 456
phs_par%t_channel = 42
phs_par%off_shell = 17
phs_par%keep_nonresonant = .false.
mapping_defs%energy_scale = 987
mapping_defs%invariant_mass_scale = 654
mapping_defs%momentum_transfer_scale = 321
mapping_defs%step_mapping = .false.
mapping_defs%step_mapping_exp = .false.
mapping_defs%enable_s_mapping = .true.
call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_1"), &
    mapping_defs, phs_par)
call phs%write (u)

call phs%final ()

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_phs_1"

```

```
end subroutine dispatch_phs_1
```

Phase-space configuration with file

```

<Dispatch phs: execute tests>+≡
  call test (dispatch_phs_2, "dispatch_phs_2", &
    "configure phase space using file", &
    u, results)

<Dispatch phs: test declarations>+≡
  public :: dispatch_phs_2

<Dispatch phs: tests>+≡
  subroutine dispatch_phs_2 (u)
    use phs_base_ut, only: init_test_process_data
    use phs_wood_ut, only: write_test_phs_file
    use phs_forests
    integer, intent(in) :: u
    type(var_list_t) :: var_list
    type(os_data_t) :: os_data
    type(process_constants_t) :: process_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    class(phs_config_t), allocatable :: phs
    integer :: u_phs

    write (u, "(A)")  "* Test output: dispatch_phs_2"
    write (u, "(A)")  "* Purpose: select 'wood' phase-space &
      &for a test process"
    write (u, "(A)")  "*           and read phs configuration from file"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize a process"
    write (u, "(A)")

    call var_list%init_defaults (0)
    call os_data%init ()
    call syntax_model_file_init ()
    call model_list%read_model &
      (var_str ("Test"), var_str ("Test.mdl"), os_data, model)

    call syntax_phs_forest_init ()

    call init_test_process_data (var_str ("dispatch_phs_2"), process_data)

    write (u, "(A)")  "* Write phase-space file"

    u_phs = free_unit ()
    open (u_phs, file = "dispatch_phs_2.phs", action = "write", status = "replace")
    call write_test_phs_file (u_phs, var_str ("dispatch_phs_2"))
    close (u_phs)

    write (u, "(A)")

```

```

write (u, "(A)")  "** Allocate PHS as phs_wood_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("phs_method"), &
    var_str ("wood"), is_known = .true.)
call var_list%set_string (&
    var_str ("phs_file"), &
    var_str ("dispatch_phs_2.phs"), is_known = .true.)
call dispatch_phs (phs, var_list, os_data, var_str ("dispatch_phs_2"))

call phs%init (process_data, model)
call phs%configure (sqrts = 1000._default)

call phs%write (u)
write (u, "(A)")
select type (phs)
type is (phs_wood_config_t)
    call phs%write_forest (u)
end select

call phs%final ()

call var_list%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: dispatch_phs_2"

end subroutine dispatch_phs_2

```

@

19.13 A lexer for O'Mega's phase-space output

This module provides three data types. One of them is the type `dag_string_t` which should contain the information of all Feynman diagrams in the factorized form which is provided by O'Mega in its phase-space output. This output is translated into a string of tokens (in the form of an array of the type `dag_token_t`) which have a certain meaning. The purpose of this module is only to identify these tokens correctly and to provide some procedures and interfaces which allow us to use these strings in a similar way as variables of the basic character type or the type `iso_varying_string`. Both `character` and `iso_varying_string` have some disadvantages at least if one wants to keep support for some older compiler versions. These can be circumvented by the `dag_string_t` type. Finally the `dag_chain_t` type is used to create a larger string in several steps without always recreating the string, which is done in the form of a simple linked list. In the end one can create a single `dag_string` out of this list, which is more useful.

```

(cascades2_lexer.f90)≡
  <File header>

```

```

module cascades2_lexer

  <Use kinds>
    use kinds, only: TC, i8

  <Standard module head>

  <Cascades2 lexer: public>

  <Cascades2 lexer: parameters>

  <Cascades2 lexer: types>

  <Cascades2 lexer: interfaces>

  contains

  <Cascades2 lexer: procedures>

end module cascades2_lexer

```

This is the token type. By default the variable `type` is `EMPTY_TK` but can obtain other values corresponding to the parameters defined below. The type of the token corresponds to a particular sequence of characters. When the token corresponds to a node of a tree, i.e. some particle in the Feynman diagram, the type is `NODE_TK` and the `particle_name` variable is holding the name of the particle. O'Megas output contains in addition to the particle name some numbers which indicate the external momenta that are flowing through this line. These numbers are translated into a binary code and saved in the variable `bincode`. In this case the number 1 corresponds to a bit set at position 0, 2 corresponds to a bit set at position 1, etc. Instead of numbers which are composed out of several digits, letters are used, i.e. A instead of 10 (bit at position 9), B instead of 11 (bit at position 10), etc.

When the DAG is reconstructed from a `dag_string` which was built from O'Mega's output, this string is modified such that a substring (a set of tokens) is replaced by a single token where the type variable is one of the three parameters `DAG_NODE_TK`, `DAG_OPTIONS_TK` and `DAG_COMBINATION_TK`. These parameters correspond to the three types `dag_node_t`, `dag_options_t` and `dag_combination_t` (see `cascades2` for more information. In this case, since these objects are organized in arrays, the `index` variable holds the corresponding position in the array.

In any case, we want to be able to reproduce the character string from which a token (or a string) has been created. The variable `char_len` is the length of this string. For tokens with the type `DAG_NODE_TK`, `DAG_OPTIONS_TK` and `DAG_COMBINATION_TK` we use output of the form `<N23>`, `<O23>` or `<C23>` which is useful for debugging the parser. Here 23 is the `index` and N, O or C obviously corresponds to the `type`.

```

<Cascades2 lexer: parameters>≡
  integer, parameter :: PRT_NAME_LEN = 20
<Cascades2 lexer: public>≡

```

```

    public :: dag_token_t
<Cascades2 lexer: types>≡
    type :: dag_token_t
        integer :: type = EMPTY_TK
        integer :: char_len = 0
        integer(TC) :: bincode = 0
        character (PRT_NAME_LEN) :: particle_name=""
        integer :: index = 0
    contains
        <Cascades2 lexer: dag token: TBP>
    end type dag_token_t

```

This is the string type. It also holds the number of characters in the corresponding character string. It contains an array of tokens. If the `dag_string` is constructed using the type `dag_chain_t`, which creates a linked list, we also need the pointer `next`.

```

<Cascades2 lexer: public>+≡
    public :: dag_string_t
<Cascades2 lexer: types>+≡
    type :: dag_string_t
        integer :: char_len = 0
        type (dag_token_t), dimension(:), allocatable :: t
        type (dag_string_t), pointer :: next => null ()
    contains
        <Cascades2 lexer: dag string: TBP>
    end type dag_string_t

```

This is the chain of `dag_strings`. It allows us to construct a large string by appending new strings to the linked list, which can later be merged to a single string. This is very useful because the file written by O'Mega contains large strings where each string contains all Feynman diagrams in a factorized form, but these large strings are cut into several pieces and distributed over many lines. As the file can become large, rewriting a new `dag_string` (or `iso_varying_string`) would consume more and more time with each additional line. For recreating a single `dag_string` out of this chain, we need the total character length and the sum of all sizes of the `dag_token` arrays `t`.

```

<Cascades2 lexer: public>+≡
    public :: dag_chain_t
<Cascades2 lexer: types>+≡
    type :: dag_chain_t
        integer :: char_len = 0
        integer :: t_size = 0
        type (dag_string_t), pointer :: first => null ()
        type (dag_string_t), pointer :: last => null ()
    contains
        <Cascades2 lexer: dag chain: TBP>
    end type dag_chain_t

```

We define two parameters holding the characters corresponding to a backslash and a blanc space.

```
<Cascades2 lexer: parameters>+≡
    character(len=1), parameter, public :: BACKSLASH_CHAR = "\\"
    character(len=1), parameter :: BLANC_CHAR = " "
```

These are the parameters which correspond to meaningful types of token.

```
<Cascades2 lexer: parameters>+≡
    integer, parameter, public :: NEW_LINE_TK = -2
    integer, parameter :: BLANC_SPACE_TK = -1
    integer, parameter :: EMPTY_TK = 0
    integer, parameter, public :: NODE_TK = 1
    integer, parameter, public :: DAG_NODE_TK = 2
    integer, parameter, public :: DAG_OPTIONS_TK = 3
    integer, parameter, public :: DAG_COMBINATION_TK = 4
    integer, parameter, public :: COLON_TK = 11
    integer, parameter, public :: COMMA_TK = 12
    integer, parameter, public :: VERTICAL_BAR_TK = 13
    integer, parameter, public :: OPEN_PAR_TK = 21
    integer, parameter, public :: CLOSED_PAR_TK = 22
    integer, parameter, public :: OPEN_CURLY_TK = 31
    integer, parameter, public :: CLOSED_CURLY_TK = 32
```

Different sorts of assignment. This contains the conversion of a character variable into a dag_token or dag_string.

```
<Cascades2 lexer: public>+≡
    public :: assignment (=)

<Cascades2 lexer: interfaces>≡
    interface assignment (=)
        module procedure dag_token_assign_from_char_string
        module procedure dag_token_assign_from_dag_token
        module procedure dag_string_assign_from_dag_token
        module procedure dag_string_assign_from_char_string
        module procedure dag_string_assign_from_dag_string
        module procedure dag_string_assign_from_dag_token_array
    end interface assignment (=)
```

```
<Cascades2 lexer: dag token: TBP>≡
    procedure :: init_dag_object_token => dag_token_init_dag_object_token
```

```
<Cascades2 lexer: procedures>≡
    subroutine dag_token_init_dag_object_token (dag_token, type, index)
        class (dag_token_t), intent (out) :: dag_token
        integer, intent (in) :: index
        integer :: type
        dag_token%type = type
        dag_token%char_len = integer_n_dec_digits (index) + 3
        dag_token%index = index
    contains
        function integer_n_dec_digits (number) result (n_digits)
            integer, intent (in) :: number
            integer :: n_digits
            integer :: div_number
```



```

n_digits = 0
div_number = number
do
    div_number = div_number / 10
    n_digits = n_digits + 1
    if (div_number == 0) exit
enddo
end function integer_n_dec_digits
end subroutine dag_token_init_dag_object_token

```

<Cascades2 lexer: procedures>+≡

```

elemental subroutine dag_token_assign_from_char_string (dag_token, char_string)
    type (dag_token_t), intent (out) :: dag_token
    character (len=*), intent (in) :: char_string
    integer :: i, j
    logical :: set_bincode
    integer :: bit_pos
    character (len=10) :: index_char
    dag_token%char_len = len (char_string)
    if (dag_token%char_len == 1) then
        select case (char_string(1:1))
            case (BACKSLASH_CHAR)
                dag_token%type = NEW_LINE_TK
            case (" ")
                dag_token%type = BLANC_SPACE_TK
            case (":")
                dag_token%type = COLON_TK
            case (",")
                dag_token%type = COMMA_TK
            case ("|")
                dag_token%type = VERTICAL_BAR_TK
            case "("
                dag_token%type = OPEN_PAR_TK
            case (")")
                dag_token%type = CLOSED_PAR_TK
            case "{"
                dag_token%type = OPEN_CURLY_TK
            case "}"
                dag_token%type = CLOSED_CURLY_TK
        end select
    else if (char_string(1:1) == "<") then
        select case (char_string(2:2))
            case ("N")
                dag_token%type = DAG_NODE_TK
            case ("O")
                dag_token%type = DAG_OPTIONS_TK
            case ("C")
                dag_token%type = DAG_COMBINATION_TK
        end select
        read(char_string(3:dag_token%char_len-1), fmt="(I10)") dag_token%index
    else
        dag_token%bincode = 0
        set_bincode = .false.
        do i=1, dag_token%char_len

```

```

select case (char_string(i:i))
case "["
    dag_token%type = NODE_TK
    if (i > 1) then
        do j = 1, i - 1
            dag_token%particle_name(j:j) = char_string(j:j)
        enddo
    end if
    set_bincode = .true.
case "]"
    set_bincode = .false.
case default
    dag_token%type = NODE_TK
    if (set_bincode) then
        select case (char_string(i:i))
        case ("1", "2", "3", "4", "5", "6", "7", "8", "9")
            read (char_string(i:i), fmt="(I1)") bit_pos
        case ("A")
            bit_pos = 10
        case ("B")
            bit_pos = 11
        case ("C")
            bit_pos = 12
        end select
        dag_token%bincode = ibset(dag_token%bincode, bit_pos - 1)
    end if
end select
if (dag_token%type /= NODE_TK) exit
enddo
end if
end subroutine dag_token_assign_from_char_string

```

<Cascades2 lexer: procedures>+≡

```

elemental subroutine dag_token_assign_from_dag_token (token_out, token_in)
    type (dag_token_t), intent (out) :: token_out
    type (dag_token_t), intent (in) :: token_in
    token_out%type = token_in%type
    token_out%char_len = token_in%char_len
    token_out%bincode = token_in%bincode
    token_out%particle_name = token_in%particle_name
    token_out%index = token_in%index
end subroutine dag_token_assign_from_dag_token

```

<Cascades2 lexer: procedures>+≡

```

elemental subroutine dag_string_assign_from_dag_token (dag_string, dag_token)
    type (dag_string_t), intent (out) :: dag_string
    type (dag_token_t), intent (in) :: dag_token
    allocate (dag_string%t(1))
    dag_string%t(1) = dag_token
    dag_string%char_len = dag_token%char_len
end subroutine dag_string_assign_from_dag_token

```

<Cascades2 lexer: procedures>+≡

```

subroutine dag_string_assign_from_dag_token_array (dag_string, dag_token)
  type (dag_string_t), intent (out) :: dag_string
  type (dag_token_t), dimension(:), intent (in) :: dag_token
  allocate (dag_string%t(size(dag_token)))
  dag_string%t = dag_token
  dag_string%char_len = sum(dag_token%char_len)
end subroutine dag_string_assign_from_dag_token_array

```

<Cascades2 lexer: procedures>+≡

```

elemental subroutine dag_string_assign_from_char_string (dag_string, char_string)
  type (dag_string_t), intent (out) :: dag_string
  character (len=*), intent (in) :: char_string
  type (dag_token_t), dimension(:), allocatable :: token
  integer :: token_pos
  integer :: i
  character (len=len(char_string)) :: node_char
  integer :: node_char_len
  node_char = ""
  dag_string%char_len = len (char_string)
  if (dag_string%char_len > 0) then
    allocate (token(dag_string%char_len))
    token_pos = 0
    node_char_len = 0
    do i=1, dag_string%char_len
      select case (char_string(i:i))
        case (BACKSLASH_CHAR, " ", ":", " ", "|", "(", ")", "{", "}")
          if (node_char_len > 0) then
            token_pos = token_pos + 1
            token(token_pos) = node_char(:node_char_len)
            node_char_len = 0
          end if
          token_pos = token_pos + 1
          token(token_pos) = char_string(i:i)
        case default
          node_char_len = node_char_len + 1
          node_char(node_char_len:node_char_len) = char_string(i:i)
      end select
    enddo
    if (node_char_len > 0) then
      token_pos = token_pos + 1
      token(token_pos) = node_char(:node_char_len)
    end if
    if (token_pos > 0) then
      allocate (dag_string%t(token_pos))
      dag_string%t = token(:token_pos)
      deallocate (token)
    end if
  end if
end subroutine dag_string_assign_from_char_string

```

<Cascades2 lexer: procedures>+≡

```

elemental subroutine dag_string_assign_from_dag_string (string_out, string_in)
  type (dag_string_t), intent (out) :: string_out

```

```

type (dag_string_t), intent (in) :: string_in
if (allocated (string_in%t)) then
    allocate (string_out%t (size(string_in%t)))
    string_out%t = string_in%t
end if
string_out%char_len = string_in%char_len
end subroutine dag_string_assign_from_dag_string

```

Concatenate strings/tokens. The result is always a **dag_string**.

<Cascades2 lexer: public>+≡

```
public :: operator (//)
```

<Cascades2 lexer: interfaces>+≡

```

interface operator (//)
    module procedure concat_dag_token_dag_token
    module procedure concat_dag_string_dag_token
    module procedure concat_dag_token_dag_string
    module procedure concat_dag_string_dag_string
end interface operator (//)

```

<Cascades2 lexer: procedures>+≡

```

function concat_dag_token_dag_token (token1, token2) result (res_string)
    type (dag_token_t), intent (in) :: token1, token2
    type (dag_string_t) :: res_string
    if (token1%type == EMPTY_TK) then
        res_string = token2
    else if (token2%type == EMPTY_TK) then
        res_string = token1
    else
        allocate (res_string%t(2))
        res_string%t(1) = token1
        res_string%t(2) = token2
        res_string%char_len = token1%char_len + token2%char_len
    end if
end function concat_dag_token_dag_token

```

<Cascades2 lexer: procedures>+≡

```

function concat_dag_string_dag_token (dag_string, dag_token) result (res_string)
    type (dag_string_t), intent (in) :: dag_string
    type (dag_token_t), intent (in) :: dag_token
    type (dag_string_t) :: res_string
    integer :: t_size
    if (dag_string%char_len == 0) then
        res_string = dag_token
    else if (dag_token%type == EMPTY_TK) then
        res_string = dag_string
    else
        t_size = size (dag_string%t)
        allocate (res_string%t(t_size+1))
        res_string%t(:t_size) = dag_string%t
        res_string%t(t_size+1) = dag_token
        res_string%char_len = dag_string%char_len + dag_token%char_len
    end if
end function

```

```
end function concat_dag_string_dag_token
```

<Cascades2 lexer: procedures>+≡

```
function concat_dag_token_dag_string (dag_token, dag_string) result (res_string)
  type (dag_token_t), intent (in) :: dag_token
  type (dag_string_t), intent (in) :: dag_string
  type (dag_string_t) :: res_string
  integer :: t_size
  if (dag_token%type == EMPTY_TK) then
    res_string = dag_string
  else if (dag_string%char_len == 0) then
    res_string = dag_token
  else
    t_size = size (dag_string%t)
    allocate (res_string%t(t_size+1))
    res_string%t(2:t_size+1) = dag_string%t
    res_string%t(1) = dag_token
    res_string%char_len = dag_token%char_len + dag_string%char_len
  end if
end function concat_dag_token_dag_string
```

<Cascades2 lexer: procedures>+≡

```
function concat_dag_string_dag_string (string1, string2) result (res_string)
  type (dag_string_t), intent (in) :: string1, string2
  type (dag_string_t) :: res_string
  integer :: t1_size, t2_size, t_size
  if (string1%char_len == 0) then
    res_string = string2
  else if (string2%char_len == 0) then
    res_string = string1
  else
    t1_size = size (string1%t)
    t2_size = size (string2%t)
    t_size = t1_size + t2_size
    if (t_size > 0) then
      allocate (res_string%t(t_size))
      res_string%t(:t1_size) = string1%t
      res_string%t(t1_size+1:) = string2%t
      res_string%char_len = string1%char_len + string2%char_len
    end if
  end if
end function concat_dag_string_dag_string
```

Compare strings/tokens/characters. Each character is relevant, including all blanc spaces. An exception is the **newline** character which is not treated by the types used in this module (not to confused with the type parameter **NEW_LINE_TK** which corresponds to the backslash character and simply tells us that the string continues on the next line in the file).

<Cascades2 lexer: public>+≡

```
public :: operator (==)
```

<Cascades2 lexer: interfaces>+≡

```
interface operator (==)
```

```

module procedure dag_token_eq_dag_token
module procedure dag_string_eq_dag_string
module procedure dag_token_eq_dag_string
module procedure dag_string_eq_dag_token
module procedure dag_token_eq_char_string
module procedure char_string_eq_dag_token
module procedure dag_string_eq_char_string
module procedure char_string_eq_dag_string
end interface operator (==)

```

<Cascades2 lexer: procedures>+≡

```

elemental function dag_token_eq_dag_token (token1, token2) result (flag)
  type (dag_token_t), intent (in) :: token1, token2
  logical :: flag
  flag = (token1%type == token2%type) .and. &
        (token1%char_len == token2%char_len) .and. &
        (token1%bincode == token2%bincode) .and. &
        (token1%index == token2%index) .and. &
        (token1%particle_name == token2%particle_name)
end function dag_token_eq_dag_token

```

<Cascades2 lexer: procedures>+≡

```

elemental function dag_string_eq_dag_string (string1, string2) result (flag)
  type (dag_string_t), intent (in) :: string1, string2
  logical :: flag
  flag = (string1%char_len == string2%char_len) .and. &
        (allocated (string1%t) .eqv. allocated (string2%t))
  if (flag) then
    if (allocated (string1%t)) flag = all (string1%t == string2%t)
  end if
end function dag_string_eq_dag_string

```

<Cascades2 lexer: procedures>+≡

```

elemental function dag_token_eq_dag_string (dag_token, dag_string) result (flag)
  type (dag_token_t), intent (in) :: dag_token
  type (dag_string_t), intent (in) :: dag_string
  logical :: flag
  flag = size (dag_string%t) == 1 .and. &
        dag_string%char_len == dag_token%char_len
  if (flag) flag = (dag_string%t(1) == dag_token)
end function dag_token_eq_dag_string

```

<Cascades2 lexer: procedures>+≡

```

elemental function dag_string_eq_dag_token (dag_string, dag_token) result (flag)
  type (dag_token_t), intent (in) :: dag_token
  type (dag_string_t), intent (in) :: dag_string
  logical :: flag
  flag = (dag_token == dag_string)
end function dag_string_eq_dag_token

```

<Cascades2 lexer: procedures>+≡

```

elemental function dag_token_eq_char_string (dag_token, char_string) result (flag)

```

```

    type (dag_token_t), intent (in) :: dag_token
    character (len=*), intent (in) :: char_string
    logical :: flag
    flag = (char (dag_token) == char_string)
end function dag_token_eq_char_string

```

<Cascades2 lexer: procedures>+≡

```

    elemental function char_string_eq_dag_token (char_string, dag_token) result (flag)
        type (dag_token_t), intent (in) :: dag_token
        character (len=*), intent (in) :: char_string
        logical :: flag
        flag = (char (dag_token) == char_string)
    end function char_string_eq_dag_token

```

<Cascades2 lexer: procedures>+≡

```

    elemental function dag_string_eq_char_string (dag_string, char_string) result (flag)
        type (dag_string_t), intent (in) :: dag_string
        character (len=*), intent (in) :: char_string
        logical :: flag
        flag = (char (dag_string) == char_string)
    end function dag_string_eq_char_string

```

<Cascades2 lexer: procedures>+≡

```

    elemental function char_string_eq_dag_string (char_string, dag_string) result (flag)
        type (dag_string_t), intent (in) :: dag_string
        character (len=*), intent (in) :: char_string
        logical :: flag
        flag = (char (dag_string) == char_string)
    end function char_string_eq_dag_string

```

<Cascades2 lexer: public>+≡

```

    public :: operator (/=)

```

<Cascades2 lexer: interfaces>+≡

```

    interface operator (/=)
        module procedure dag_token_ne_dag_token
        module procedure dag_string_ne_dag_string
        module procedure dag_token_ne_dag_string
        module procedure dag_string_ne_dag_token
        module procedure dag_token_ne_char_string
        module procedure char_string_ne_dag_token
        module procedure dag_string_ne_char_string
        module procedure char_string_ne_dag_string
    end interface operator (/=)

```

<Cascades2 lexer: procedures>+≡

```

    elemental function dag_token_ne_dag_token (token1, token2) result (flag)
        type (dag_token_t), intent (in) :: token1, token2
        logical :: flag
        flag = .not. (token1 == token2)
    end function dag_token_ne_dag_token

```

```

<Cascades2 lexer: procedures>+≡
  elemental function dag_string_ne_dag_string (string1, string2) result (flag)
    type (dag_string_t), intent (in) :: string1, string2
    logical :: flag
    flag = .not. (string1 == string2)
  end function dag_string_ne_dag_string

<Cascades2 lexer: procedures>+≡
  elemental function dag_token_ne_dag_string (dag_token, dag_string) result (flag)
    type (dag_token_t), intent (in) :: dag_token
    type (dag_string_t), intent (in) :: dag_string
    logical :: flag
    flag = .not. (dag_token == dag_string)
  end function dag_token_ne_dag_string

<Cascades2 lexer: procedures>+≡
  elemental function dag_string_ne_dag_token (dag_string, dag_token) result (flag)
    type (dag_token_t), intent (in) :: dag_token
    type (dag_string_t), intent (in) :: dag_string
    logical :: flag
    flag = .not. (dag_string == dag_token)
  end function dag_string_ne_dag_token

<Cascades2 lexer: procedures>+≡
  elemental function dag_token_ne_char_string (dag_token, char_string) result (flag)
    type (dag_token_t), intent (in) :: dag_token
    character (len=*), intent (in) :: char_string
    logical :: flag
    flag = .not. (dag_token == char_string)
  end function dag_token_ne_char_string

<Cascades2 lexer: procedures>+≡
  elemental function char_string_ne_dag_token (char_string, dag_token) result (flag)
    type (dag_token_t), intent (in) :: dag_token
    character (len=*), intent (in) :: char_string
    logical :: flag
    flag = .not. (char_string == dag_token)
  end function char_string_ne_dag_token

<Cascades2 lexer: procedures>+≡
  elemental function dag_string_ne_char_string (dag_string, char_string) result (flag)
    type (dag_string_t), intent (in) :: dag_string
    character (len=*), intent (in) :: char_string
    logical :: flag
    flag = .not. (dag_string == char_string)
  end function dag_string_ne_char_string

<Cascades2 lexer: procedures>+≡
  elemental function char_string_ne_dag_string (char_string, dag_string) result (flag)
    type (dag_string_t), intent (in) :: dag_string
    character (len=*), intent (in) :: char_string
    logical :: flag

```



```

        flag = .not. (char_string == dag_string)
    end function char_string_ne_dag_string

```

Convert a dag_token or dag_string to character.

<Cascades2 lexer: public>+≡

```

    public :: char

```

<Cascades2 lexer: interfaces>+≡

```

    interface char
        module procedure char_dag_token
        module procedure char_dag_string
    end interface char

```

<Cascades2 lexer: procedures>+≡

```

    pure function char_dag_token (dag_token) result (char_string)
        type (dag_token_t), intent (in) :: dag_token
        character (dag_token%char_len) :: char_string
        integer :: i
        integer :: name_len
        integer :: bc_pos
        integer :: n_digits
        character (len=9) :: fmt_spec
        select case (dag_token%type)
        case (EMPTY_TK)
            char_string = ""
        case (NEW_LINE_TK)
            char_string = BACKSLASH_CHAR
        case (BLANC_SPACE_TK)
            char_string = " "
        case (COLON_TK)
            char_string = ":"
        case (COMMA_TK)
            char_string = ","
        case (VERTICAL_BAR_TK)
            char_string = "|"
        case (OPEN_PAR_TK)
            char_string = "("
        case (CLOSED_PAR_TK)
            char_string = ")"
        case (OPEN_CURLY_TK)
            char_string = "{"
        case (CLOSED_CURLY_TK)
            char_string = "}"
        case (DAG_NODE_TK, DAG_OPTIONS_TK, DAG_COMBINATION_TK)
            n_digits = dag_token%char_len - 3
            fmt_spec = ""
            if (n_digits > 9) then
                write (fmt_spec, fmt="(A,I2,A)") "(A,I", n_digits, ",A)"
            else
                write (fmt_spec, fmt="(A,I1,A)") "(A,I", n_digits, ",A)"
            end if
            select case (dag_token%type)
            case (DAG_NODE_TK)
                write (char_string, fmt=fmt_spec) "<N", dag_token%index, ">"

```

```

        case (DAG_OPTIONS_TK)
            write (char_string, fmt=fmt_spec) "<0", dag_token%index, ">"
        case (DAG_COMBINATION_TK)
            write (char_string, fmt=fmt_spec) "<C", dag_token%index, ">"
        end select
    case (NODE_TK)
        name_len = len_trim (dag_token%particle_name)
        char_string = dag_token%particle_name
        bc_pos = name_len + 1
        char_string(bc_pos:bc_pos) = "["
        do i=0, bit_size (dag_token%bincode) - 1
            if (btest (dag_token%bincode, i)) then
                bc_pos = bc_pos + 1
                select case (i)
                    case (0, 1, 2, 3, 4, 5, 6, 7, 8)
                        write (char_string(bc_pos:bc_pos), fmt="(I1)") i + 1
                    case (9)
                        write (char_string(bc_pos:bc_pos), fmt="(A1)") "A"
                    case (10)
                        write (char_string(bc_pos:bc_pos), fmt="(A1)") "B"
                    case (11)
                        write (char_string(bc_pos:bc_pos), fmt="(A1)") "C"
                end select
                bc_pos = bc_pos + 1
            if (bc_pos == dag_token%char_len) then
                write (char_string(bc_pos:bc_pos), fmt="(A1)") "]"
                return
            else
                write (char_string(bc_pos:bc_pos), fmt="(A1)") "/"
            end if
        end if
    enddo
end select
end function char_dag_token

```

<Cascades2 lexer: procedures>+≡

```

pure function char_dag_string (dag_string) result (char_string)
    type (dag_string_t), intent (in) :: dag_string
    character (dag_string%char_len) :: char_string
    integer :: pos
    integer :: i
    char_string = ""
    pos = 0
    do i=1, size(dag_string%t)
        char_string(pos+1:pos+dag_string%t(i)%char_len) = char (dag_string%t(i))
        pos = pos + dag_string%t(i)%char_len
    enddo
end function char_dag_string

```

Remove all tokens which are irrelevant for parsing. These are of type NEW_LINE_TK, BLANC_SPACE_TK and EMPTY_TK.

<Cascades2 lexer: dag string: TBP>≡

```

procedure :: clean => dag_string_clean

```

```

<Cascades2 lexer: procedures>+≡
subroutine dag_string_clean (dag_string)
  class (dag_string_t), intent (inout) :: dag_string
  type (dag_token_t), dimension(:), allocatable :: tmp_token
  integer :: n_keep
  integer :: i
  n_keep = 0
  dag_string%char_len = 0
  allocate (tmp_token (size(dag_string%t)))
  do i=1, size (dag_string%t)
    select case (dag_string%t(i)%type)
      case(NEW_LINE_TK, BLANC_SPACE_TK, EMPTY_TK)
      case default
        n_keep = n_keep + 1
        tmp_token(n_keep) = dag_string%t(i)
        dag_string%char_len = dag_string%char_len + dag_string%t(i)%char_len
    end select
  enddo
  deallocate (dag_string%t)
  allocate (dag_string%t(n_keep))
  dag_string%t = tmp_token(:n_keep)
end subroutine dag_string_clean

```

If we operate explicitly on the token array `t` of a `dag_string`, the variable `char_len` is not automatically modified. It can however be determined afterwards using the following subroutine.

```

<Cascades2 lexer: dag_string: TBP>+≡
  procedure :: update_char_len => dag_string_update_char_len

<Cascades2 lexer: procedures>+≡
subroutine dag_string_update_char_len (dag_string)
  class (dag_string_t), intent (inout) :: dag_string
  integer :: char_len
  integer :: i
  char_len = 0
  if (allocated (dag_string%t)) then
    do i=1, size (dag_string%t)
      char_len = char_len + dag_string%t(i)%char_len
    enddo
  end if
  dag_string%char_len = char_len
end subroutine dag_string_update_char_len

```

Append a `dag_string` to a `dag_chain`. The argument `char_string` is of type `character` because the subroutine is used for reading from the file produced by O'Mega which is first read line by line to a character variable.

```

<Cascades2 lexer: dag_chain: TBP>≡
  procedure :: append => dag_chain_append_string

<Cascades2 lexer: procedures>+≡
subroutine dag_chain_append_string (dag_chain, char_string)
  class (dag_chain_t), intent (inout) :: dag_chain
  character (len=*), intent (in) :: char_string

```

```

if (.not. associated (dag_chain%first)) then
  allocate (dag_chain%first)
  dag_chain%last => dag_chain%first
else
  allocate (dag_chain%last%next)
  dag_chain%last => dag_chain%last%next
end if
dag_chain%last = char_string
dag_chain%char_len = dag_chain%char_len + dag_chain%last%char_len
dag_chain%t_size = dag_chain%t_size + size (dag_chain%last%t)
end subroutine dag_chain_append_string

```

Reduce the linked list of dag_string objects which are attached to a given dag_chain object to a single dag_string.

```

<Cascades2 lexer: dag_chain: TBP>+≡
  procedure :: compress => dag_chain_compress

<Cascades2 lexer: procedures>+≡
  subroutine dag_chain_compress (dag_chain)
    class (dag_chain_t), intent (inout) :: dag_chain
    type (dag_string_t), pointer :: current
    type (dag_string_t), pointer :: remove
    integer :: filled_t
    current => dag_chain%first
    dag_chain%first => null ()
    allocate (dag_chain%first)
    dag_chain%last => dag_chain%first
    dag_chain%first%char_len = dag_chain%char_len
    allocate (dag_chain%first%t (dag_chain%t_size))
    filled_t = 0
    do while (associated (current))
      dag_chain%first%t(filled_t+1:filled_t+size(current%t)) = current%t
      filled_t = filled_t + size (current%t)
      remove => current
      current => current%next
      deallocate (remove)
    enddo
  end subroutine dag_chain_compress

```

Finalizer for dag_string_t.

```

<Cascades2 lexer: dag_string: TBP>+≡
  procedure :: final => dag_string_final

<Cascades2 lexer: procedures>+≡
  subroutine dag_string_final (dag_string)
    class (dag_string_t), intent (inout) :: dag_string
    if (allocated (dag_string%t)) deallocate (dag_string%t)
    dag_string%next => null ()
  end subroutine dag_string_final

```

Finalizer for dag_chain_t.

```

<Cascades2 lexer: dag_chain: TBP>+≡
  procedure :: final => dag_chain_final

```

```

<Cascades2 lexer: procedures>+≡
  subroutine dag_chain_final (dag_chain)
    class (dag_chain_t), intent (inout) :: dag_chain
    type (dag_string_t), pointer :: current
    current => dag_chain%first
    do while (associated (current))
      dag_chain%first => dag_chain%first%next
      call current%final ()
      deallocate (current)
      current => dag_chain%first
    enddo
    dag_chain%last => null ()
  end subroutine dag_chain_final

```

```

<cascades2_lexer_ut.f90>≡
  <File header>

```

```

  module cascades2_lexer_ut
    use unit_tests
    use cascades2_lexer_util

```

```

  <Standard module head>

```

```

  <Cascades2 lexer: public test>

```

```

  contains

```

```

  <Cascades2 lexer: test driver>

```

```

  end module cascades2_lexer_ut

```

```

<cascades2_lexer_util.f90>≡
  <File header>

```

```

  module cascades2_lexer_util

```

```

    <Use kinds>

```

```

    <Use strings>

```

```

    use numeric_utils

```

```

    use cascades2_lexer

```

```

  <Standard module head>

```

```

  <Cascades2 lexer: test declarations>

```

```

  contains

```

```

  <Cascades2 lexer: tests>

```

```

  end module cascades2_lexer_util

```

API: driver for the unit tests below.

```

<Cascades2 lexer: public test>≡
  public :: cascades2_lexer_test

```

```

<Cascades2 lexer: test driver>≡
  subroutine cascades2_lexer_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Cascades2 lexer: execute tests>
  end subroutine cascades2_lexer_test

<Cascades2 lexer: execute tests>≡
  call test (cascades2_lexer_1, "cascades2_lexer_1", &
    "make phase-space", u, results)

<Cascades2 lexer: test declarations>≡
  public :: cascades2_lexer_1

<Cascades2 lexer: tests>≡
  subroutine cascades2_lexer_1 (u)
    integer, intent(in) :: u
    integer :: u_in = 8
    character (len=300) :: line
    integer :: stat
    logical :: fail
    type (dag_string_t) :: dag_string

    write (u, "(A)")  "* Test output: cascades2_lexer_1"
    write (u, "(A)")  "* Purpose: read lines of O'Mega's phase space output, translate"
    write (u, "(A)")  "*           to dag_string, retranslate to character string and"
    write (u, "(A)")  "*           compare"
    write (u, "(A)")

    open (unit=u_in, file="cascades2_lexer_1.fds", status='old', action='read')

    stat = 0
    fail = .false.
    read (unit=u_in, fmt="(A)", iostat=stat) line
    do while (stat == 0 .and. .not. fail)
      read (unit=u_in, fmt="(A)", iostat=stat) line
      if (stat /= 0) exit
      dag_string = line
      fail = (char(dag_string) /= line)
    enddo
    if (fail) then
      write (u, "(A)")  "* Test result: Test failed!"
    else
      write (u, "(A)")  "* Test result: Test passed"
    end if

    close (u_in)
    write (u, *)
    write (u, "(A)")  "* Test output end: cascades2_lexer_1"
  end subroutine cascades2_lexer_1

```

@

19.14 An alternative cascades module

This module might replace the module `cascades`, which generates suitable phase space parametrizations and generates the phase space file. The mappings, as well as the criteria to determine these, do not change.

The advantage of this module is that it makes use of the `O'Mega` matrix element generator which provides the relevant Feynman diagrams (the ones which can be constructed only from 3-vertices). In principle, the construction of these diagrams is also one of the tasks of the existing `cascades` module, in which the diagrams would correspond to a set of cascades. It starts by creating cascades which correspond to the outgoing particles. These are combined to a new cascade using the vertices of the model. In this way, since each cascade knows the daughter cascades from which it is built, complete Feynman diagrams are represented by sets of cascades, as soon as the existing cascades can be recombined with the incoming particle(s).

In this module, the Feynman diagrams are represented by the type `feyngraph.t`, which represents the Feynman diagrams as a tree of nodes. The object which contains the necessary kinematical information to determine mappings, and hence sensible phase space parametrizations is of another type, called `kingraph.t`, which is built from a corresponding `feyngraph` object.

There are two types of output which can be produced by `O'Mega` and are potentially relevant here. The first type contains all tree diagrams for the process under consideration, where each line of the output corresponds to one Feynman diagram. This output is easy to read, but can be very large, depending on the number of particles involved in the process. Moreover, it repeats substructures of the diagrams which are part of more than one diagram. One could in principle work with this output and construct a `feyngraph` from each line, if allowed, i.e. if there are only 3-vertices.

The other output contains also all of these Feynman diagrams, but in a factorized form. This means that the substructures which appear in several Feynman diagrams, are written only once, if possible. This leads to a much shorter input file, which speeds up the parsing process. Furthermore it makes it possible to reconstruct the `feyngraphs` in such a way that the calculations concerning subdiagrams which reappear in other `feyngraphs` have to be performed only once. This is already the case in the existing `cascades` module but can be exploited more efficiently here because the possible graphs are well known from the input file, whereas the `cascades` module would create a large number of `cascades` which do not lead to a complete Feynman diagram of the given process.

```
<cascades2.f90>≡  
  <File header>  
  
  module cascades2  
  
    <Use kinds>  
    use kinds, only: TC, i8  
    <Use debug>  
    use cascades2_lexer  
    use sorting  
    use flavors  
    use model_data
```

```

use iso_varying_string, string_t => varying_string
use io_units
use physics_defs, only: SCALAR, SPINOR, VECTOR, VECTORSPINOR, TENSOR
use phs_forests, only: phs_parameters_t
use diagnostics
use hashes
use cascades, only: phase_space_vanishes, MAX_WARN_RESONANCE
use, intrinsic :: iso_fortran_env, only : input_unit, output_unit, error_unit
use resonances, only: resonance_info_t
use resonances, only: resonance_history_t
use resonances, only: resonance_history_set_t

<Standard module head>

<Cascades2: public>

<Cascades2: parameters>

<Cascades2: types>

<Cascades2: interfaces>

contains

<Cascades2: procedures>

end module cascades2

```

19.14.1 Particle properties

We define a type holding the properties of the particles which are needed for parsing and finding the phase space parametrizations and mappings. The properties of all particles which appear in the parsed Feynman diagrams for the given process will be stored in a central place, and only pointers to these objects are used.

```

<Cascades2: types>≡
  type :: part_prop_t
    character (len=LABEL_LEN) :: particle_label
    integer :: pdg = 0
    real(default) :: mass = 0.
    real :: width = 0.
    integer :: spin_type = 0
    logical :: is_vector = .false.
    logical :: empty = .true.
    type (part_prop_t), pointer :: anti => null ()
    type (string_t) :: tex_name
  contains
  <Cascades2: part prop: TBP>
end type part_prop_t

```

The `particle_label` in `part_prop_t` is simply the particle name (e.g. 'W+'). The corresponding variable in the type `f_node_t` contains some additional infor-

mation related to the external momenta, see below. The length of the `character` variable is fixed as:

```

<Cascades2: parameters>≡
    integer, parameter :: LABEL_LEN=30

<Cascades2: part prop: TBP>≡
    procedure :: final => part_prop_final

<Cascades2: procedures>≡
    subroutine part_prop_final (part)
        class(part_prop_t), intent(inout) :: part
        part%anti => null ()
    end subroutine part_prop_final

```

19.14.2 The mapping modes

The possible mappings are essentially the same as in `cascades`, but we introduce in addition the mapping constant `NON_RESONANT`, which does not refer to a new mapping; it corresponds to the nonresonant version of a potentially resonant particle (or `k_node`). This becomes relevant when we compare `k_nodes` to eliminate equivalences.

```

<Cascades2: parameters>+≡
    integer, parameter :: &
        & NONRESONANT = -2, EXTERNAL_PRT = -1, &
        & NO_MAPPING = 0, S_CHANNEL = 1, T_CHANNEL = 2, U_CHANNEL = 3, &
        & RADIATION = 4, COLLINEAR = 5, INFRARED = 6, &
        & STEP_MAPPING_E = 11, STEP_MAPPING_H = 12, &
        & ON_SHELL = 99

```

19.14.3 Grove properties

The channels or `kingraphs` will be grouped in groves, i.e. sets of channels, which share some characteristic numbers. These numbers are stored in the following type:

```

<Cascades2: types>+≡
    type :: grove_prop_t
        integer :: multiplicity = 0
        integer :: n_resonances = 0
        integer :: n_log_enhanced = 0
        integer :: n_off_shell = 0
        integer :: n_t_channel = 0
        integer :: res_hash = 0
    end type grove_prop_t

```

19.14.4 The tree type

This type contains all the information which is needed to reconstruct a `feyngraph` or `kingraph`. We store bincodes, pdg codes and mappings for all nodes of a valid `kingraph`. If we label the external particles as given in the process definition with integer numbers representing their position in the process definition, the

bincode would be the number that one obtains by setting the bit at the position that is given by this number. If we combine two particles/nodes to a third one (using a three-vertex of the given model), the bincode is the number which one obtains by setting all the bits which are set for the two particles. The **pdg** and **mapping** are simply the pdg-code and mapping at the position (i.e. propagator or external particle) which is specified by the corresponding bincode. We use **tree_t** not only for completed **kingraphs**, but also for all **k_nodes**, which are a subtree of a **kingraph**.

```

<Cascades2: types>+≡
  type :: tree_t
    integer(TC), dimension(:), allocatable :: bc
    integer, dimension(:), allocatable :: pdg
    integer, dimension(:), allocatable :: mapping
    integer :: n_entries = 0
    logical :: keep = .true.
    logical :: empty = .true.
  contains
    <Cascades2: tree: TBP>
  end type tree_t

<Cascades2: tree: TBP>≡
  procedure :: final => tree_final

<Cascades2: procedures>+≡
  subroutine tree_final (tree)
    class (tree_t), intent (inout) :: tree
    if (allocated (tree%bc)) deallocate (tree%bc)
    if (allocated (tree%pdg)) deallocate (tree%pdg)
    if (allocated (tree%mapping)) deallocate (tree%mapping)
  end subroutine tree_final

<Cascades2: interfaces>≡
  interface assignment (=)
    module procedure tree_assign
  end interface assignment (=)

<Cascades2: procedures>+≡
  subroutine tree_assign (tree1, tree2)
    type (tree_t), intent (inout) :: tree1
    type (tree_t), intent (in) :: tree2
    if (allocated (tree2%bc)) then
      allocate (tree1%bc(size(tree2%bc)))
      tree1%bc = tree2%bc
    end if
    if (allocated (tree2%pdg)) then
      allocate (tree1%pdg(size(tree2%pdg)))
      tree1%pdg = tree2%pdg
    end if
    if (allocated (tree2%mapping)) then
      allocate (tree1%mapping(size(tree2%mapping)))
      tree1%mapping = tree2%mapping
    end if
    tree1%n_entries = tree2%n_entries
  end subroutine tree_assign

```

```

    tree1%keep = tree2%keep
    tree1%empty = tree2%empty
end subroutine tree_assign

```

19.14.5 Add entries to the tree

The following procedures fill the arrays in `tree_t` with entries resulting from the bincode and mapping assignment.

```

<Cascades2: tree: TBP>+≡
  procedure :: add_entry_from_numbers => tree_add_entry_from_numbers
  procedure :: add_entry_from_node => tree_add_entry_from_node
  generic :: add_entry => add_entry_from_numbers, add_entry_from_node

```

Here we add a single entry to each of the arrays. This will exclusively be used for external particles.

```

<Cascades2: procedures>+≡
  subroutine tree_add_entry_from_numbers (tree, bincode, pdg, mapping)
    class (tree_t), intent (inout) :: tree
    integer(TC), intent (in) :: bincode
    integer, intent (in) :: pdg
    integer, intent (in) :: mapping
    integer :: pos
    if (tree%empty) then
      allocate (tree%bc(1))
      allocate (tree%pdg(1))
      allocate (tree%mapping(1))
      pos = tree%n_entries + 1
      tree%bc(pos) = bincode
      tree%pdg(pos) = pdg
      tree%mapping(pos) = mapping
      tree%n_entries = pos
      tree%empty = .false.
    end if
  end subroutine tree_add_entry_from_numbers

```

Here we merge two existing subtrees and a single entry (bc, pdg and mapping).

```

<Cascades2: procedures>+≡
  subroutine tree_merge (tree, tree1, tree2, bc, pdg, mapping)
    class (tree_t), intent (inout) :: tree
    type (tree_t), intent (in) :: tree1, tree2
    integer(TC), intent (in) :: bc
    integer, intent (in) :: pdg, mapping
    integer :: tree_size
    integer :: i1, i2
    if (tree%empty) then
      i1 = tree1%n_entries
      i2 = tree1%n_entries + tree2%n_entries
      !! Proof: tree_size > 0 (always)
      tree_size = tree1%n_entries + tree2%n_entries + 1
      allocate (tree%bc (tree_size))
      allocate (tree%pdg (tree_size))
      allocate (tree%mapping (tree_size))
    end if
  end subroutine tree_merge

```

```

      if (.not. tree1%empty) then
        tree%bc(:i1) = tree1%bc
        tree%pdg(:i1) = tree1%pdg
        tree%mapping(:i1) = tree1%mapping
      end if
      if (.not. tree2%empty) then
        tree%bc(i1+1:i2) = tree2%bc
        tree%pdg(i1+1:i2) = tree2%pdg
        tree%mapping(i1+1:i2) = tree2%mapping
      end if
      tree%bc(tree_size) = bc
      tree%pdg(tree_size) = pdg
      tree%mapping(tree_size) = mapping
      tree%n_entries = tree_size
      tree%empty = .false.
    end if
  end subroutine tree_merge

```

Here we add entries to a tree for a given `k_node`, which means that we first have to determine whether the node is external or internal. The arrays are sorted after the entries have been added (see below for details).

```

<Cascades2: procedures>+≡
subroutine tree_add_entry_from_node (tree, node)
  class (tree_t), intent (inout) :: tree
  type (k_node_t), intent (in) :: node
  integer :: pdg
  if (node%t_line) then
    pdg = abs (node%particle%pdg)
  else
    pdg = node%particle%pdg
  end if
  if (associated (node%daughter1) .and. &
    associated (node%daughter2)) then
    call tree_merge (tree, node%daughter1%subtree, &
      node%daughter2%subtree, node%bincode, &
      node%particle%pdg, node%mapping)
  else
    call tree_add_entry_from_numbers (tree, node%bincode, &
      node%particle%pdg, node%mapping)
  end if
  call tree%sort ()
end subroutine tree_add_entry_from_node

```

For a well-defined order of the elements of the arrays in `tree_t`, the elements can be sorted. The bincodes (entries of `bc`) are simply ordered by size, the `pdg` and `mapping` entries go to the positions of the corresponding `bc` values.

```

<Cascades2: tree: TBP>+≡
  procedure :: sort => tree_sort

<Cascades2: procedures>+≡
subroutine tree_sort (tree)
  class (tree_t), intent (inout) :: tree
  integer(TC), dimension(size(tree%bc)) :: bc_tmp

```

```

integer, dimension(size(tree%pdg)) :: pdg_tmp, mapping_tmp
integer, dimension(1) :: pos
integer :: i
bc_tmp = tree%bc
pdg_tmp = tree%pdg
mapping_tmp = tree%mapping
do i = size(tree%bc),1,-1
  pos = maxloc (bc_tmp)
  tree%bc(i) = bc_tmp (pos(1))
  tree%pdg(i) = pdg_tmp (pos(1))
  tree%mapping(i) = mapping_tmp (pos(1))
  bc_tmp(pos(1)) = 0
end do
end subroutine tree_sort

```

19.14.6 Graph types

We define an abstract type which will give rise to two different types: The type `feyngraph_t` contains the pure information of the corresponding Feynman diagram, but also a list of objects of the `kingraph` type which contain the kinematically relevant data for the mapping calculation as well as the mappings themselves. Every graph should have an index which is unique. Graphs which are not needed any more can be disabled by setting the `keep` variable to `false`.

```

<Cascades2: types>+≡
type, abstract :: graph_t
  integer :: index = 0
  integer :: n_nodes = 0
  logical :: keep = .true.
end type graph_t

```

This is the type representing the Feynman diagrams which are read from an input file created by O'Mega. It is a tree of nodes, which we call `f_nodes`, so that `feyngraph_t` contains a pointer to the root of this tree, and each node can have two daughter nodes. The case of only one associated daughter should never appear, because in the method of phase space parametrization which is used here, we combine always two particle momenta to a third one. The `feyngraphs` will be arranged in a linked list. This is why we have a pointer to the next graph. The `kingraphs` on the other hand are arranged in linked lists which are attached to the corresponding `feyngraph`. In general, a `feyngraph` can give rise to more than one `kingraph` because we make a copy every time a particle can be resonant, so that in the copy we keep the particle nonresonant.

```

<Cascades2: types>+≡
type, extends (graph_t) :: feyngraph_t
  type (string_t) :: omega_feyngraph_output
  type (f_node_t), pointer :: root => null ()
  type (feyngraph_t), pointer :: next => null ()
  type (kingraph_t), pointer :: kin_first => null ()
  type (kingraph_t), pointer :: kin_last => null ()
contains
  <Cascades2: feyngraph: TBP>

```

```
end type feyngraph_t
```

A container for a pointer of type `feyngraph_t`. This is used to realize arrays of these pointers.

```
<Cascades2: types>+≡
  type :: feyngraph_ptr_t
    type (feyngraph_t), pointer :: graph => null ()
  end type feyngraph_ptr_t
```

The length of a string describing a Feynman diagram which is produced by O'Mega is fixed by the parameter

```
<Cascades2: parameters>+≡
  integer, parameter :: FEYNGRAPH_LEN=300

<Cascades2: feyngraph: TBP>≡
  procedure :: final => feyngraph_final

<Cascades2: procedures>+≡
  subroutine feyngraph_final (graph)
    class(feyngraph_t), intent(inout) :: graph
    type (kingraph_t), pointer :: current
    graph%root => null ()
    graph%kin_last => null ()
    do while (associated (graph%kin_first))
      current => graph%kin_first
      graph%kin_first => graph%kin_first%next
      call current%final ()
      deallocate (current)
    enddo
  end subroutine feyngraph_final
```

This is the type of graph which is used to find the phase space channels, or in other words, each kingraph could correspond to a channel, if it is not eliminated for kinematical reasons or due to an equivalence. For the linked list which is attached to the corresponding `feyngraph`, we need the `next` pointer, whereas `grove_next` points to the next kingraph within a grove. The information which is relevant for the specification of a channel is stored in `tree`. We use `grove_prop` to sort the `kingraph` in a grove in which all `kingraphs` are characterized by the numbers contained in `grove_prop`. Later these groves are further subdivided using the resonance hash. A `kingraph` which is constructed directly from the output of O'Mega, is not `inverse`. In this case the first incoming particle is the root of the tree. In a scattering process, we can also construct a `kingraph` where the root of the tree is the second incoming particle. In this case the value of `inverse` is `.true..`

```
<Cascades2: types>+≡
  type, extends (graph_t) :: kingraph_t
    type (k_node_t), pointer :: root => null ()
    type (kingraph_t), pointer :: next => null()
    type (kingraph_t), pointer :: grove_next => null ()
    type (tree_t) :: tree
    type (grove_prop_t) :: grove_prop
    logical :: inverse = .false.
```

```

        integer :: prc_component = 0
        contains
        <Cascades2: kingraph: TBP>
    end type kingraph_t

```

Another container for a pointer to emulate arrays of pointers:

```

<Cascades2: types>+≡
    type :: kingraph_ptr_t
        type (kingraph_t), pointer :: graph => null ()
    end type kingraph_ptr_t

<Cascades2: kingraph: TBP>≡
    procedure :: final => kingraph_final

<Cascades2: procedures>+≡
    subroutine kingraph_final (graph)
        class(kingraph_t), intent(inout) :: graph
        graph%root => null ()
        graph%next => null ()
        graph%grove_next => null ()
        call graph%tree%final ()
    end subroutine kingraph_final

```

19.14.7 The node types

We define an abstract type containing variables which are needed for `f_node_t` as well as `k_node_t`. We say that a node is on the t-line if it lies between the two nodes which correspond to the two incoming particles. `incoming` and `tline` are used only for scattering processes and remain `.false.` in decay processes. The variable `n_subtree_nodes` holds the number of nodes (including the node itself) of the subtree of which the node is the root.

```

<Cascades2: types>+≡
    type, abstract :: node_t
        type (part_prop_t), pointer :: particle => null ()
        logical :: incoming = .false.
        logical :: t_line = .false.
        integer :: index = 0
        logical :: keep = .true.
        integer :: n_subtree_nodes = 1
    end type node_t

```

We use two different list types for the different kinds of nodes. We therefore start with an abstract type:

```

<Cascades2: types>+≡
    type, abstract :: list_t
        integer :: n_entries = 0
    end type list_t

```

Since the contents of the lists are different, we introduce two different entry types. Since the trees of nodes use pointers, the nodes should only be allocated by a type-bound procedure of the corresponding list type, such that we can keep track of all nodes, eventually reuse and in the end deallocate nodes correctly, without forgetting any nodes. Here is the type for the `k_nodes`. The list is a linked list. We want to reuse (recycle) the `k_nodes` which are neither incoming nor `t_line`.

```

<Cascades2: types>+≡
  type :: k_node_entry_t
    type (k_node_t), pointer :: node => null ()
    type (k_node_entry_t), pointer :: next => null ()
    logical :: recycle = .false.
  contains
    <Cascades2: k node entry: TBP>
  end type k_node_entry_t

<Cascades2: k node entry: TBP>≡
  procedure :: final => k_node_entry_final

<Cascades2: procedures>+≡
  subroutine k_node_entry_final (entry)
    class(k_node_entry_t), intent(inout) :: entry
    if (associated (entry%node)) then
      call entry%node%final
      deallocate (entry%node)
    end if
    entry%next => null ()
  end subroutine k_node_entry_final

<Cascades2: k node entry: TBP>+≡
  procedure :: write => k_node_entry_write

<Cascades2: procedures>+≡
  subroutine k_node_entry_write (k_node_entry, u)
    class (k_node_entry_t), intent (in) :: k_node_entry
    integer, intent (in) :: u
  end subroutine k_node_entry_write

```

Here is the list type for `k_nodes`. A `k_node_list` can be declared to be an observer. In this case it does not create any nodes by itself, but the entries set their pointers to existing nodes. In this way we can use the list structure and the type bound procedures for existing nodes.

```

<Cascades2: types>+≡
  type, extends (list_t) :: k_node_list_t
    type (k_node_entry_t), pointer :: first => null ()
    type (k_node_entry_t), pointer :: last => null ()
    integer :: n_recycle
    logical :: observer = .false.
  contains
    <Cascades2: k node list: TBP>
  end type k_node_list_t

```



```

<Cascades2: k node list: TBP>≡
  procedure :: final => k_node_list_final

<Cascades2: procedures>+≡
  subroutine k_node_list_final (list)
    class(k_node_list_t), intent(inout) :: list
    type (k_node_entry_t), pointer :: current
    do while (associated (list%first))
      current => list%first
      list%first => list%first%next
      if (list%observer) current%node => null ()
      call current%final ()
      deallocate (current)
    enddo
  end subroutine k_node_list_final

```

The `f_node_t` type contains the `particle_label` variable which is extracted from the input file. It consists not only of the particle name, but also of some numbers in brackets. These numbers indicate which external particles are part of the subtree of this node. The `f_node` contains also a list of `k_nodes`. Therefore, if the nodes are not incoming or t_line, the mapping calculations for these `k_nodes` which can appear in several kingraphs have to be performed only once.

```

<Cascades2: types>+≡
  type, extends (node_t) :: f_node_t
    type (f_node_t), pointer :: daughter1 => null ()
    type (f_node_t), pointer :: daughter2 => null ()
    character (len=LABEL_LEN) :: particle_label
    type (k_node_list_t) :: k_node_list
  contains
    <Cascades2: f node: TBP>
  end type f_node_t

```

The finalizer nullifies the daughter pointers, since they are deallocated, like the `f_node` itself, with the finalizer of the `f_node_list`.

```

<Cascades2: f node: TBP>≡
  procedure :: final => f_node_final

<Cascades2: procedures>+≡
  recursive subroutine f_node_final (node)
    class(f_node_t), intent(inout) :: node
    call node%k_node_list%final ()
    node%daughter1 => null ()
    node%daughter2 => null ()
  end subroutine f_node_final

```

Finaliser for `f_node_entry`.

```

<Cascades2: f node entry: TBP>≡
  procedure :: final => f_node_entry_final

<Cascades2: procedures>+≡
  subroutine f_node_entry_final (entry)
    class(f_node_entry_t), intent(inout) :: entry

```

```

        if (associated (entry%node)) then
            call entry%node%final ()
            deallocate (entry%node)
        end if
        entry%next => null ()
    end subroutine f_node_entry_final

```

Set index if not yet done, i.e. if it is zero.

```

<Cascades2: f node: TBP>+≡
    procedure :: set_index => f_node_set_index

<Cascades2: procedures>+≡
    subroutine f_node_set_index (f_node)
        class (f_node_t), intent (inout) :: f_node
        integer, save :: counter = 0
        if (f_node%index == 0) then
            counter = counter + 1
            f_node%index = counter
        end if
    end subroutine f_node_set_index

```

Type for the nodes of the tree (lines of the Feynman diagrams). We also need a type containing a pointer to a node, which is needed for creating arrays of pointers. This will be used for scattering processes where we can take either the first or the second particle to be the root of the tree. Since we need both cases for the calculations and O'Mega only gives us one of these, we have to perform a transformation of the graph in which some nodes (on the line which we hereafter call t-line) need to know their mother and sister nodes, which become their daughters within this transformation.

```

<Cascades2: types>+≡
    type :: f_node_ptr_t
        type (f_node_t), pointer :: node => null ()
        contains
            <Cascades2: f node ptr: TBP>
    end type f_node_ptr_t

<Cascades2: f node ptr: TBP>≡
    procedure :: final => f_node_ptr_final

<Cascades2: procedures>+≡
    subroutine f_node_ptr_final (f_node_ptr)
        class (f_node_ptr_t), intent (inout) :: f_node_ptr
        f_node_ptr%node => null ()
    end subroutine f_node_ptr_final

<Cascades2: interfaces>+≡
    interface assignment (=)
        module procedure f_node_ptr_assign
    end interface assignment (=)

<Cascades2: procedures>+≡
    subroutine f_node_ptr_assign (ptr1, ptr2)
        type (f_node_ptr_t), intent (out) :: ptr1

```

```

    type (f_node_ptr_t), intent (in) :: ptr2
    ptr1%node => ptr2%node
end subroutine f_node_ptr_assign

```

<Cascades2: types>+≡

```

type :: k_node_ptr_t
    type (k_node_t), pointer :: node => null ()
end type k_node_ptr_t

```

<Cascades2: types>+≡

```

type, extends (node_t) :: k_node_t
    type (k_node_t), pointer :: daughter1 => null ()
    type (k_node_t), pointer :: daughter2 => null ()
    type (k_node_t), pointer :: inverse_daughter1 => null ()
    type (k_node_t), pointer :: inverse_daughter2 => null ()
    type (f_node_t), pointer :: f_node => null ()
    type (tree_t) :: subtree
    real (default) :: ext_mass_sum = 0.
    real (default) :: effective_mass = 0.
    logical :: resonant = .false.
    logical :: on_shell = .false.
    logical :: log_enhanced = .false.
    integer :: mapping = NO_MAPPING
    integer(TC) :: bincode = 0
    logical :: mapping_assigned = .false.
    logical :: is_nonresonant_copy = .false.
    logical :: subtree_checked = .false.
    integer :: n_off_shell = 0
    integer :: n_log_enhanced = 0
    integer :: n_resonances = 0
    integer :: multiplicity = 0
    integer :: n_t_channel = 0
    integer :: f_node_index = 0
contains
    <Cascades2: k node: TBP>
end type k_node_t

```

Subroutine for k_node assignment.

<Cascades2: interfaces>+≡

```

interface assignment (=)
    module procedure k_node_assign
end interface assignment (=)

```

<Cascades2: procedures>+≡

```

subroutine k_node_assign (k_node1, k_node2)
    type (k_node_t), intent (inout) :: k_node1
    type (k_node_t), intent (in) :: k_node2
    k_node1%f_node => k_node2%f_node
    k_node1%particle => k_node2%particle
    k_node1%incoming = k_node2%incoming
    k_node1%t_line = k_node2%t_line
    k_node1%keep = k_node2%keep
    k_node1%n_subtree_nodes = k_node2%n_subtree_nodes

```

```

k_node1%ext_mass_sum = k_node2%ext_mass_sum
k_node1%effective_mass = k_node2%effective_mass
k_node1%resonant = k_node2%resonant
k_node1%on_shell = k_node2%on_shell
k_node1%log_enhanced = k_node2%log_enhanced
k_node1%mapping = k_node2%mapping
k_node1%bincode = k_node2%bincode
k_node1%mapping_assigned = k_node2%mapping_assigned
k_node1%is_nonresonant_copy = k_node2%is_nonresonant_copy
k_node1%n_off_shell = k_node2%n_off_shell
k_node1%n_log_enhanced = k_node2%n_log_enhanced
k_node1%n_resonances = k_node2%n_resonances
k_node1%multiplicity = k_node2%multiplicity
k_node1%n_t_channel = k_node2%n_t_channel
k_node1%f_node_index = k_node2%f_node_index
end subroutine k_node_assign

```

The finalizer of `k_node_t` nullifies all pointers to nodes, since the deallocation of these nodes takes place in the finalizer of the list by which they were created.

```

⟨Cascades2: k node: TBP⟩≡
  procedure :: final => k_node_final

⟨Cascades2: procedures⟩+≡
  recursive subroutine k_node_final (k_node)
    class(k_node_t), intent(inout) :: k_node
    k_node%daughter1 => null ()
    k_node%daughter2 => null ()
    k_node%inverse_daughter1 => null ()
    k_node%inverse_daughter2 => null ()
    k_node%f_node => null ()
  end subroutine k_node_final

```

Set an index to a `k_node`, if not yet done, i.e. if it is zero. The indices are simply positive integer numbers starting from 1.

```

⟨Cascades2: k node: TBP⟩+≡
  procedure :: set_index => k_node_set_index

⟨Cascades2: procedures⟩+≡
  subroutine k_node_set_index (k_node)
    class (k_node_t), intent (inout) :: k_node
    integer, save :: counter = 0
    if (k_node%index == 0) then
      counter = counter + 1
      k_node%index = counter
    end if
  end subroutine k_node_set_index

```

The process type (decay or scattering) is given by an integer which is equal to the number of incoming particles.

```

⟨Cascades2: public⟩≡
  public :: DECAY, SCATTERING

```

```

<Cascades2: parameters>+≡
    integer, parameter :: DECAY=1, SCATTERING=2

```

The entries of the `f_node_list` contain the substring of the input file from which the node's subtree will be constructed (or a modified string containing placeholders for substrings). We use the length of this string for fast comparison to find the nodes in the `f_node_list` which we want to reuse.

```

<Cascades2: types>+≡
    type :: f_node_entry_t
        character (len=FEYNGRAPH_LEN) :: subtree_string
        integer :: string_len = 0
        type (f_node_t), pointer :: node => null ()
        type (f_node_entry_t), pointer :: next => null ()
        integer :: subtree_size = 0
    contains
        <Cascades2: f node entry: TBP>
    end type f_node_entry_t

```

A write method for `f_node_entry`.

```

<Cascades2: f node entry: TBP>+≡
    procedure :: write => f_node_entry_write

<Cascades2: procedures>+≡
    subroutine f_node_entry_write (f_node_entry, u)
        class (f_node_entry_t), intent (in) :: f_node_entry
        integer, intent (in) :: u
        write (unit=u, fmt='(A)') trim(f_node_entry%subtree_string)
    end subroutine f_node_entry_write

```

```

<Cascades2: interfaces>+≡
    interface assignment (=)
        module procedure f_node_entry_assign
    end interface assignment (=)

```

```

<Cascades2: procedures>+≡
    subroutine f_node_entry_assign (entry1, entry2)
        type (f_node_entry_t), intent (out) :: entry1
        type (f_node_entry_t), intent (in) :: entry2
        entry1%node => entry2%node
        entry1%subtree_string = entry2%subtree_string
        entry1%string_len = entry2%string_len
        entry1%subtree_size = entry2%subtree_size
    end subroutine f_node_entry_assign

```

This is the list type for `f_nodes`. The variable `max_tree_size` is the number of nodes which appear in a complete graph.

```

<Cascades2: types>+≡
    type, extends (list_t) :: f_node_list_t
        type (f_node_entry_t), pointer :: first => null ()
        type (f_node_entry_t), pointer :: last => null ()
        type (k_node_list_t), pointer :: k_node_list => null ()
        integer :: max_tree_size = 0

```

```

contains
  <Cascades2: f node list: TBP>
end type f_node_list_t

```

Add an entry to the `f_node_list`. If the node might be reused, we check first using the `subtree_string` if there is already a node in the list which is the root of exactly the same subtree. Otherwise we add an entry to the list and allocate the node. In both cases we return a pointer to the node which allows to access the node.

```

<Cascades2: f node list: TBP>≡
  procedure :: add_entry => f_node_list_add_entry

<Cascades2: procedures>+≡
  subroutine f_node_list_add_entry (list, subtree_string, ptr_to_node, &
    recycle, subtree_size)
    class (f_node_list_t), intent (inout) :: list
    character (len=*), intent (in) :: subtree_string
    type (f_node_t), pointer, intent (out) :: ptr_to_node
    logical, intent (in) :: recycle
    integer, intent (in), optional :: subtree_size
    type (f_node_entry_t), pointer :: current
    type (f_node_entry_t), pointer :: second
    integer :: subtree_len
    ptr_to_node => null ()
    if (recycle) then
      subtree_len = len_trim (subtree_string)
      current => list%first
      do while (associated (current))
        if (present (subtree_size)) then
          if (current%subtree_size /= subtree_size) exit
        end if
        if (current%string_len == subtree_len) then
          if (trim (current%subtree_string) == trim (subtree_string)) then
            ptr_to_node => current%node
            exit
          end if
        end if
        current => current%next
      enddo
    end if
    if (.not. associated (ptr_to_node)) then
      if (list%n_entries == 0) then
        allocate (list%first)
        list%last => list%first
      else
        second => list%first
        list%first => null ()
        allocate (list%first)
        list%first%next => second
      end if
      list%n_entries = list%n_entries + 1
      list%first%subtree_string = trim(subtree_string)
      list%first%string_len = subtree_len
      if (present (subtree_size)) list%first%subtree_size = subtree_size
    end if
  end subroutine

```

```

        allocate (list%first%node)
        call list%first%node%set_index ()
        ptr_to_node => list%first%node
    end if
end subroutine f_node_list_add_entry

```

A write method for debugging.

```

<Cascades2: f node list: TBP>+≡
    procedure :: write => f_node_list_write

<Cascades2: procedures>+≡
    subroutine f_node_list_write (f_node_list, u)
        class (f_node_list_t), intent (in) :: f_node_list
        integer, intent (in) :: u
        type (f_node_entry_t), pointer :: current
        integer :: pos = 0
        current => f_node_list%first
        do while (associated (current))
            pos = pos + 1
            write (unit=u, fmt='(A,I10)') 'entry #: ', pos
            call current%write (u)
            write (unit=u, fmt=*)
            current => current%next
        enddo
    end subroutine f_node_list_write

```

```

<Cascades2: interfaces>+≡
    interface assignment (=)
        module procedure k_node_entry_assign
    end interface assignment (=)

```

```

<Cascades2: procedures>+≡
    subroutine k_node_entry_assign (entry1, entry2)
        type (k_node_entry_t), intent (out) :: entry1
        type (k_node_entry_t), intent (in) :: entry2
        entry1%node => entry2%node
        entry1%recycle = entry2%recycle
    end subroutine k_node_entry_assign

```

Add an entry to the `k_node_list`. We have to specify if the node can be reused. The check for existing reusable nodes happens with `k_node_list_get_nodes` (see below).

```

<Cascades2: k node list: TBP>+≡
    procedure :: add_entry => k_node_list_add_entry

<Cascades2: procedures>+≡
    recursive subroutine k_node_list_add_entry (list, ptr_to_node, recycle)
        class (k_node_list_t), intent (inout) :: list
        type (k_node_t), pointer, intent (out) :: ptr_to_node
        logical, intent (in) :: recycle
        if (list%n_entries == 0) then
            allocate (list%first)
            list%last => list%first
        else

```

```

        allocate (list%last%next)
        list%last => list%last%next
    end if
    list%n_entries = list%n_entries + 1
    list%last%recycle = recycle
    allocate (list%last%node)
    call list%last%node%set_index ()
    ptr_to_node => list%last%node
end subroutine k_node_list_add_entry

```

We need a similar subroutine for adding only a pointer to a list. This is needed for a `k_node_list` which is only an observer, i.e. it does not create any nodes by itself.

```

<Cascades2: k node list: TBP>+≡
    procedure :: add_pointer => k_node_list_add_pointer

<Cascades2: procedures>+≡
    subroutine k_node_list_add_pointer (list, ptr_to_node, recycle)
        class (k_node_list_t), intent (inout) :: list
        type (k_node_t), pointer, intent (in) :: ptr_to_node
        logical, optional, intent (in) :: recycle
        logical :: rec
        if (present (recycle)) then
            rec = recycle
        else
            rec = .false.
        end if
        if (list%n_entries == 0) then
            allocate (list%first)
            list%last => list%first
        else
            allocate (list%last%next)
            list%last => list%last%next
        end if
        list%n_entries = list%n_entries + 1
        list%last%recycle = rec
        list%last%node => ptr_to_node
    end subroutine k_node_list_add_pointer

```

The `k_node_list` can also be used to collect `k_nodes` which belong to different `f_nodes` in order to compare these. This is done only for nodes which have the same number of subtree nodes. We compare all nodes of the list with each other (as long as the node is not deactivated, i.e. if the `keep` variable is set to `.true.`) using the subroutine `subtree_select`. If it turns out that two nodes are equivalent, we keep only one of them. The term equivalent in this module refers to trees or subtrees which differ in the pdg codes at positions where the trivial mapping is used (`NO_MAPPING` or `NON_RESONANT`) so that the mass of the particle does not matter. Depending on the available couplings, two equivalent subtrees could eventually lead to the same phase space channels, which is why only one of them is kept.

```

<Cascades2: k node list: TBP>+≡
    procedure :: check_subtree_equivalences => k_node_list_check_subtree_equivalences

```



```

<Cascades2: procedures>+≡
subroutine k_node_list_check_subtree_equivalences (list, model)
  class (k_node_list_t), intent (inout) :: list
  type (model_data_t), intent (in) :: model
  type (k_node_ptr_t), dimension (:), allocatable :: set
  type (k_node_entry_t), pointer :: current
  integer :: pos
  integer :: i,j
  if (list%n_entries == 0) return
  allocate (set (list%n_entries))
  current => list%first
  pos = 0
  do while (associated (current))
    pos = pos + 1
    set(pos)%node => current%node
    current => current%next
  enddo
  do i=1, list%n_entries
    if (set(i)%node%keep) then
      do j=i+1, list%n_entries
        if (set(j)%node%keep) then
          if (set(i)%node%bincode == set(j)%node%bincode) then
            call subtree_select (set(i)%node%subtree,set(j)%node%subtree, model)
            if (.not. set(i)%node%subtree%keep) then
              set(i)%node%keep = .false.
              exit
            else if (.not. set(j)%node%subtree%keep) then
              set(j)%node%keep = .false.
            end if
          end if
        end if
      enddo
    end if
  enddo
  deallocate (set)
end subroutine k_node_list_check_subtree_equivalences

```

This subroutine is used to obtain all `k_nodes` of a `k_node_list` which can be recycled and are not disabled for some reason. We pass an allocatable array of the type `k_node_ptr_t` which will be allocated if there are any such nodes in the list and the pointers will be associated with these nodes.

```

<Cascades2: k node list: TBP>+≡
  procedure :: get_nodes => k_node_list_get_nodes

<Cascades2: procedures>+≡
subroutine k_node_list_get_nodes (list, nodes)
  class (k_node_list_t), intent (inout) :: list
  type (k_node_ptr_t), dimension(:), allocatable, intent (out) :: nodes
  integer :: n_nodes
  integer :: pos
  type (k_node_entry_t), pointer :: current, garbage
  n_nodes = 0
  current => list%first
  do while (associated (current))

```

```

        if (current%recycle .and. current%node%keep) n_nodes = n_nodes + 1
        current => current%next
    enddo
    if (n_nodes /= 0) then
        pos = 1
        allocate (nodes (n_nodes))
        do while (associated (list%first) .and. .not. list%first%node%keep)
            garbage => list%first
            list%first => list%first%next
            call garbage%final ()
            deallocate (garbage)
        enddo
        current => list%first
        do while (associated (current))
            do while (associated (current%next))
                if (.not. current%next%node%keep) then
                    garbage => current%next
                    current%next => current%next%next
                    call garbage%final
                    deallocate (garbage)
                else
                    exit
                end if
            enddo
            if (current%recycle .and. current%node%keep) then
                nodes(pos)%node => current%node
                pos = pos + 1
            end if
            current => current%next
        enddo
    end if
end subroutine k_node_list_get_nodes

```

```

<Cascades2: f node list: TBP>+≡
    procedure :: final => f_node_list_final

<Cascades2: procedures>+≡
    subroutine f_node_list_final (list)
        class (f_node_list_t) :: list
        type (f_node_entry_t), pointer :: current
        list%k_node_list => null ()
        do while (associated (list%first))
            current => list%first
            list%first => list%first%next
            call current%final ()
            deallocate (current)
        enddo
    end subroutine f_node_list_final

```

19.14.8 The grove list

First a type is introduced in order to speed up the comparison of kingraphs with the purpose to quickly find the graphs that might be equivalent. This is

done solely on the basis of a number (which is given by the value of **depth** in **compare_tree_t**) of bincodes, which are the highest ones that do not belong to external particles. The highest such value determines the index of the element in the **entry** array of the **compare_tree**. The next lower such value determines the index of the element in the **entry** array of this **entry**, and so on and so forth. This results in a tree structure where the number of levels is given by **depth** and should not be too large for reasons of memory. This is the entry type.

```

<Cascades2: types>+≡
  type :: compare_tree_entry_t
    type (compare_tree_entry_t), dimension(:), pointer :: entry => null ()
    type (kingraph_ptr_t), dimension(:), allocatable :: graph_entry
  contains
    <Cascades2: compare tree entry: TBP>
  end type compare_tree_entry_t

```

This is the tree type.

```

<Cascades2: types>+≡
  type :: compare_tree_t
    integer :: depth = 3
    type (compare_tree_entry_t), dimension(:), pointer :: entry => null ()
  contains
    <Cascades2: compare tree: TBP>
  end type compare_tree_t

```

Finalizers for both types. The one for the entry type has to be recursive.

```

<Cascades2: compare tree: TBP>≡
  procedure :: final => compare_tree_final

<Cascades2: procedures>+≡
  subroutine compare_tree_final (ctree)
    class (compare_tree_t), intent (inout) :: ctree
    integer :: i
    if (associated (ctree%entry)) then
      do i=1, size (ctree%entry)
        call ctree%entry(i)%final ()
        deallocate (ctree%entry)
      end do
    end if
  end subroutine compare_tree_final

<Cascades2: compare tree entry: TBP>≡
  procedure :: final => compare_tree_entry_final

<Cascades2: procedures>+≡
  recursive subroutine compare_tree_entry_final (ct_entry)
    class (compare_tree_entry_t), intent (inout) :: ct_entry
    integer :: i
    if (associated (ct_entry%entry)) then
      do i=1, size (ct_entry%entry)
        call ct_entry%entry(i)%final ()
      enddo
    deallocate (ct_entry%entry)
  end subroutine compare_tree_entry_final

```

```

else
  deallocate (ct_entry%graph_entry)
end if
end subroutine compare_tree_entry_final

```

Check the presence of a graph which is considered as equivalent and select between the two. If there is no such graph, the current one is added to the list. First the entry has to be found:

```

<Cascades2: compare tree: TBP>+≡
  procedure :: check_kingraph => compare_tree_check_kingraph

<Cascades2: procedures>+≡
  subroutine compare_tree_check_kingraph (ctree, kingraph, model, preliminary)
    class (compare_tree_t), intent (inout) :: ctree
    type (kingraph_t), intent (inout), pointer :: kingraph
    type (model_data_t), intent (in) :: model
    logical, intent (in) :: preliminary
    integer :: i
    integer :: pos
    integer(TC) :: sz
    integer(TC), dimension(:), allocatable :: identifier
    if (.not. associated (ctree%entry)) then
      sz = 0_TC
      do i = size(kingraph%tree%bc), 1, -1
        sz = ior (sz, kingraph%tree%bc(i))
      enddo
      if (sz > 0) then
        allocate (ctree%entry (sz))
      else
        call msg_bug ("Compare tree could not be created")
      end if
    end if
    allocate (identifier (ctree%depth))
    pos = 0
    do i = size(kingraph%tree%bc), 1, -1
      if (popcnt (kingraph%tree%bc(i)) /= 1) then
        pos = pos + 1
        identifier(pos) = kingraph%tree%bc(i)
        if (pos == ctree%depth) exit
      end if
    enddo
    if (size (identifier) > 1) then
      call ctree%entry(identifier(1))%check_kingraph (kingraph, model, &
        preliminary, identifier(1), identifier(2:))
    else if (size (identifier) == 1) then
      call ctree%entry(identifier(1))%check_kingraph (kingraph, model, preliminary)
    end if
    deallocate (identifier)
  end subroutine compare_tree_check_kingraph

```

Then the graphs of the entry are checked.

```

<Cascades2: compare tree entry: TBP>+≡
  procedure :: check_kingraph => compare_tree_entry_check_kingraph

```

<Cascades2: procedures>+≡

```

recursive subroutine compare_tree_entry_check_kingraph (ct_entry, kingraph, &
    model, preliminary, subtree_size, identifier)
    class (compare_tree_entry_t), intent (inout) :: ct_entry
    type (kingraph_t), pointer, intent (inout) :: kingraph
    type (model_data_t), intent (in) :: model
    logical, intent (in) :: preliminary
    integer, intent (in), optional :: subtree_size
    integer, dimension (:), intent (in), optional :: identifier
    if (present (identifier)) then
        if (.not. associated (ct_entry%entry)) &
            allocate (ct_entry%entry(subtree_size))
        if (size (identifier) > 1) then
            call ct_entry%entry(identifier(1))%check_kingraph (kingraph, &
                model, preliminary, identifier(1), identifier(2:))
        else if (size (identifier) == 1) then
            call ct_entry%entry(identifier(1))%check_kingraph (kingraph, &
                model, preliminary)
        end if
    else
        if (allocated (ct_entry%graph_entry)) then
            call perform_check
        else
            allocate (ct_entry%graph_entry(1))
            ct_entry%graph_entry(1)%graph => kingraph
        end if
    end if
end if

```

contains

```

subroutine perform_check
    integer :: i
    logical :: rebuild
    rebuild = .true.
    do i=1, size(ct_entry%graph_entry)
        if (ct_entry%graph_entry(i)%graph%keep) then
            if (preliminary .or. &
                ct_entry%graph_entry(i)%graph%prc_component /= kingraph%prc_component) then
                call kingraph_select (ct_entry%graph_entry(i)%graph, kingraph, model, preliminary)
            if (.not. kingraph%keep) then
                return
            else if (rebuild .and. .not. ct_entry%graph_entry(i)%graph%keep) then
                ct_entry%graph_entry(i)%graph => kingraph
                rebuild = .false.
            end if
        end if
    end if
end if
enddo
if (rebuild) call rebuild_graph_entry
end subroutine perform_check

subroutine rebuild_graph_entry
    type (kingraph_ptr_t), dimension(:), allocatable :: tmp_ptr
    integer :: i

```

```

integer :: pos
allocate (tmp_ptr(size(ct_entry%graph_entry)+1))
pos = 0
do i=1, size(ct_entry%graph_entry)
    pos = pos + 1
    tmp_ptr(pos)%graph => ct_entry%graph_entry(i)%graph
enddo
pos = pos + 1
tmp_ptr(pos)%graph => kingraph
deallocate (ct_entry%graph_entry)
allocate (ct_entry%graph_entry (pos))
do i=1, pos
    ct_entry%graph_entry(i)%graph => tmp_ptr(i)%graph
enddo
deallocate (tmp_ptr)
end subroutine rebuild_graph_entry
end subroutine compare_tree_entry_check_kingraph

```

The grove to which a completed `kingraph` will be added is determined by the entries of `grove_prop`. We use another list type (linked list) to arrange the groves. Each grove contains again a linked list of `kingraphs`.

```

<Cascades2: types>+≡
type :: grove_t
    type (grove_prop_t) :: grove_prop
    type (grove_t), pointer :: next => null ()
    type (kingraph_t), pointer :: first => null ()
    type (kingraph_t), pointer :: last => null ()
    type (compare_tree_t) :: compare_tree
contains
    <Cascades2: grove: TBP>
end type grove_t

```

Container for a pointer of type `grove_t`:

```

<Cascades2: types>+≡
type :: grove_ptr_t
    type (grove_t), pointer :: grove => null ()
end type grove_ptr_t

```

```

<Cascades2: grove: TBP>≡
procedure :: final => grove_final

```

```

<Cascades2: procedures>+≡
subroutine grove_final (grove)
    class(grove_t), intent(inout) :: grove
    grove%first => null ()
    grove%last  => null ()
    grove%next  => null ()
end subroutine grove_final

```

This is the list type:

```

<Cascades2: types>+≡
type :: grove_list_t

```

```

        type (grove_t), pointer :: first => null ()
contains
    <Cascades2: grove list: TBP>
end type grove_list_t

<Cascades2: grove list: TBP>≡
    procedure :: final => grove_list_final

<Cascades2: procedures>+≡
    subroutine grove_list_final (list)
        class(grove_list_t), intent(inout) :: list
        class(grove_t), pointer :: current
        do while (associated (list%first))
            current => list%first
            list%first => list%first%next
            call current%final ()
            deallocate (current)
        end do
    end subroutine grove_list_final

```

19.14.9 The feyngraph set

The fundament of the module is the public type `feyngraph_set_t`. It is not only a linked list of all `feyngraphs` but contains an array of all particle properties (`particle`), an `f_node_list` and a pointer of the type `grove_list_t`, since several `feyngraph_sets` can share a common `grove_list`. In addition it keeps the data which unambiguously specifies the process, as well as the model which provides information which allows us to choose between equivalent subtrees or complete `kingraphs`.

```

<Cascades2: public>+≡
    public :: feyngraph_set_t

<Cascades2: types>+≡
    type :: feyngraph_set_t
        type (model_data_t), pointer :: model => null ()
        type(flavor_t), dimension(:, :), allocatable :: flv
        integer :: n_in = 0
        integer :: n_out = 0
        integer :: process_type = DECAY
        type (phs_parameters_t) :: phs_par
        logical :: fatal_beam_decay = .true.
        type (part_prop_t), dimension (:), pointer :: particle => null ()
        type (f_node_list_t) :: f_node_list
        type (feyngraph_t), pointer :: first => null ()
        type (feyngraph_t), pointer :: last => null ()
        integer :: n_graphs = 0
        type (grove_list_t), pointer :: grove_list => null ()
        logical :: use_dag = .true.
        type (dag_t), pointer :: dag => null ()
        type (feyngraph_set_t), dimension (:), pointer :: fset => null ()
contains
    <Cascades2: feyngraph set: TBP>

```

```
end type feyngraph_set_t
```

This final procedure contains calls to all other necessary final procedures.

```
<Cascades2: feyngraph set: TBP>≡
```

```
procedure :: final => feyngraph_set_final
```

```
<Cascades2: procedures>+≡
```

```
recursive subroutine feyngraph_set_final (set)
  class(feyngraph_set_t), intent(inout) :: set
  class(feyngraph_t), pointer :: current
  integer :: i
  if (associated (set%fset)) then
    do i=1, size (set%fset)
      call set%fset(i)%final ()
    enddo
    deallocate (set%fset)
  else
    set%particle => null ()
    set%grove_list => null ()
  end if
  set%model => null ()
  if (allocated (set%flv)) deallocate (set%flv)
  set%last => null ()
  do while (associated (set%first))
    current => set%first
    set%first => set%first%next
    call current%final ()
    deallocate (current)
  end do
  if (associated (set%particle)) then
    do i = 1, size (set%particle)
      call set%particle(i)%final ()
    end do
    deallocate (set%particle)
  end if
  if (associated (set%grove_list)) then
    if (debug_on) call msg_debug (D_PHASESPACE, "grove_list: final")
    call set%grove_list%final ()
    deallocate (set%grove_list)
  end if
  if (debug_on) call msg_debug (D_PHASESPACE, "f_node_list: final")
  call set%f_node_list%final ()
  if (associated (set%dag)) then
    if (debug_on) call msg_debug (D_PHASESPACE, "dag: final")
    if (associated (set%dag)) then
      call set%dag%final ()
      deallocate (set%dag)
    end if
  end if
end subroutine feyngraph_set_final
```


19.14.10 Construct the feyngraph set

We construct the `feyngraph_set` from an input file. Therefore we pass a unit to `feyngraph_set_build`. The parsing subroutines are chosen depending on the value of `use_dag`. In the DAG output, which is the one that is produced by default, we have to work on a string of one line, where the length of this string becomes larger the more particles are involved in the process. The other output (which is now only used in a unit test) contains one Feynman diagram per line and each line starts with an open parenthesis so that we read the file line per line and create a `feyngraph` for every line. Only after this, nodes are created. In both decay and scattering processes the diagrams are represented like in a decay process, i.e. in a scattering process one of the incoming particles appears as an outgoing particle.

```

(Cascades2: feyngraph set: TBP)+≡
    procedure :: build => feyngraph_set_build

(Cascades2: procedures)+≡
    subroutine feyngraph_set_build (feyngraph_set, u_in)
        class (feyngraph_set_t), intent (inout) :: feyngraph_set
        integer, intent (in) :: u_in
        integer :: stat = 0
        character (len=FEYNGRAPH_LEN) :: omega_feyngraph_output
        type (feyngraph_t), pointer :: current_graph
        type (feyngraph_t), pointer :: compare_graph
        logical :: present
        if (feyngraph_set%use_dag) then
            allocate (feyngraph_set%dag)
            if (.not. associated (feyngraph_set%first)) then
                call feyngraph_set%dag%read_string (u_in, feyngraph_set%flv(:,1))
                call feyngraph_set%dag%construct (feyngraph_set)
                call feyngraph_set%dag%make_feyngraphs (feyngraph_set)
            end if
        else
            if (.not. associated (feyngraph_set%first)) then
                read (unit=u_in, fmt='(A)', iostat=stat, advance='yes') omega_feyngraph_output
                if (omega_feyngraph_output(1:1) == '(') then
                    allocate (feyngraph_set%first)
                    feyngraph_set%first%omega_feyngraph_output = trim(omega_feyngraph_output)
                    feyngraph_set%last => feyngraph_set%first
                    feyngraph_set%n_graphs = feyngraph_set%n_graphs + 1
                else
                    call msg_fatal ("Invalid input file")
                end if
                read (unit=u_in, fmt='(A)', iostat=stat, advance='yes') omega_feyngraph_output
                do while (stat == 0)
                    if (omega_feyngraph_output(1:1) == '(') then
                        compare_graph => feyngraph_set%first
                        present = .false.
                        do while (associated (compare_graph))
                            if (len_trim(compare_graph%omega_feyngraph_output) &
                                == len_trim(omega_feyngraph_output)) then
                                if (compare_graph%omega_feyngraph_output == omega_feyngraph_output) then
                                    present = .true.
                                end if
                            end if
                            compare_graph => compare_graph%next
                        end do
                    end if
                end do
            end if
        end if
    end subroutine

```

```

        end if
    end if
    compare_graph => compare_graph%next
enddo
if (.not. present) then
    allocate (feyngraph_set%last%next)
    feyngraph_set%last => feyngraph_set%last%next
    feyngraph_set%last%omega_feyngraph_output = trim(omega_feyngraph_output)
    feyngraph_set%n_graphs = feyngraph_set%n_graphs + 1
end if
end if
read (unit=u_in, fmt='(A)', iostat=stat, advance='yes') omega_feyngraph_output
else
    exit
end if
enddo
current_graph => feyngraph_set%first
do while (associated (current_graph))
    call feyngraph_construct (feyngraph_set, current_graph)
    current_graph => current_graph%next
enddo
feyngraph_set%f_node_list%max_tree_size = feyngraph_set%first%n_nodes
end if
end if
end subroutine feyngraph_set_build

```

Read the string from the file. The output which is produced by O'Mega contains the DAG in a factorised form as a long string, distributed over several lines (in addition, in the case of a scattering process, it contains a similar string for the same process, but with the other incoming particle as the root of the tree structure). In general, such a file can contain many of these strings, belonging to different process components. Therefore we first have to find the correct position of the string for the process in question. Therefore we look for a line containing a pair of colons, in which case the line contains a process string. Then we check if the process string describes the correct process, which is done by checking for all the incoming and outgoing particle names. If the process is correct, the dag output should start in the following line. As long as we do not find the correct process string, we continue searching. If we reach the end of the file, we rewind the unit once, and repeat searching. If the process is still not found, there must be some sort of error.

```

<Cascades2: dag: TBP>≡
    procedure :: read_string => dag_read_string

<Cascades2: procedures>+≡
    subroutine dag_read_string (dag, u_in, flv)
        class (dag_t), intent (inout) :: dag
        integer, intent (in) :: u_in
        type(flavor_t), dimension(:), intent(in) :: flv
        character (len=BUFFER_LEN) :: process_string
        logical :: process_found
        logical :: rewind
    !!! find process string in file
        process_found = .false.
        rewind = .false.
    end subroutine

```

```

do while (.not. process_found)
  process_string = ""
  read (unit=u_in, fmt='(A)') process_string
  if (len_trim(process_string) /= 0) then
    if (index (process_string, "::") > 0) then
      process_found = process_string_match (trim (process_string), flv)
    end if
  else if (.not. rewind) then
    rewind (u_in)
    rewind = .true.
  else
    call msg_bug ("Process string not found in O'Mega input file.")
  end if
enddo
call fds_file_get_line (u_in, dag%string)
call dag%string%clean ()
if (.not. allocated (dag%string%t) .or. dag%string%char_len == 0) &
  call msg_bug ("Process string not found in O'Mega input file.")
end subroutine dag_read_string

```

The output of factorized Feynman diagrams which is created by O'Mega for a given process could in principle be written to a single line in the file. This can however lead to different problems with different compilers as soon as such lines become too long. This is the reason why the line is cut into smaller pieces. This means that a new line starts after each vertical bar. For this long string the type `dag_string_t` has been introduced. In order to read the file quickly into such a `dag_string` we use another type, `dag_chain_t` which is a linked list of such `dag_strings`. This has the advantage that we do not have to recreate a new `dag_string` for every line which has been read from file. Only in the end of this operation we compress the list of strings to a single string, removing useless `dag_tokens`, such as blanc space tokens. This subroutine reads all lines starting from the position in the file the unit is connected to, until no backslash character is found at the end of a line (the backslash means that the next line also belongs to the current string).

```

<Cascades2: parameters>+≡
  integer, parameter :: BUFFER_LEN = 1000
  integer, parameter :: STACK_SIZE = 100

<Cascades2: procedures>+≡
  subroutine fds_file_get_line (u, string)
    integer, intent (in) :: u
    type (dag_string_t), intent (out) :: string
    type (dag_chain_t) :: chain
    integer :: string_size, current_len
    character (len=BUFFER_LEN) :: buffer
    integer :: fragment_len
    integer :: stat
    current_len = 0
    stat = 0
    string_size = 0
    do while (stat == 0)
      read (unit=u, fmt='(A)', iostat=stat) buffer
      if (stat /= 0) exit
    enddo
  end subroutine

```

```

        fragment_len = len_trim (buffer)
        if (fragment_len == 0) then
            exit
        else if (buffer (fragment_len:fragment_len) == BACKSLASH_CHAR) then
            fragment_len = fragment_len - 1
        end if
        call chain%append (buffer(:fragment_len))
        if (buffer(fragment_len+1:fragment_len+1) /= BACKSLASH_CHAR) exit
    enddo
    if (associated (chain%first)) then
        call chain%compress ()
        string = chain%first
        call chain%final ()
    end if
end subroutine fds_file_get_line

```

We check, if the process string which has been read from file corresponds to the process for which we want to extract the Feynman diagrams.

```

<Cascades2: procedures>+≡
function process_string_match (string, flv) result (match)
    character (len=*), intent(in) :: string
    type(flavor_t), dimension(:), intent(in) :: flv
    logical :: match
    integer :: pos
    integer :: occurrence
    integer :: i
    pos = 1
    match = .false.
    do i=1, size (flv)
        occurrence = index (string(pos:), char(flvl(i)%get_name()))
        if (occurrence > 0) then
            pos = pos + occurrence
            match = .true.
        else
            match = .false.
            exit
        end if
    enddo
end function process_string_match

```

19.14.11 Particle properties

This subroutine initializes a model instance with the Standard Model data. It is only relevant for a unit test. We do not have to care about the model initialization in this module because the `model` is passed to `feyngraph.set_generate` when it is called.

```

<Cascades2: public>+≡
    public :: init_sm_full_test

<Cascades2: procedures>+≡
    subroutine init_sm_full_test (model)
        class(model_data_t), intent(out) :: model
    end subroutine

```

```

type(field_data_t), pointer :: field
integer, parameter :: n_real = 17
integer, parameter :: n_field = 21
integer, parameter :: n_vtx = 56
integer :: i
call model%init (var_str ("SM_vertex_test"), &
    n_real, 0, n_field, n_vtx)
call model%init_par (1, var_str ("mZ"), 91.1882_default)
call model%init_par (2, var_str ("mW"), 80.419_default)
call model%init_par (3, var_str ("mH"), 125._default)
call model%init_par (4, var_str ("me"), 0.000510997_default)
call model%init_par (5, var_str ("mmu"), 0.105658389_default)
call model%init_par (6, var_str ("mtau"), 1.77705_default)
call model%init_par (7, var_str ("ms"), 0.095_default)
call model%init_par (8, var_str ("mc"), 1.2_default)
call model%init_par (9, var_str ("mb"), 4.2_default)
call model%init_par (10, var_str ("mtop"), 173.1_default)
call model%init_par (11, var_str ("wtop"), 1.523_default)
call model%init_par (12, var_str ("wZ"), 2.443_default)
call model%init_par (13, var_str ("wW"), 2.049_default)
call model%init_par (14, var_str ("wH"), 0.004143_default)
call model%init_par (15, var_str ("ee"), 0.3079561542961_default)
call model%init_par (16, var_str ("cw"), 8.819013863636E-01_default)
call model%init_par (17, var_str ("sw"), 4.714339240339E-01_default)
i = 0
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("D_QUARK"), 1)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (name = [var_str ("d")], anti = [var_str ("dbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("U_QUARK"), 2)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (name = [var_str ("u")], anti = [var_str ("ubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("S_QUARK"), 3)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (mass_data=model%get_par_real_ptr (7))
call field%set (name = [var_str ("s")], anti = [var_str ("sbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("C_QUARK"), 4)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (mass_data=model%get_par_real_ptr (8))
call field%set (name = [var_str ("c")], anti = [var_str ("cbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("B_QUARK"), 5)
call field%set (spin_type=2, color_type=3, charge_type=-2, isospin_type=-2)
call field%set (mass_data=model%get_par_real_ptr (9))
call field%set (name = [var_str ("b")], anti = [var_str ("bbar")])
i = i + 1

```

```

field => model%get_field_ptr_by_index (i)
call field%init (var_str ("T_QUARK"), 6)
call field%set (spin_type=2, color_type=3, charge_type=3, isospin_type=2)
call field%set (mass_data=model%get_par_real_ptr (10))
call field%set (width_data=model%get_par_real_ptr (11))
call field%set (name = [var_str ("t")], anti = [var_str ("tbar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_LEPTON"), 11)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (4))
call field%set (name = [var_str ("e-")], anti = [var_str ("e+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("E_NEUTRINO"), 12)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("nue")], anti = [var_str ("nuebar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("MU_LEPTON"), 13)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (5))
call field%set (name = [var_str ("mu-")], anti = [var_str ("mu+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("MU_NEUTRINO"), 14)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("numu")], anti = [var_str ("numubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("TAU_LEPTON"), 15)
call field%set (spin_type=2)
call field%set (mass_data=model%get_par_real_ptr (6))
call field%set (name = [var_str ("tau-")], anti = [var_str ("tau+")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("TAU_NEUTRINO"), 16)
call field%set (spin_type=2, is_left_handed=.true.)
call field%set (name = [var_str ("nutau")], anti = [var_str ("nutaubar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("GLUON"), 21)
call field%set (spin_type=3, color_type=8)
call field%set (name = [var_str ("gl")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PHOTON"), 22)
call field%set (spin_type=3)
call field%set (name = [var_str ("A")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("Z_BOSON"), 23)
call field%set (spin_type=3)
call field%set (mass_data=model%get_par_real_ptr (1))

```

```

call field%set (width_data=model%get_par_real_ptr (12))
call field%set (name = [var_str ("Z")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("W_BOSON"), 24)
call field%set (spin_type=3)
call field%set (mass_data=model%get_par_real_ptr (2))
call field%set (width_data=model%get_par_real_ptr (13))
call field%set (name = [var_str ("W+")] , anti = [var_str ("W-")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HIGGS"), 25)
call field%set (spin_type=1)
call field%set (mass_data=model%get_par_real_ptr (3))
call field%set (width_data=model%get_par_real_ptr (14))
call field%set (name = [var_str ("H")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("PROTON"), 2212)
call field%set (spin_type=2)
call field%set (name = [var_str ("p")] , anti = [var_str ("pbar")])
!   call field%set (mass_data=model%get_par_real_ptr (12))
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_SINGLET"), 91)
call field%set (color_type=1)
call field%set (name = [var_str ("hr1")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_TRIPLET"), 92)
call field%set (color_type=3)
call field%set (name = [var_str ("hr3")] , anti = [var_str ("hr3bar")])
i = i + 1
field => model%get_field_ptr_by_index (i)
call field%init (var_str ("HADRON_REMNANT_OCTET"), 93)
call field%set (color_type=8)
call field%set (name = [var_str ("hr8")])
call model%freeze_fields ()
i = 0
i = i + 1
!!! QED
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("sbar"), var_str ("s"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("cbar"), var_str ("c"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("b"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("t"), var_str ("A")])
i = i + 1
!!!

```

```

call model%set_vertex (i, [var_str ("e+"), var_str ("e-"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("mu+"), var_str ("mu-"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("tau+"), var_str ("tau-"), var_str ("A")])
i = i + 1
!!! QCD
call model%set_vertex (i, [var_str ("gl"), var_str ("gl"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("gl"), var_str ("gl"), &
var_str ("gl"), var_str ("gl")])
i = i + 1
!!!
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("sbar"), var_str ("s"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("cbar"), var_str ("c"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("b"), var_str ("gl")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("t"), var_str ("gl")])
i = i + 1
!!! Neutral currents
call model%set_vertex (i, [var_str ("dbar"), var_str ("d"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("ubar"), var_str ("u"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("sbar"), var_str ("s"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("cbar"), var_str ("c"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("b"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("t"), var_str ("Z")])
i = i + 1
!!!
call model%set_vertex (i, [var_str ("e+"), var_str ("e-"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("mu+"), var_str ("mu-"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("tau+"), var_str ("tau-"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("nuebar"), var_str ("nue"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("numubar"), var_str ("numu"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("nutaubar"), var_str ("nutau"), &
var_str ("Z")])
i = i + 1
!!! Charged currents
call model%set_vertex (i, [var_str ("ubar"), var_str ("d"), var_str ("W+")])

```



```

i = i + 1
call model%set_vertex (i, [var_str ("cbar"), var_str ("s"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("b"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("dbar"), var_str ("u"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("sbar"), var_str ("c"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("t"), var_str ("W-")])
i = i + 1
!!!
call model%set_vertex (i, [var_str ("nuebar"), var_str ("e-"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("numubar"), var_str ("mu-"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("nutaubar"), var_str ("tau-"), var_str ("W+")])
i = i + 1
call model%set_vertex (i, [var_str ("e+"), var_str ("nue"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("mu+"), var_str ("numu"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("tau+"), var_str ("nutau"), var_str ("W-")])
i = i + 1
!!! Yukawa
!!! keeping only 3rd generation for the moment
! call model%set_vertex (i, [var_str ("sbar"), var_str ("s"), var_str ("H")])
! i = i + 1
! call model%set_vertex (i, [var_str ("cbar"), var_str ("c"), var_str ("H")])
! i = i + 1
call model%set_vertex (i, [var_str ("bbar"), var_str ("b"), var_str ("H")])
i = i + 1
call model%set_vertex (i, [var_str ("tbar"), var_str ("t"), var_str ("H")])
i = i + 1
! call model%set_vertex (i, [var_str ("mubar"), var_str ("mu"), var_str ("H")])
! i = i + 1
call model%set_vertex (i, [var_str ("taubar"), var_str ("tau"), var_str ("H")])
i = i + 1
!!! Vector-boson self-interactions
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("W+"), var_str ("W+"), var_str ("W-"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("Z"), var_str ("A")])
i = i + 1
call model%set_vertex (i, [var_str ("W+"), var_str ("W-"), var_str ("A"), var_str ("A")])
i = i + 1
!!! Higgs - vector boson
! call model%set_vertex (i, [var_str ("H"), var_str ("Z"), var_str ("A")])

```

```

! i = i + 1
! call model%set_vertex (i, [var_str ("H"), var_str ("A"), var_str ("A")])
! i = i + 1
! call model%set_vertex (i, [var_str ("H"), var_str ("gl"), var_str ("gl")])
! i = i + 1
!!!
call model%set_vertex (i, [var_str ("H"), var_str ("W+"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("H"), var_str ("Z"), var_str ("Z")])
i = i + 1
call model%set_vertex (i, [var_str ("H"), var_str ("H"), var_str ("W+"), var_str ("W-")])
i = i + 1
call model%set_vertex (i, [var_str ("H"), var_str ("H"), var_str ("Z"), var_str ("Z")])
i = i + 1
!!! Higgs self-interactions
call model%set_vertex (i, [var_str ("H"), var_str ("H"), var_str ("H")])
i = i + 1
call model%set_vertex (i, [var_str ("H"), var_str ("H"), var_str ("H"), var_str ("H")])
i = i + 1
call model%freeze_vertices ()
end subroutine init_sm_full_test

```

Initialize a `part_prop` object by passing a `particle_label`, which is simply the particle name. `part_prop` should be part of the `particle` array of `feyngraph_set`. We use the `model` of `feyngraph_set` to obtain the relevant data of the particle which is needed to find `phase_space` parametrizations. When a `part_prop` is initialized, we add and initialize also the corresponding anti- particle `part_prop` if it is not yet in the array.

```

<Cascades2: part_prop: TBP>+≡
  procedure :: init => part_prop_init

<Cascades2: procedures>+≡
  recursive subroutine part_prop_init (part_prop, feyngraph_set, particle_label)
    class (part_prop_t), intent (out), target :: part_prop
    type (feyngraph_set_t), intent (inout) :: feyngraph_set
    character (len=*), intent (in) :: particle_label
    type (flavor_t) :: flv, anti
    type (string_t) :: name
    integer :: i
    name = particle_label
    call flv%init (name, feyngraph_set%model)
    part_prop%particle_label = particle_label
    part_prop%pdg = flv%get_pdg ()
    part_prop%mass = flv%get_mass ()
    part_prop%width = flv%get_width()
    part_prop%spin_type = flv%get_spin_type ()
    part_prop%is_vector = flv%get_spin_type () == VECTOR
    part_prop%empty = .false.
    part_prop%tex_name = flv%get_tex_name ()
    anti = flv%anti ()
    if (flv%get_pdg() == anti%get_pdg()) then
      select type (part_prop)
        type is (part_prop_t)
          part_prop%anti => part_prop

```

```

        end select
    else
        do i=1, size (feyngraph_set%particle)
            if (feyngraph_set%particle(i)%pdg == (- part_prop%pdg)) then
                part_prop%anti => feyngraph_set%particle(i)
                exit
            else if (feyngraph_set%particle(i)%empty) then
                part_prop%anti => feyngraph_set%particle(i)
                call feyngraph_set%particle(i)%init (feyngraph_set, char(anti%get_name()))
                exit
            end if
        enddo
    end if
end subroutine part_prop_init

```

This subroutine assigns to a node the particle properties. Since these properties do not change and are simply read from the model file, we use pointers to the elements of the `particle` array of the `feyngraph_set`. If there is no corresponding array element, we have to initialize the first empty element of the array.

```

<Cascades2: parameters>+≡
    integer, parameter :: PRT_ARRAY_SIZE = 200

<Cascades2: f node: TBP>+≡
    procedure :: assign_particle_properties => f_node_assign_particle_properties

<Cascades2: procedures>+≡
    subroutine f_node_assign_particle_properties (node, feyngraph_set)
        class (f_node_t), intent (inout) :: node
        type (feyngraph_set_t), intent (inout) :: feyngraph_set
        character (len=LABEL_LEN) :: particle_label
        integer :: i
        particle_label = node%particle_label(1:index (node%particle_label, '[')-1)
        if (.not. associated (feyngraph_set%particle)) then
            allocate (feyngraph_set%particle (PRT_ARRAY_SIZE))
        end if
        do i = 1, size (feyngraph_set%particle)
            if (particle_label == feyngraph_set%particle(i)%particle_label) then
                node%particle => feyngraph_set%particle(i)
                exit
            else if (feyngraph_set%particle(i)%empty) then
                call feyngraph_set%particle(i)%init (feyngraph_set, particle_label)
                node%particle => feyngraph_set%particle(i)
                exit
            end if
        enddo
        !!! Since the O'Mega output uses the anti-particles instead of the particles specified
        !!! in the process definition, we revert this here. An exception is the first particle
        !!! in the parsable DAG output
        node%particle => node%particle%anti
    end subroutine f_node_assign_particle_properties

```

From the output of a Feynman diagram (in the non-factorized output) we need to find out how many daughter nodes would be required to reconstruct it cor-

rectly, to make sure that we keep only those **feyngraphs** which are constructed solely on the basis of the 3-vertices which are provided by the model. The number of daughter particles can easily be determined from the syntax of O'Mega's output: The particle which appears before the colon ':' is the mother particle. The particles or subtrees (i.e. whole parentheses) follow after the colon and are separated by commas.

```

<Cascades2: procedures>+≡
function get_n_daughters (subtree_string, pos_first_colon) &
    result (n_daughters)
character (len=*), intent (in) :: subtree_string
integer, intent (in) :: pos_first_colon
integer :: n_daughters
integer :: n_open_par
integer :: i
n_open_par = 1
n_daughters = 0
if (len_trim(subtree_string) > 0) then
    if (pos_first_colon > 0) then
        do i=pos_first_colon, len_trim(subtree_string)
            if (subtree_string(i:i) == ',') then
                if (n_open_par == 1) n_daughters = n_daughters + 1
            else if (subtree_string(i:i) == '(') then
                n_open_par = n_open_par + 1
            else if (subtree_string(i:i) == ')') then
                n_open_par = n_open_par - 1
            end if
        end do
        if (n_open_par == 0) then
            n_daughters = n_daughters + 1
        end if
    end if
end if
end function get_n_daughters

```

19.14.12 Reconstruction of trees

The reconstruction of a tree or subtree with the non-factorized input can be done recursively, i.e. we first find the root of the tree in the string and create an **f_node**. Then we look for daughters, which in the string appear either as single particles or subtrees (which are of the same form as the tree which we want to reconstruct. Therefore the subroutine can simply be called again and again until there are no more daughter nodes to create. When we meet a vertex which requires more than two daughter particles, we stop the recursion and disable the node using its **keep** variable. Whenever a daughter node is not kept, we do not keep the mother node as well.

```

<Cascades2: procedures>+≡
recursive subroutine node_construct_subtree_rec (feyngraph_set, &
    feyngraph, subtree_string, mother_node)
type (feyngraph_set_t), intent (inout) :: feyngraph_set
type (feyngraph_t), intent (inout) :: feyngraph
character (len=*), intent (in) :: subtree_string

```

```

type (f_node_t), pointer, intent (inout) :: mother_node
integer :: n_daughters
integer :: pos_first_colon
integer :: current_daughter
integer :: pos_subtree_begin, pos_subtree_end
integer :: i
integer :: n_open_par
if (.not. associated (mother_node)) then
  call feyngraph_set%f_node_list%add_entry (subtree_string, mother_node, .true.)
  current_daughter = 1
  n_open_par = 1
  pos_first_colon = index (subtree_string, ':')
  n_daughters = get_n_daughters (subtree_string, pos_first_colon)
  if (pos_first_colon == 0) then
    mother_node%particle_label = subtree_string
  else
    mother_node%particle_label = subtree_string(2:pos_first_colon-1)
  end if
  if (.not. associated (mother_node%particle)) then
    call mother_node%assign_particle_properties (feyngraph_set)
  end if
  if (n_daughters /= 2 .and. n_daughters /= 0) then
    mother_node%keep = .false.
    feyngraph%keep = .false.
    return
  end if
  pos_subtree_begin = pos_first_colon + 1
  do i = pos_first_colon + 1, len(trim(subtree_string))
    if (current_daughter == 2) then
      pos_subtree_end = len(trim(subtree_string)) - 1
      call node_construct_subtree_rec (feyngraph_set, feyngraph, &
        subtree_string(pos_subtree_begin:pos_subtree_end), &
        mother_node%daughter2)
      exit
    else if (subtree_string(i:i) == ',') then
      if (n_open_par == 1) then
        pos_subtree_end = i - 1
        call node_construct_subtree_rec (feyngraph_set, feyngraph, &
          subtree_string(pos_subtree_begin:pos_subtree_end), &
          mother_node%daughter1)
        current_daughter = 2
        pos_subtree_begin = i + 1
      end if
    else if (subtree_string(i:i) == '(') then
      n_open_par = n_open_par + 1
    else if (subtree_string(i:i) == ')') then
      n_open_par = n_open_par - 1
    end if
  end do
end if
if (associated (mother_node%daughter1)) then
  if (.not. mother_node%daughter1%keep) then
    mother_node%keep = .false.
  end if
end if

```

```

end if
if (associated (mother_node%daughter2)) then
  if (.not. mother_node%daughter2%keep) then
    mother_node%keep = .false.
  end if
end if
if (associated (mother_node%daughter1) .and. &
    associated (mother_node%daughter2)) then
  mother_node%n_subtree_nodes = &
    mother_node%daughter1%n_subtree_nodes &
    + mother_node%daughter2%n_subtree_nodes + 1
end if
if (.not. mother_node%keep) then
  feyngraph%keep = .false.
end if
end subroutine node_construct_subtree_rec

```

When the non-factorized version of the O'Mega output is used, the `feyngraph` is reconstructed from the contents of its `string_t` variable `omega_feyngraph_output`. This can be used for the recursive reconstruction of the tree of `k_nodes` with `node_construct_subtree_rec`.

```

<Cascades2: procedures>+≡
subroutine feyngraph_construct (feyngraph_set, feyngraph)
  type (feyngraph_set_t), intent (inout) :: feyngraph_set
  type (feyngraph_t), pointer, intent (inout) :: feyngraph
  call node_construct_subtree_rec (feyngraph_set, feyngraph, &
    char(feyngraph%omega_feyngraph_output), feyngraph%root)
  feyngraph%n_nodes = feyngraph%root%n_subtree_nodes
end subroutine feyngraph_construct

```

We introduce another node type, which is called `dag_node_t` and is used to reproduce the dag structure which is represented by the input. The `dag_nodes` can have several combinations of daughters 1 and 2. The `dag` type contains an array of `dag_nodes` and is only used for the reconstruction of `feyngraphs` which are factorized as well, but in the other direction as the original output. This means in particular that the outgoing particles in the output file (which there can appear many times) exist only once as `f_nodes`. To represent combinations of daughters and alternatives (options), we further use the types `dag_options_t` and `dag_combination_t`. The `dag_nodes`, `dag_options` and `dag_combinations` correspond to a substring of the string which has been read from file (and transformed into an object of type `dag_string_t`, which is simply another compact representation of this string), or a modified version of this substring. The aim is to create only one object for a given substring, even if it appears several times in the original string and then create trees of `f_nodes`, which build up the `feyngraph`, such that as many `f_nodes` as possible can be reused. An outgoing particle (always interpreting the input as a decay) is called a `leaf` in the context of a `dag`.

```

<Cascades2: types>+≡
type :: dag_node_t
  integer :: string_len
  type (dag_string_t) :: string

```

```

        logical :: leaf = .false.
        type (f_node_ptr_t), dimension (:), allocatable :: f_node
        integer :: subtree_size = 0
    contains
        <Cascades2: dag node: TBP>
    end type dag_node_t

```

```

<Cascades2: dag node: TBP>≡
    procedure :: final => dag_node_final

<Cascades2: procedures>+≡
    subroutine dag_node_final (dag_node)
        class (dag_node_t), intent (inout) :: dag_node
        integer :: i
        call dag_node%string%final ()
        if (allocated (dag_node%f_node)) then
            do i=1, size (dag_node%f_node)
                if (associated (dag_node%f_node(i)%node)) then
                    call dag_node%f_node(i)%node%final ()
                    deallocate (dag_node%f_node(i)%node)
                end if
            enddo
            deallocate (dag_node%f_node)
        end if
    end subroutine dag_node_final

```

Whenever there are more than one possible subtrees (represented by a `dag_node`) or combinations of subtrees to daughters (represented by `dag_combination_t`), we use the type `dag_options_t`. In the syntax of the factorized output, options are listed within curly braces, separated by horizontal bars.

```

<Cascades2: types>+≡
    type :: dag_options_t
        integer :: string_len
        type (dag_string_t) :: string
        type (f_node_ptr_t), dimension (:), allocatable :: f_node_ptr1
        type (f_node_ptr_t), dimension (:), allocatable :: f_node_ptr2
    contains
        <Cascades2: dag options: TBP>
    end type dag_options_t

```

```

<Cascades2: dag options: TBP>≡
    procedure :: final => dag_options_final

<Cascades2: procedures>+≡
    subroutine dag_options_final (dag_options)
        class (dag_options_t), intent (inout) :: dag_options
        integer :: i
        call dag_options%string%final ()
        if (allocated (dag_options%f_node_ptr1)) then
            do i=1, size (dag_options%f_node_ptr1)
                dag_options%f_node_ptr1(i)%node => null ()
            enddo
            deallocate (dag_options%f_node_ptr1)
        end if
    end subroutine dag_options_final

```

```

end if
  if (allocated (dag_options%f_node_ptr2)) then
    do i=1, size (dag_options%f_node_ptr2)
      dag_options%f_node_ptr2(i)%node => null ()
    enddo
    deallocate (dag_options%f_node_ptr2)
  end if
end subroutine dag_options_final

```

A pair of two daughters (which can be `dag_nodes` or `dag_options`) is represented by the type `dag_combination_t`. In the original string, a `dag_combination` appears between parentheses, which contain a comma, but not a colon. If we find a colon between these parentheses, it is a `dag_node` instead.

```

<Cascades2: types>+≡
type :: dag_combination_t
  integer :: string_len
  type (dag_string_t) :: string
  integer, dimension (2) :: combination
  type (f_node_ptr_t), dimension (:), allocatable :: f_node_ptr1
  type (f_node_ptr_t), dimension (:), allocatable :: f_node_ptr2
contains
  <Cascades2: dag combination: TBP>
end type dag_combination_t

```

```

<Cascades2: dag combination: TBP>≡
procedure :: final => dag_combination_final

```

```

<Cascades2: procedures>+≡
subroutine dag_combination_final (dag_combination)
  class (dag_combination_t), intent (inout) :: dag_combination
  integer :: i
  call dag_combination%string%final ()
  if (allocated (dag_combination%f_node_ptr1)) then
    do i=1, size (dag_combination%f_node_ptr1)
      dag_combination%f_node_ptr1(i)%node => null ()
    enddo
    deallocate (dag_combination%f_node_ptr1)
  end if
  if (allocated (dag_combination%f_node_ptr2)) then
    do i=1, size (dag_combination%f_node_ptr2)
      dag_combination%f_node_ptr2(i)%node => null ()
    enddo
    deallocate (dag_combination%f_node_ptr2)
  end if
end subroutine dag_combination_final

```

Here is the type representing the DAG, i.e. it holds arrays of the `dag_nodes`, `dag_options` and `dag_combinations`. The root node of the `dag` is the last filled element of the `node` array.

```

<Cascades2: types>+≡
type :: dag_t
  type (dag_string_t) :: string

```



```

        type (dag_node_t), dimension (:), allocatable :: node
        type (dag_options_t), dimension (:), allocatable :: options
        type (dag_combination_t), dimension (:), allocatable :: combination
        integer :: n_nodes = 0
        integer :: n_options = 0
        integer :: n_combinations = 0
    contains
        <Cascades2: dag: TBP>
    end type dag_t

<Cascades2: dag: TBP>+≡
    procedure :: final => dag_final

<Cascades2: procedures>+≡
    subroutine dag_final (dag)
        class (dag_t), intent (inout) :: dag
        integer :: i
        call dag%string%final ()
        if (allocated (dag%node)) then
            do i=1, size (dag%node)
                call dag%node(i)%final ()
            enddo
            deallocate (dag%node)
        end if
        if (allocated (dag%options)) then
            do i=1, size (dag%options)
                call dag%options(i)%final ()
            enddo
            deallocate (dag%options)
        end if
        if (allocated (dag%combination)) then
            do i=1, size (dag%combination)
                call dag%combination(i)%final ()
            enddo
            deallocate (dag%combination)
        end if
    end subroutine dag_final

```

We construct the DAG from the given `dag_string` which is modified several times so that in the end the remaining string corresponds to a simple `dag_node`, the root of the factorized tree. This means that we first identify the leaves, i.e. outgoing particles. Then we identify `dag_nodes`, `dag_combinations` and `options` until the number of these objects does not change any more. Identifying means that we add a corresponding object to the array (if not yet present), which can be identified with the corresponding substring, and replace the substring in the original `dag_string` by a `dag_token` of the corresponding type (in the char output of this token, this corresponds to a place holder like e.g. `'iO23i'` which in this particular case corresponds to an option and can be found at the position 23 in the array). The character output of the substrings turns out to be very useful for debugging.

```

<Cascades2: dag: TBP>+≡
    procedure :: construct => dag_construct

```

```

<Cascades2: procedures>+≡
subroutine dag_construct (dag, feyngraph_set)
  class (dag_t), intent (inout) :: dag
  type (feyngraph_set_t), intent (inout) :: feyngraph_set
  integer :: n_nodes
  integer :: n_options
  integer :: n_combinations
  logical :: continue_loop
  integer :: subtree_size
  integer :: i,j
  subtree_size = 1
  call dag%get_nodes_and_combinations (leaves = .true.)
  do i=1, dag%n_nodes
    call dag%node(i)%make_f_nodes (feyngraph_set, dag)
  enddo
  continue_loop = .true.
  subtree_size = subtree_size + 2
  do while (continue_loop)
    n_nodes = dag%n_nodes
    n_options = dag%n_options
    n_combinations = dag%n_combinations
    call dag%get_nodes_and_combinations (leaves = .false.)
    if (n_nodes /= dag%n_nodes) then
      dag%node(n_nodes+1:dag%n_nodes)%subtree_size = subtree_size
      do i = n_nodes+1, dag%n_nodes
        call dag%node(i)%make_f_nodes (feyngraph_set, dag)
      enddo
      subtree_size = subtree_size + 2
    end if
    if (n_combinations /= dag%n_combinations) then
      !$OMP PARALLEL DO
      do i = n_combinations+1, dag%n_combinations
        call dag%combination(i)%make_f_nodes (feyngraph_set, dag)
      enddo
      !$OMP END PARALLEL DO
    end if
    call dag%get_options ()
    if (n_options /= dag%n_options) then
      !$OMP PARALLEL DO
      do i = n_options+1, dag%n_options
        call dag%options(i)%make_f_nodes (feyngraph_set, dag)
      enddo
      !$OMP END PARALLEL DO
    end if
    if (n_nodes == dag%n_nodes .and. n_options == dag%n_options &
      .and. n_combinations == dag%n_combinations) then
      continue_loop = .false.
    end if
  enddo
  !!! add root node to dag
  call dag%add_node (dag%string%t, leaf = .false.)
  dag%node(dag%n_nodes)%subtree_size = subtree_size
  call dag%node(dag%n_nodes)%make_f_nodes (feyngraph_set, dag)
  if (debug2_active (D_PHASESPACE)) then

```

```

        call dag%write (output_unit)
    end if
    !!! set indices for all f_nodes
    do i=1, dag%n_nodes
        if (allocated (dag%node(i)%f_node)) then
            do j=1, size (dag%node(i)%f_node)
                if (associated (dag%node(i)%f_node(j)%node)) &
                    call dag%node(i)%f_node(j)%node%set_index ()
            enddo
        end if
    enddo
end subroutine dag_construct

```

Identify `dag_nodes` and `dag_combinations`. Leaves are simply nodes (i.e. of type `NODE_TK`) where only one bit in the bincode is set. The `dag_nodes` and `dag_combinations` have in common that they are surrounded by parentheses. There is however a way to distinguish between them because the corresponding substring contains a colon (or `dag_token` with type `COLON_TK`) if it is a `dag_node`. Otherwise it is a `dag_combination`. The string of the `dag_node` or `dag_combination` should not contain curly braces, because these correspond to `dag_options` and should be identified before.

```

<Cascades2: dag: TBP>+≡
    procedure :: get_nodes_and_combinations => dag_get_nodes_and_combinations

<Cascades2: procedures>+≡
    subroutine dag_get_nodes_and_combinations (dag, leaves)
        class (dag_t), intent (inout) :: dag
        logical, intent (in) :: leaves
        type (dag_string_t) :: new_string
        integer :: i, j, k
        integer :: i_node
        integer :: new_size
        integer :: first_colon
        logical :: combination
    !!! Create nodes also for external particles, except for the incoming one which
    !!! appears as the root of the tree. These can easily be identified by their
    !!! bincodes, since they should contain only one bit which is set.
        if (leaves) then
            first_colon = minloc (dag%string%t%type, 1, dag%string%t%type == COLON_TK)
            do i = first_colon + 1, size (dag%string%t)
                if (dag%string%t(i)%type == NODE_TK) then
                    if (popcnt(dag%string%t(i)%bincode) == 1) then
                        call dag%add_node (dag%string%t(i:i), .true., i_node)
                        call dag%string%t(i)%init_dag_object_token (DAG_NODE_TK, i_node)
                    end if
                end if
            enddo
            call dag%string%update_char_len ()
        else
    !!! Create a node or combination for every closed pair of parentheses
    !!! which do not contain any other parentheses or curly braces.
    !!! A node (not outgoing) contains a colon. This is not the case
    !!! for combinations, which we use as the criteria to distinguish

```

```

!!! between both.
    allocate (new_string%t (size (dag%string%t)))
    i = 1
    new_size = 0
    do while (i <= size(dag%string%t))
        if (dag%string%t(i)%type == OPEN_PAR_TK) then
            combination = .true.
            do j = i+1, size (dag%string%t)
                select case (dag%string%t(j)%type)
                    case (CLOSED_PAR_TK)
                        new_size = new_size + 1
                        if (combination) then
                            call dag%add_combination (dag%string%t(i:j), i_node)
                            call new_string%t(new_size)%init_dag_object_token (DAG_COMBINATION_TK, i_node)
                        else
                            call dag%add_node (dag%string%t(i:j), leaves, i_node)
                            call new_string%t(new_size)%init_dag_object_token (DAG_NODE_TK, i_node)
                        end if
                        i = j + 1
                    exit
                case (OPEN_PAR_TK, OPEN_CURLY_TK, CLOSED_CURLY_TK)
                    new_size = new_size + 1
                    new_string%t(new_size) = dag%string%t(i)
                    i = i + 1
                    exit
                case (COLON_TK)
                    combination = .false.
            end select
        enddo
    else
        new_size = new_size + 1
        new_string%t(new_size) = dag%string%t(i)
        i = i + 1
    end if
enddo
dag%string = new_string%t(:new_size)
call dag%string%update_char_len ()
end if
end subroutine dag_get_nodes_and_combinations

```

Identify `dag_options`, i.e. lists of rival nodes or combinations of nodes. These are identified by the surrounding curly braces. They should not contain any parentheses any more, because these correspond either to nodes or to combinations and should be identified before.

```

<Cascades2: dag: TBP>+≡
    procedure :: get_options => dag_get_options

<Cascades2: procedures>+≡
    subroutine dag_get_options (dag)
        class (dag_t), intent (inout) :: dag
        type (dag_string_t) :: new_string
        integer :: i, j, k
        integer :: new_size
        integer :: i_options
    end subroutine

```

```

character (len=10) :: index_char
integer :: index_start, index_end
!!! Create a node or combination for every closed pair of parentheses
!!! which do not contain any other parentheses or curly braces.
!!! A node (not outgoing) contains a colon. This is not the case
!!! for combinations, which we use as the criteria to distinguish
!!! between both.
allocate (new_string%t (size (dag%string%t)))
i = 1
new_size = 0
do while (i <= size(dag%string%t))
  if (dag%string%t(i)%type == OPEN_CURLY_TK) then
    do j = i+1, size (dag%string%t)
      select case (dag%string%t(j)%type)
      case (CLOSED_CURLY_TK)
        new_size = new_size + 1
        call dag%add_options (dag%string%t(i:j), i_options)
        call new_string%t(new_size)%init_dag_object_token (DAG_OPTIONS_TK, i_options)
        i = j + 1
        exit
      case (OPEN_PAR_TK, CLOSED_PAR_TK, OPEN_CURLY_TK)
        new_size = new_size + 1
        new_string%t(new_size) = dag%string%t(i)
        i = i + 1
        exit
      end select
    enddo
  else
    new_size = new_size + 1
    new_string%t(new_size) = dag%string%t(i)
    i = i + 1
  end if
enddo
dag%string = new_string%t(:new_size)
call dag%string%update_char_len ()
end subroutine dag_get_options

```

Add a `dag_node` to the list. The optional argument returns the index of the node. The node might already exist. In this case we only return the index.

<Cascades2: dag: TBP>+≡

```
procedure :: add_node => dag_add_node
```

<Cascades2: parameters>+≡

```
integer, parameter :: DAG_STACK_SIZE = 1000
```

<Cascades2: procedures>+≡

```

subroutine dag_add_node (dag, string, leaf, i_node)
  class (dag_t), intent (inout) :: dag
  type (dag_token_t), dimension (:), intent (in) :: string
  logical, intent (in) :: leaf
  integer, intent (out), optional :: i_node
  type (dag_node_t), dimension (:), allocatable :: tmp_node
  integer :: string_len
  integer :: i
  string_len = sum (string%char_len)

```

```

if (.not. allocated (dag%node)) then
    allocate (dag%node (DAG_STACK_SIZE))
else if (dag%n_nodes == size (dag%node)) then
    allocate (tmp_node (dag%n_nodes))
    tmp_node = dag%node
    deallocate (dag%node)
    allocate (dag%node (dag%n_nodes+DAG_STACK_SIZE))
    dag%node(:dag%n_nodes) = tmp_node
    deallocate (tmp_node)
end if
do i = 1, dag%n_nodes
    if (dag%node(i)%string_len == string_len) then
        if (size (dag%node(i)%string%t) == size (string)) then
            if (all(dag%node(i)%string%t == string)) then
                if (present (i_node)) i_node = i
                return
            end if
        end if
    end if
end if
enddo
dag%n_nodes = dag%n_nodes + 1
dag%node(dag%n_nodes)%string = string
dag%node(dag%n_nodes)%string_len = string_len
if (present (i_node)) i_node = dag%n_nodes
dag%node(dag%n_nodes)%leaf = leaf
end subroutine dag_add_node

```

A similar subroutine for options.

<Cascades2: dag: TBP>+≡

```

procedure :: add_options => dag_add_options

```

<Cascades2: procedures>+≡

```

subroutine dag_add_options (dag, string, i_options)
    class (dag_t), intent (inout) :: dag
    type (dag_token_t), dimension (:), intent (in) :: string
    integer, intent (out), optional :: i_options
    type (dag_options_t), dimension (:), allocatable :: tmp_options
    integer :: string_len
    integer :: i
    string_len = sum (string%char_len)
    if (.not. allocated (dag%options)) then
        allocate (dag%options (DAG_STACK_SIZE))
    else if (dag%n_options == size (dag%options)) then
        allocate (tmp_options (dag%n_options))
        tmp_options = dag%options
        deallocate (dag%options)
        allocate (dag%options (dag%n_options+DAG_STACK_SIZE))
        dag%options(:dag%n_options) = tmp_options
        deallocate (tmp_options)
    end if
    do i = 1, dag%n_options
        if (dag%options(i)%string_len == string_len) then
            if (size (dag%options(i)%string%t) == size (string)) then
                if (all(dag%options(i)%string%t == string)) then

```

```

        if (present (i_options)) i_options = i
        return
    end if
end if
end if
enddo
dag%n_options = dag%n_options + 1
dag%options(dag%n_options)%string = string
dag%options(dag%n_options)%string_len = string_len
if (present (i_options)) i_options = dag%n_options
end subroutine dag_add_options

```

A similar subroutine for combinations.

```

<Cascades2: dag: TBP>+=
    procedure :: add_combination => dag_add_combination

<Cascades2: procedures>+=
    subroutine dag_add_combination (dag, string, i_combination)
        class (dag_t), intent (inout) :: dag
        type (dag_token_t), dimension (:), intent (in) :: string
        integer, intent (out), optional :: i_combination
        type (dag_combination_t), dimension (:), allocatable :: tmp_combination
        integer :: string_len
        integer :: i
        string_len = sum (string%char_len)
        if (.not. allocated (dag%combination)) then
            allocate (dag%combination (DAG_STACK_SIZE))
        else if (dag%n_combinations == size (dag%combination)) then
            allocate (tmp_combination (dag%n_combinations))
            tmp_combination = dag%combination
            deallocate (dag%combination)
            allocate (dag%combination (dag%n_combinations+DAG_STACK_SIZE))
            dag%combination(:dag%n_combinations) = tmp_combination
            deallocate (tmp_combination)
        end if
        do i = 1, dag%n_combinations
            if (dag%combination(i)%string_len == string_len) then
                if (size (dag%combination(i)%string%t) == size (string)) then
                    if (all(dag%combination(i)%string%t == string)) then
                        i_combination = i
                        return
                    end if
                end if
            end if
        end do
        dag%n_combinations = dag%n_combinations + 1
        dag%combination(dag%n_combinations)%string = string
        dag%combination(dag%n_combinations)%string_len = string_len
        if (present (i_combination)) i_combination = dag%n_combinations
    end subroutine dag_add_combination

```

For a given `dag_node` we want to create all `f_nodes`. If the node is not a leaf, it contains in its string placeholders for options or combinations. For these

objects there are similar subroutines which are needed here to obtain the sets of daughter nodes. If the `dag_node` is a leaf, it corresponds to an external particle and the token contains the particle name.

(Cascades2: dag node: TBP)+≡

```
procedure :: make_f_nodes => dag_node_make_f_nodes
```

(Cascades2: procedures)+≡

```
subroutine dag_node_make_f_nodes (dag_node, feyngraph_set, dag)
  class (dag_node_t), intent (inout) :: dag_node
  type (feyngraph_set_t), intent (inout) :: feyngraph_set
  type (dag_t), intent (inout) :: dag
  character (len=LABEL_LEN) :: particle_label
  integer :: i, j
  integer, dimension (2) :: obj
  integer, dimension (2) :: i_obj
  integer :: n_obj
  integer :: pos
  integer :: new_size, size1, size2
  integer, dimension (:), allocatable :: match
  if (allocated (dag_node%f_node)) return
  pos = minloc (dag_node%string%t%type, 1, dag_node%string%t%type == NODE_TK)
  particle_label = char (dag_node%string%t(pos))
  if (dag_node%leaf) then
```

```
!!! construct subtree with procedure similar to the one for the old output
```

```
  allocate (dag_node%f_node(1))
  allocate (dag_node%f_node(1)%node)
  dag_node%f_node(1)%node%particle_label = particle_label
  call dag_node%f_node(1)%node%assign_particle_properties (feyngraph_set)
  if (.not. dag_node%f_node(1)%node%keep) then
    deallocate (dag_node%f_node)
    return
  end if
```

```
else
```

```
  n_obj = 0
  do i = 1, size (dag_node%string%t)
    select case (dag_node%string%t(i)%type)
      case (DAG_NODE_TK, DAG_OPTIONS_TK, DAG_COMBINATION_TK)
        n_obj = n_obj + 1
        if (n_obj > 2) return
        obj(n_obj) = dag_node%string%t(i)%type
        i_obj(n_obj) = dag_node%string%t(i)%index
    end select
  enddo
```

```
enddo
```

```
if (n_obj == 1) then
```

```
  if (obj(1) == DAG_OPTIONS_TK) then
```

```
    if (allocated (dag%options(i_obj(1))%f_node_ptr1)) then
```

```
      size1 = size(dag%options(i_obj(1))%f_node_ptr1)
```

```
      allocate (dag_node%f_node(size1))
```

```
      do i=1, size1
```

```
        allocate (dag_node%f_node(i)%node)
```

```
        dag_node%f_node(i)%node%particle_label = particle_label
```

```
        call dag_node%f_node(i)%node%assign_particle_properties (feyngraph_set)
```

```
        dag_node%f_node(i)%node%daughter1 => dag%options(i_obj(1))%f_node_ptr1(i)%node
```

```
        dag_node%f_node(i)%node%daughter2 => dag%options(i_obj(1))%f_node_ptr2(i)%node
```



```

        dag_node%f_node(i)%node%n_subtree_nodes = &
        dag%options(i_obj(1))%f_node_ptr1(i)%node%n_subtree_nodes &
        + dag%options(i_obj(1))%f_node_ptr2(i)%node%n_subtree_nodes + 1
    enddo
end if
else if (obj(1) == DAG_COMBINATION_TK) then
    if (allocated (dag%combination(i_obj(1))%f_node_ptr1)) then
        size1 = size(dag%combination(i_obj(1))%f_node_ptr1)
        allocate (dag_node%f_node(size1))
        do i=1, size1
            allocate (dag_node%f_node(i)%node)
            dag_node%f_node(i)%node%particle_label = particle_label
            call dag_node%f_node(i)%node%assign_particle_properties (feyngraph_set)
            dag_node%f_node(i)%node%daughter1 => dag%combination(i_obj(1))%f_node_ptr1(i)%n
            dag_node%f_node(i)%node%daughter2 => dag%combination(i_obj(1))%f_node_ptr2(i)%n
            dag_node%f_node(i)%node%n_subtree_nodes = &
                dag%combination(i_obj(1))%f_node_ptr1(i)%node%n_subtree_nodes &
                + dag%combination(i_obj(1))%f_node_ptr2(i)%node%n_subtree_nodes + 1
        enddo
    end if
end if
!!! simply set daughter pointers, daughters are already combined correctly
else if (n_obj == 2) then
    size1 = 0
    size2 = 0
    if (obj(1) == DAG_NODE_TK) then
        if (allocated (dag%node(i_obj(1))%f_node)) then
            do i=1, size (dag%node(i_obj(1))%f_node)
                if (dag%node(i_obj(1))%f_node(i)%node%keep) size1 = size1 + 1
            enddo
        end if
    else if (obj(1) == DAG_OPTIONS_TK) then
        if (allocated (dag%options(i_obj(1))%f_node_ptr1)) then
            do i=1, size (dag%options(i_obj(1))%f_node_ptr1)
                if (dag%options(i_obj(1))%f_node_ptr1(i)%node%keep) size1 = size1 + 1
            enddo
        end if
    end if
    if (obj(2) == DAG_NODE_TK) then
        if (allocated (dag%node(i_obj(2))%f_node)) then
            do i=1, size (dag%node(i_obj(2))%f_node)
                if (dag%node(i_obj(2))%f_node(i)%node%keep) size2 = size2 + 1
            enddo
        end if
    else if (obj(2) == DAG_OPTIONS_TK) then
        if (allocated (dag%options(i_obj(2))%f_node_ptr1)) then
            do i=1, size (dag%options(i_obj(2))%f_node_ptr1)
                if (dag%options(i_obj(2))%f_node_ptr1(i)%node%keep) size2 = size2 + 1
            enddo
        end if
    end if
    !!! make all combinations of daughters
    select case (obj(1))
    case (DAG_NODE_TK)

```

```

        select case (obj(2))
        case (DAG_NODE_TK)
            call combine_all_daughters(dag%node(i_obj(1))%f_node, &
                dag%node(i_obj(2))%f_node)
        case (DAG_OPTIONS_TK)
            call combine_all_daughters(dag%node(i_obj(1))%f_node, &
                dag%options(i_obj(2))%f_node_ptr1)
        end select
    case (DAG_OPTIONS_TK)
        select case (obj(2))
        case (DAG_NODE_TK)
            call combine_all_daughters(dag%options(i_obj(1))%f_node_ptr1, &
                dag%node(i_obj(2))%f_node)
        case (DAG_OPTIONS_TK)
            call combine_all_daughters(dag%options(i_obj(1))%f_node_ptr1, &
                dag%options(i_obj(2))%f_node_ptr1)
        end select
    end select
end if
end if

contains

subroutine combine_all_daughters (daughter1_ptr, daughter2_ptr)
    type (f_node_ptr_t), dimension (:), intent (in) :: daughter1_ptr
    type (f_node_ptr_t), dimension (:), intent (in) :: daughter2_ptr
    integer :: i, j
    integer :: pos
    new_size = size1*size2
    allocate (dag_node%f_node(new_size))
    pos = 0
    do i = 1, size (daughter1_ptr)
        if (daughter1_ptr(i)%node%keep) then
            do j = 1, size (daughter2_ptr)
                if (daughter2_ptr(j)%node%keep) then
                    pos = pos + 1
                    allocate (dag_node%f_node(pos)%node)
                    dag_node%f_node(pos)%node%particle_label = particle_label
                    call dag_node%f_node(pos)%node%assign_particle_properties (feyngraph_set)
                    dag_node%f_node(pos)%node%daughter1 => daughter1_ptr(i)%node
                    dag_node%f_node(pos)%node%daughter2 => daughter2_ptr(j)%node
                    dag_node%f_node(pos)%node%n_subtree_nodes = daughter1_ptr(i)%node%n_subtree_nodes
                        + daughter2_ptr(j)%node%n_subtree_nodes + 1
                    call feyngraph_set%model%match_vertex (daughter1_ptr(i)%node%particle%pdg, &
                        daughter2_ptr(j)%node%particle%pdg, match)
                    if (allocated (match)) then
                        if (any (abs(match) == abs(dag_node%f_node(pos)%node%particle%pdg))) then
                            dag_node%f_node(pos)%node%keep = .true.
                        else
                            dag_node%f_node(pos)%node%keep = .false.
                        end if
                    end if
                    deallocate (match)
                else
                    dag_node%f_node(pos)%node%keep = .false.
                end if
            end do
        end do
    end do
end subroutine

```

```

        end if
    end if
enddo
end if
enddo
end subroutine combine_all_daughters
end subroutine dag_node_make_f_nodes

```

In `dag_options.make_f_nodes.single` we obtain all `f_nodes` for `dag_nodes` which correspond to a set of rival subtrees or nodes, which is the first possibility for which `dag_options` can appear. In `dag_options.make_f_nodes.pair` the options are rival pairs (`daughter1`, `daughter2`). Therefore we have to pass two allocatable arrays of type `f_node_ptr_t` to the subroutine.

```

<Cascades2: dag_options: TBP>+≡
    procedure :: make_f_nodes => dag_options_make_f_nodes

<Cascades2: procedures>+≡
    subroutine dag_options_make_f_nodes (dag_options, &
        feyngraph_set, dag)
        class (dag_options_t), intent (inout) :: dag_options
        type (feyngraph_set_t), intent (inout) :: feyngraph_set
        type (dag_t), intent (inout) :: dag
        integer, dimension (:), allocatable :: obj, i_obj
        integer :: n_obj
        integer :: i
        integer :: pos
    !!! read options
    if (allocated (dag_options%f_node_ptr1)) return
    n_obj = count ((dag_options%string%t%type == DAG_NODE_TK) .or. &
        (dag_options%string%t%type == DAG_OPTIONS_TK) .or. &
        (dag_options%string%t%type == DAG_COMBINATION_TK), 1)
    allocate (obj(n_obj)); allocate (i_obj(n_obj))
    pos = 0
    do i = 1, size (dag_options%string%t)
        select case (dag_options%string%t(i)%type)
            case (DAG_NODE_TK, DAG_OPTIONS_TK, DAG_COMBINATION_TK)
                pos = pos + 1
                obj(pos) = dag_options%string%t(i)%type
                i_obj(pos) = dag_options%string%t(i)%index
        end select
    enddo
    if (any (dag_options%string%t%type == DAG_NODE_TK)) then
        call dag_options_make_f_nodes_single
    else if (any (dag_options%string%t%type == DAG_COMBINATION_TK)) then
        call dag_options_make_f_nodes_pair
    end if
    deallocate (obj, i_obj)

contains

    subroutine dag_options_make_f_nodes_single
        integer :: i_start, i_end
        integer :: n_nodes
        n_nodes = 0

```

```

do i=1, n_obj
  if (allocated (dag%node(i_obj(i))%f_node)) then
    n_nodes = n_nodes + size (dag%node(i_obj(i))%f_node)
  end if
enddo
if (n_nodes /= 0) then
  allocate (dag_options%f_node_ptr1 (n_nodes))
  i_end = 0
  do i = 1, n_obj
    if (allocated (dag%node(i_obj(i))%f_node)) then
      i_start = i_end + 1
      i_end = i_end + size (dag%node(i_obj(i))%f_node)
      dag_options%f_node_ptr1(i_start:i_end) = dag%node(i_obj(i))%f_node
    end if
  enddo
end if
end subroutine dag_options_make_f_nodes_single

subroutine dag_options_make_f_nodes_pair
  integer :: i_start, i_end
  integer :: n_nodes
  !!! get f_nodes from each combination
  n_nodes = 0
  do i=1, n_obj
    if (allocated (dag%combination(i_obj(i))%f_node_ptr1)) then
      n_nodes = n_nodes + size (dag%combination(i_obj(i))%f_node_ptr1)
    end if
  enddo
  if (n_nodes /= 0) then
    allocate (dag_options%f_node_ptr1 (n_nodes))
    allocate (dag_options%f_node_ptr2 (n_nodes))
    i_end = 0
    do i=1, n_obj
      if (allocated (dag%combination(i_obj(i))%f_node_ptr1)) then
        i_start = i_end + 1
        i_end = i_end + size (dag%combination(i_obj(i))%f_node_ptr1)
        dag_options%f_node_ptr1(i_start:i_end) = dag%combination(i_obj(i))%f_node_ptr1
        dag_options%f_node_ptr2(i_start:i_end) = dag%combination(i_obj(i))%f_node_ptr2
      end if
    enddo
  end if
end subroutine dag_options_make_f_nodes_pair
end subroutine dag_options_make_f_nodes

```

We create all combinations of daughter **f_nodes** for a combination. In the combination each daughter can be either a single **dag_node** or **dag_options** which are a set of single **dag_nodes**. Therefore, we first create all possible **f_nodes** for daughter1, then all possible **f_nodes** for daughter2. In the end we combine all **daughter1** nodes with all **daughter2** nodes.

<Cascades2: dag combination: TBP>+≡

```
procedure :: make_f_nodes => dag_combination_make_f_nodes
```

<Cascades2: procedures>+≡

```
subroutine dag_combination_make_f_nodes (dag_combination, &
```

```

        feyngraph_set, dag)
class (dag_combination_t), intent (inout) :: dag_combination
type (feyngraph_set_t), intent (inout) :: feyngraph_set
type (dag_t), intent (inout) :: dag
integer, dimension (2) :: obj, i_obj
integer :: n_obj
integer :: new_size, size1, size2
integer :: i, j, pos
if (allocated (dag_combination%f_node_ptr1)) return
n_obj = 0
do i = 1, size (dag_combination%string%t)
    select case (dag_combination%string%t(i)%type)
    case (DAG_NODE_TK, DAG_OPTIONS_TK, DAG_COMBINATION_TK)
        n_obj = n_obj + 1
        if (n_obj > 2) return
        obj(n_obj) = dag_combination%string%t(i)%type
        i_obj(n_obj) = dag_combination%string%t(i)%index
    end select
enddo
size1 = 0
size2 = 0
if (obj(1) == DAG_NODE_TK) then
    if (allocated (dag%node(i_obj(1))%f_node)) &
        size1 = size (dag%node(i_obj(1))%f_node)
else if (obj(1) == DAG_OPTIONS_TK) then
    if (allocated (dag%options(i_obj(1))%f_node_ptr1)) &
        size1 = size (dag%options(i_obj(1))%f_node_ptr1)
end if
if (obj(2) == DAG_NODE_TK) then
    if (allocated (dag%node(i_obj(2))%f_node)) &
        size2 = size (dag%node(i_obj(2))%f_node)
else if (obj(2) == DAG_OPTIONS_TK) then
    if (allocated (dag%options(i_obj(2))%f_node_ptr1)) &
        size2 = size (dag%options(i_obj(2))%f_node_ptr1)
end if
!!! combine the 2 arrays of f_nodes
new_size = size1*size2
if (new_size /= 0) then
    allocate (dag_combination%f_node_ptr1 (new_size))
    allocate (dag_combination%f_node_ptr2 (new_size))
    pos = 0
    select case (obj(1))
    case (DAG_NODE_TK)
        select case (obj(2))
        case (DAG_NODE_TK)
            do i = 1, size1
                do j = 1, size2
                    pos = pos + 1
                    dag_combination%f_node_ptr1(pos) = dag%node(i_obj(1))%f_node(i)
                    dag_combination%f_node_ptr2(pos) = dag%node(i_obj(2))%f_node(j)
                enddo
            enddo
        case (DAG_OPTIONS_TK)
            do i = 1, size1

```

```

        do j = 1, size2
            pos = pos + 1
            dag_combination%f_node_ptr1(pos) = dag%node(i_obj(1))%f_node(i)
            dag_combination%f_node_ptr2(pos) = dag%options(i_obj(2))%f_node_ptr1(j)
        enddo
    enddo
end select
case (DAG_OPTIONS_TK)
select case (obj(2))
case (DAG_NODE_TK)
do i = 1, size1
do j = 1, size2
pos = pos + 1
dag_combination%f_node_ptr1(pos) = dag%options(i_obj(1))%f_node_ptr1(i)
dag_combination%f_node_ptr2(pos) = dag%node(i_obj(2))%f_node(j)
enddo
enddo
case (DAG_OPTIONS_TK)
do i = 1, size1
do j = 1, size2
pos = pos + 1
dag_combination%f_node_ptr1(pos) = dag%options(i_obj(1))%f_node_ptr1(i)
dag_combination%f_node_ptr2(pos) = dag%options(i_obj(2))%f_node_ptr1(j)
enddo
enddo
end select
end select
end if
end subroutine dag_combination_make_f_nodes

```

Here we create the **feyngraphs**. After the construction of the **dag** the remaining **dag.string** should contain a token for a single **dag_node** which corresponds to the roots of the **feyngraphs**. Therefore we make all **f_nodes** for this **dag_node** and create a **feyngraph** for each **f_node**. Note that only 3-vertices are accepted. All other vertices are rejected. The starting point is the last dag node which has been added to the list, since this corresponds to the root of the tree. Is is important to understand that the structure of feyngraphs is not the same as the structure of the dag which is read from file, because for the calculations which are performed in this module we want to reuse the nodes for the outgoing particles, which means that they appear only once. In O'Mega's output, it is the first incoming particle which appears only once and the outgoing particles appear many times. This transition is incorporated in the subroutines which create **f_nodes** from the different dag objects.

```

<Cascades2: dag: TBP>+≡
    procedure :: make_feyngraphs => dag_make_feyngraphs

<Cascades2: procedures>+≡
    subroutine dag_make_feyngraphs (dag, feyngraph_set)
        class (dag_t), intent (inout) :: dag
        type (feyngraph_set_t), intent (inout) :: feyngraph_set
        integer :: i
        integer :: max_subtree_size
        max_subtree_size = dag%node(dag%n_nodes)%subtree_size
    end subroutine

```

```

if (allocated (dag%node(dag%n_nodes)%f_node)) then
  do i = 1, size (dag%node(dag%n_nodes)%f_node)
    if (.not. associated (feyngraph_set%first)) then
      allocate (feyngraph_set%last)
      feyngraph_set%first => feyngraph_set%last
    else
      allocate (feyngraph_set%last%next)
      feyngraph_set%last => feyngraph_set%last%next
    end if
    feyngraph_set%last%root => dag%node(dag%n_nodes)%f_node(i)%node
!!! The first particle was correct in the 0'Mega parsable DAG output. It was however
!!! changed to its anti-particle in f_node_assign_particle_properties, which we revert here.
    feyngraph_set%last%root%particle => feyngraph_set%last%root%particle%anti
    feyngraph_set%last%n_nodes = feyngraph_set%last%root%n_subtree_nodes
    feyngraph_set%n_graphs = feyngraph_set%n_graphs + 1
  enddo
  feyngraph_set%f_node_list%max_tree_size = feyngraph_set%first%n_nodes
end if
end subroutine dag_make_feyngraphs

```

A write procedure of the dag for debugging.

```

<Cascades2: dag: TBP>+≡
  procedure :: write => dag_write

<Cascades2: procedures>+≡
  subroutine dag_write (dag, u)
    class (dag_t), intent (in) :: dag
    integer, intent(in) :: u
    integer :: i
    write (u,fmt='(A)') 'nodes'
    do i=1, dag%n_nodes
      write (u,fmt='(I5,3X,A)') i, char (dag%node(i)%string)
    enddo
    write (u,fmt='(A)') 'options'
    do i=1, dag%n_options
      write (u,fmt='(I5,3X,A)') i, char (dag%options(i)%string)
    enddo
    write (u,fmt='(A)') 'combination'
    do i=1, dag%n_combinations
      write (u,fmt='(I5,3X,A)') i, char (dag%combination(i)%string)
    enddo
  end subroutine dag_write

```

Make a copy of a resonant **k_node**, where the copy is kept nonresonant.

```

<Cascades2: procedures>+≡
  subroutine k_node_make_nonresonant_copy (k_node)
    type (k_node_t), intent (in) :: k_node
    type (k_node_t), pointer :: copy
    call k_node%f_node%k_node_list%add_entry (copy, recycle=.true.)
    copy%daughter1 => k_node%daughter1
    copy%daughter2 => k_node%daughter2
    copy = k_node
    copy%mapping = NONRESONANT
  end subroutine k_node_make_nonresonant_copy

```

```

    copy%resonant = .false.
    copy%on_shell = .false.
    copy%mapping_assigned = .true.
    copy%is_nonresonant_copy = .true.
end subroutine k_node_make_nonresonant_copy

```

For a given `feyngraph` we create all possible `kingraphs`. Here we use existing `k_nodes` which have already been created when the mapping calculations of the pure s-channel subgraphs are performed. The nodes for the incoming particles or the nodes on the t-line will have to be created in all cases because they are not used in several graphs. To obtain the existing `k_nodes`, we use the subroutine `k_node_init_from_f_node` which itself uses `f_node_list.get_nodes` to obtain all active `k_nodes` in the `k_node_list` of the `f_node`. The created `kingraphs` are attached to the linked list of the `feyngraph`. For scattering processes we have to split up the t-line, because since all graphs are represented as a decay, different nodes can share daughter nodes. This happens also for the t-line or the incoming particle which appears as an outgoing particle. For the `t_line` or `incoming` nodes we do not want to recycle nodes but rather create a copy of this line for each `kingraph`.

```

<Cascades2: feyngraph: TBP>+≡
    procedure :: make_kingraphs => feyngraph_make_kingraphs

<Cascades2: procedures>+≡
    subroutine feyngraph_make_kingraphs (feyngraph, feyngraph_set)
        class (feyngraph_t), intent (inout) :: feynngraph
        type (feyngraph_set_t), intent (in) :: feynngraph_set
        type (k_node_ptr_t), dimension (:), allocatable :: kingraph_root
        integer :: i
        if (.not. associated (feyngraph%kin_first)) then
            call k_node_init_from_f_node (feyngraph%root, &
                kingraph_root, feynngraph_set)
            if (.not. feynngraph%root%keep) return
            if (feyngraph_set%process_type == SCATTERING) then
                call split_up_t_lines (kingraph_root)
            end if
            do i=1, size (kingraph_root)
                if (associated (feyngraph%kin_last)) then
                    allocate (feyngraph%kin_last%next)
                    feynngraph%kin_last => feynngraph%kin_last%next
                else
                    allocate (feyngraph%kin_last)
                    feynngraph%kin_first => feynngraph%kin_last
                end if
                feynngraph%kin_last%root => kingraph_root(i)%node
                feynngraph%kin_last%n_nodes = feynngraph%n_nodes
                feynngraph%kin_last%keep = feynngraph%keep
                if (feyngraph_set%process_type == SCATTERING) then
                    feynngraph%kin_last%root%bincode = &
                        f_node_get_external_bincode (feyngraph_set, feynngraph%root)
                end if
            enddo
            deallocate (kingraph_root)
        end if
    end subroutine

```



```
end subroutine feyngraph_make_kingraphs
```

Create all **k_nodes** for a given **f_node**. We return these nodes using **k_node_ptr**. If the node is external, we assign also the bincode to the **k_nodes** because this is determined from substrings of the input file which belong to the **feyngraphs** and **f_nodes**.

(Cascades2: procedures)+≡

```
recursive subroutine k_node_init_from_f_node (f_node, k_node_ptr, feyngraph_set)
  type (f_node_t), target, intent (inout) :: f_node
  type (k_node_ptr_t), allocatable, dimension (:), intent (out) :: k_node_ptr
  type (feyngraph_set_t), intent (in) :: feyngraph_set
  type (k_node_ptr_t), allocatable, dimension(:) :: daughter_ptr1, daughter_ptr2
  integer :: n_nodes
  integer :: i, j
  integer :: pos
  integer, save :: counter = 0
  if (.not. (f_node%incoming .or. f_node%t_line)) then
    call f_node%k_node_list%get_nodes (k_node_ptr)
    if (.not. allocated (k_node_ptr) .and. f_node%k_node_list%n_entries > 0) then
      f_node%keep = .false.
      return
    end if
  end if
  if (.not. allocated (k_node_ptr)) then
    if (associated (f_node%daughter1) .and. associated (f_node%daughter2)) then
      call k_node_init_from_f_node (f_node%daughter1, daughter_ptr1, &
        feyngraph_set)
      call k_node_init_from_f_node (f_node%daughter2, daughter_ptr2, &
        feyngraph_set)
      if (.not. (f_node%daughter1%keep .and. f_node%daughter2%keep)) then
        f_node%keep = .false.
        return
      end if
      n_nodes = size (daughter_ptr1) * size (daughter_ptr2)
      allocate (k_node_ptr (n_nodes))
      pos = 1
      do i=1, size (daughter_ptr1)
        do j=1, size (daughter_ptr2)
          if (f_node%incoming .or. f_node%t_line) then
            call f_node%k_node_list%add_entry (k_node_ptr(pos)%node, recycle = .false.)
          else
            call f_node%k_node_list%add_entry (k_node_ptr(pos)%node, recycle = .true.)
          end if
          k_node_ptr(pos)%node%f_node => f_node
          k_node_ptr(pos)%node%daughter1 => daughter_ptr1(i)%node
          k_node_ptr(pos)%node%daughter2 => daughter_ptr2(j)%node
          k_node_ptr(pos)%node%f_node_index = f_node%index
          k_node_ptr(pos)%node%incoming = f_node%incoming
          k_node_ptr(pos)%node%t_line = f_node%t_line
          k_node_ptr(pos)%node%particle => f_node%particle
          pos = pos + 1
        enddo
      enddo
    enddo
  enddo
```

```

        deallocate (daughter_ptr1, daughter_ptr2)
    else
        allocate (k_node_ptr(1))
        if (f_node%incoming .or. f_node%t_line) then
            call f_node%k_node_list%add_entry (k_node_ptr(1)%node, recycle=.false.)
        else
            call f_node%k_node_list%add_entry (k_node_ptr(1)%node, recycle=.true.)
        end if
        k_node_ptr(1)%node%f_node => f_node
        k_node_ptr(1)%node%f_node_index = f_node%index
        k_node_ptr(1)%node%incoming = f_node%incoming
        k_node_ptr(1)%node%t_line = f_node%t_line
        k_node_ptr(1)%node%particle => f_node%particle
        k_node_ptr(1)%node%bincode = f_node_get_external_bincode (feyngraph_set, &
            f_node)
    end if
end if
end subroutine k_node_init_from_f_node

```

The graphs resulting from `k_node_init_from_f_node` are fine if they are used only in one direction. This is however not the case when one wants to invert the graphs, i.e. take the other incoming particle of a scattering process as the decaying particle, because the outgoing `f_nodes` (and hence also the `k_nodes`) exist only once. This problem is solved here by creating a distinct t-line for each of the graphs. The following subroutine disentangles the data structure by creating new nodes such that the different t-lines are not connected any more.

(*Cascades2: procedures*) +=

```

recursive subroutine split_up_t_lines (t_node)
    type (k_node_ptr_t), dimension(:), intent (inout) :: t_node
    type (k_node_t), pointer :: ref_node => null ()
    type (k_node_t), pointer :: ref_daughter => null ()
    type (k_node_t), pointer :: new_daughter => null ()
    type (k_node_ptr_t), dimension(:), allocatable :: t_daughter
    integer :: ref_daughter_index
    integer :: i, j
    allocate (t_daughter (size (t_node)))
    do i=1, size (t_node)
        ref_node => t_node(i)%node
        if (associated (ref_node%daughter1) .and. associated (ref_node%daughter2)) then
            ref_daughter => null ()
            if (ref_node%daughter1%incoming .or. ref_node%daughter1%t_line) then
                ref_daughter => ref_node%daughter1
                ref_daughter_index = 1
            else if (ref_node%daughter2%incoming .or. ref_node%daughter2%t_line) then
                ref_daughter => ref_node%daughter2
                ref_daughter_index = 2
            end if
            do j=1, size (t_daughter)
                if (.not. associated (t_daughter(j)%node)) then
                    t_daughter(j)%node => ref_daughter
                    exit
                else if (t_daughter(j)%node%index == ref_daughter%index) then
                    new_daughter => null ()

```

```

        call ref_daughter%f_node%k_node_list%add_entry (new_daughter, recycle=.false.)
        new_daughter = ref_daughter
        new_daughter%daughter1 => ref_daughter%daughter1
        new_daughter%daughter2 => ref_daughter%daughter2
        if (ref_daughter_index == 1) then
            ref_node%daughter1 => new_daughter
        else if (ref_daughter_index == 2) then
            ref_node%daughter2 => new_daughter
        end if
        ref_daughter => new_daughter
    end if
enddo
else
    return
end if
enddo
call split_up_t_lines (t_daughter)
deallocate (t_daughter)
end subroutine split_up_t_lines

```

This subroutine sets the `inverse_daughters` of a `k_node`. If we invert a kingraph such that not the first but the second incoming particle appears as the root of the tree, the `incoming` and `t_line` particles obtain other daughters. These are the former mother node and the sister node `s_daughter`. Here we set only the pointers for the `inverse_daughters`. The inversion happens in `kingraph_make_inverse_copy` and `node_inverse_deep_copy`.

(*Cascades2: procedures*) +=

```

subroutine kingraph_set_inverse_daughters (kingraph)
    type (kingraph_t), intent (inout) :: kingraph
    type (k_node_t), pointer :: mother
    type (k_node_t), pointer :: t_daughter
    type (k_node_t), pointer :: s_daughter
    mother => kingraph%root
    do while (associated (mother))
        if (associated (mother%daughter1) .and. &
            associated (mother%daughter2)) then
            if (mother%daughter1%t_line .or. mother%daughter1%incoming) then
                t_daughter => mother%daughter1; s_daughter => mother%daughter2
            else if (mother%daughter2%t_line .or. mother%daughter2%incoming) then
                t_daughter => mother%daughter2; s_daughter => mother%daughter1
            else
                exit
            end if
            t_daughter%inverse_daughter1 => mother
            t_daughter%inverse_daughter2 => s_daughter
            mother => t_daughter
        else
            exit
        end if
    enddo
end subroutine kingraph_set_inverse_daughters

```

Set the bincode of an `f_node` which corresponds to an external particle. This

is done on the basis of the `particle_label` which is a substring of the input file. Here it is not the particle name which is important, but the number(s) in brackets which in general indicate the external particles which are connected to the current node. This function is however only used for external particles, so there can either be one or `n_out + 1` particles in the brackets (in the DAG input file always one, because also for the root there is only a single number). In all cases we check the number of particles (in the DAG input the numbers are separated by a slash).

```

<Cascades2: procedures>+≡
function f_node_get_external_bincode (feyngraph_set, f_node) result (bincode)
  type (feyngraph_set_t), intent (in) :: feyngraph_set
  type (f_node_t), intent (in) :: f_node
  integer (TC) :: bincode
  character (len=LABEL_LEN) :: particle_label
  integer :: start_pos, end_pos, n_out_decay
  integer :: n_prt ! for DAG
  integer :: i
  bincode = 0
  if (feyngraph_set%process_type == DECAY) then
    n_out_decay = feyngraph_set%n_out
  else
    n_out_decay = feyngraph_set%n_out + 1
  end if
  particle_label = f_node%particle_label
  start_pos = index (particle_label, '[') + 1
  end_pos = index (particle_label, ']') - 1
  particle_label = particle_label(start_pos:end_pos)
  !!! n_out_decay is the number of outgoing particles in the
  !!! 0'Mega output, which is always represented as a decay
  if (feyngraph_set%use_dag) then
    n_prt = 1
    do i=1, len(particle_label)
      if (particle_label(i:i) == '/') n_prt = n_prt + 1
    enddo
  else
    n_prt = end_pos - start_pos + 1
  end if
  if (n_prt == 1) then
    bincode = calculate_external_bincode (particle_label, &
      feyngraph_set%process_type, n_out_decay)
  else if (n_prt == n_out_decay) then
    bincode = ibset (0, n_out_decay)
  end if
end function f_node_get_external_bincode

```

Assign a bincode to an internal node, which is calculated from the bincodes of `daughter1` and `daughter2`.

```

<Cascades2: procedures>+≡
subroutine node_assign_bincode (node)
  type (k_node_t), intent (inout) :: node
  if (associated (node%daughter1) .and. associated (node%daughter2) &
    .and. .not. node%incoming) then
    node%bincode = ior(node%daughter1%bincode, node%daughter2%bincode)
  end if
end subroutine node_assign_bincode

```

```

    end if
end subroutine node_assign_bincode

```

Calculate the `bincode` from the number in the brackets of the `particle_label`, if the node is external. For the root in the non-factorized output, this is calculated directly in `f_node_get_external_bincode` because in this case all the other external particle numbers appear between the brackets.

(Cascades2: procedures)+≡

```

function calculate_external_bincode (label_number_string, process_type, n_out_decay) result (bin
character (len=*), intent (in) :: label_number_string
integer, intent (in) :: process_type
integer, intent (in) :: n_out_decay
character :: number_char
integer :: number_int
integer (kind=TC) :: bincode
bincode = 0
read (label_number_string, fmt='(A)') number_char
!!! check if the character is a letter (A,B,C,...) or a number (1...9)
!!! numbers 1 and 2 are special cases
select case (number_char)
case ('1')
    if (process_type == SCATTERING) then
        number_int = n_out_decay + 3
    else
        number_int = n_out_decay + 2
    end if
case ('2')
    if (process_type == SCATTERING) then
        number_int = n_out_decay + 2
    else
        number_int = 2
    end if
case ('A')
    number_int = 10
case ('B')
    number_int = 11
case ('C')
    number_int = 12
case ('D')
    number_int = 13
case default
    read (number_char, fmt='(I1)') number_int
end select
bincode = ibset (bincode, number_int - process_type - 1)
end function calculate_external_bincode

```

19.14.13 Mapping calculations

Once a `k_node` and its subtree nodes have been created, we can perform the kinematical calculations and assign mappings, depending on the particle properties and the results for the subtree nodes. This could in principle be done recursively, calling the procedure first for the daughter nodes and then perform

the calculations for the actual node. But for parallization and comparing the nodes, this will be done simultaneously for all nodes with the same number of subtree nodes, and the number of subtree nodes increases, starting from one, in steps of two. The actual mapping calculations are done in complete analogy to cascades.

```

(Cascades2: procedures)+≡
subroutine node_assign_mapping_s (feyngraph, node, feyngraph_set)
  type (feyngraph_t), intent (inout) :: feyngraph
  type (k_node_t), intent (inout) :: node
  type (feyngraph_set_t), intent (inout) :: feyngraph_set
  real(default) :: eff_mass_sum
  logical :: keep
  if (.not. node%mapping_assigned) then
    if (node%particle%mass > feyngraph_set%phs_par%m_threshold_s) then
      node%effective_mass = node%particle%mass
    end if
    if (associated (node%daughter1) .and. associated (node%daughter2)) then
      if (.not. (node%daughter1%keep .and. node%daughter2%keep)) then
        node%keep = .false.; return
      end if
      node%ext_mass_sum = node%daughter1%ext_mass_sum &
        + node%daughter2%ext_mass_sum
      keep = .false.
    !!! Potentially resonant cases [sqrts = m_rea for on-shell decay]
    if (node%particle%mass > node%ext_mass_sum &
      .and. node%particle%mass <= feyngraph_set%phs_par%sqrts) then
      if (node%particle%width /= 0) then
        if (node%daughter1%on_shell .or. node%daughter2%on_shell) then
          keep = .true.
          node%mapping = S_CHANNEL
          node%resonant = .true.
        end if
      else
        call warn_decay (node%particle)
      end if
    !!! Collinear and IR singular cases
    else if (node%particle%mass < feyngraph_set%phs_par%sqrts) then
    !!! Massless splitting
      if (node%daughter1%effective_mass == 0 &
        .and. node%daughter2%effective_mass == 0 &
        .and. .not. associated (node%daughter1%daughter1) &
        .and. .not. associated (node%daughter1%daughter2) &
        .and. .not. associated (node%daughter2%daughter1) &
        .and. .not. associated (node%daughter2%daughter2)) then
        keep = .true.
        node%log_enhanced = .true.
        if (node%particle%is_vector) then
          if (node%daughter1%particle%is_vector &
            .and. node%daughter2%particle%is_vector) then
            node%mapping = COLLINEAR    !!! three-vector-splitting
          else
            node%mapping = INFRARED    !!! vector splitting into matter
          end if
        end if
      end if
    end if
  end if

```

```

else
  if (node%daughter1%particle%is_vector &
      .or. node%daughter2%particle%is_vector) then
    node%mapping = COLLINEAR    !!! vector radiation off matter
  else
    node%mapping = INFRARED     !!! scalar radiation/splitting
  end if
end if
!!! IR radiation off massive particle [cascades]
else if (node%effective_mass > 0 .and. &
  node%daughter1%effective_mass > 0 .and. &
  node%daughter2%effective_mass == 0 .and. &
  (node%daughter1%on_shell .or. &
  node%daughter1%mapping == RADIATION) .and. &
  abs (node%effective_mass - &
  node%daughter1%effective_mass) < feyngraph_set%phs_par%m_threshold_s) &
  then
    keep = .true.
    node%log_enhanced = .true.
    node%mapping = RADIATION
  else if (node%effective_mass > 0 .and. &
    node%daughter2%effective_mass > 0 .and. &
    node%daughter1%effective_mass == 0 .and. &
    (node%daughter2%on_shell .or. &
    node%daughter2%mapping == RADIATION) .and. &
    abs (node%effective_mass - &
    node%daughter2%effective_mass) < feyngraph_set%phs_par%m_threshold_s) &
    then
      keep = .true.
      node%log_enhanced = .true.
      node%mapping = RADIATION
    end if
  end if
!!! Non-singular cases, including failed resonances [from cascades]
  if (.not. keep) then
!!! Two on-shell particles from a virtual mother [from cascades, here eventually more than 2]
    if (node%daughter1%on_shell .or. node%daughter2%on_shell) then
      keep = .true.
      eff_mass_sum = node%daughter1%effective_mass &
        + node%daughter2%effective_mass
      node%effective_mass = max (node%ext_mass_sum, eff_mass_sum)
      if (node%effective_mass < feyngraph_set%phs_par%m_threshold_s) then
        node%effective_mass = 0
      end if
    end if
  end if
!!! Complete and register feyngraph (make copy in case of resonance)
  if (keep) then
    node%on_shell = node%resonant .or. node%log_enhanced
    if (node%resonant) then
      if (feyngraph_set%phs_par%keep_nonresonant) then
        call k_node_make_nonresonant_copy (node)
      end if
      node%ext_mass_sum = node%particle%mass
    end if
  end if

```

```

        end if
    end if
    node%mapping_assigned = .true.
    call node_assign_bincode (node)
    call node%subtree%add_entry (node)
else !!! external (outgoing) particle
    node%ext_mass_sum = node%particle%mass
    node%mapping = EXTERNAL_PRT
    node%multiplicity = 1
    node%mapping_assigned = .true.
    call node%subtree%add_entry (node)
    node%on_shell = .true.
    if (node%particle%mass >= feyngraph_set%phs_par%m_threshold_s) then
        node%effective_mass = node%particle%mass
    end if
end if
else if (node%is_nonresonant_copy) then
    call node_assign_bincode (node)
    call node%subtree%add_entry (node)
    node%is_nonresonant_copy = .false.
end if
call node_count_specific_properties (node)
if (node%n_off_shell > feyngraph_set%phs_par%off_shell) then
    node%keep = .false.
end if
contains
subroutine warn_decay (particle)
    type(part_prop_t), intent(in) :: particle
    integer :: i
    integer, dimension(MAX_WARN_RESONANCE), save :: warned_code = 0
    LOOP_WARNED: do i = 1, MAX_WARN_RESONANCE
        if (warned_code(i) == 0) then
            warned_code(i) = particle%pdg
            write (msg_buffer, "(A)" &
                & " Intermediate decay of zero-width particle " &
                & // trim(particle%particle_label) &
                & // " may be possible."
            )
            call msg_warning
            exit LOOP_WARNED
        else if (warned_code(i) == particle%pdg) then
            exit LOOP_WARNED
        end if
    end do LOOP_WARNED
end subroutine warn_decay
end subroutine node_assign_mapping_s

```

We determine the numbers `n_resonances`, `multiplicity`, `n_off_shell` and `n_log_enhanced` for a given node.

(Cascades2: procedures) +≡

```

subroutine node_count_specific_properties (node)
    type(k_node_t), intent(inout) :: node
    if (associated (node%daughter1) .and. associated(node%daughter2)) then
        if (node%resonant) then

```



```

        node%multiplicity = 1
        node%n_resonances &
            = node%daughter1%n_resonances &
              + node%daughter2%n_resonances + 1
    else
        node%multiplicity &
            = node%daughter1%multiplicity &
              + node%daughter2%multiplicity
        node%n_resonances &
            = node%daughter1%n_resonances &
              + node%daughter2%n_resonances
    end if
    if (node%log_enhanced) then
        node%n_log_enhanced &
            = node%daughter1%n_log_enhanced &
              + node%daughter2%n_log_enhanced + 1
    else
        node%n_log_enhanced &
            = node%daughter1%n_log_enhanced &
              + node%daughter2%n_log_enhanced
    end if
    if (node%resonant) then
        node%n_off_shell = 0
    else if (node%log_enhanced) then
        node%n_off_shell &
            = node%daughter1%n_off_shell &
              + node%daughter2%n_off_shell
    else
        node%n_off_shell &
            = node%daughter1%n_off_shell &
              + node%daughter2%n_off_shell + 1
    end if
    if (node%t_line) then
        if (node%daughter1%t_line .or. node%daughter1%incoming) then
            node%n_t_channel = node%daughter1%n_t_channel + 1
        else if (node%daughter2%t_line .or. node%daughter2%incoming) then
            node%n_t_channel = node%daughter2%n_t_channel + 1
        end if
    end if
end if
end if
end subroutine node_count_specific_properties

```

The subroutine `kingraph_assign_mappings_s` completes kinematical calculations for a decay process, considering the root node.

(*Cascades2: procedures*) +=

```

subroutine kingraph_assign_mappings_s (feyngraph, kingraph, feyngraph_set)
    type (feyngraph_t), intent (inout) :: feyngraph
    type (kingraph_t), pointer, intent (inout) :: kingraph
    type (feyngraph_set_t), intent (inout) :: feyngraph_set
    if (.not. (kingraph%root%daughter1%keep .and. kingraph%root%daughter2%keep)) then
        kingraph%keep = .false.
        call kingraph%tree%final ()
    end if
end if

```

```

if (kingraph%keep) then
  kingraph%root%on_shell = .true.
  kingraph%root%mapping = EXTERNAL_PRT
  kingraph%root%mapping_assigned = .true.
  call node_assign_bincode (kingraph%root)
  kingraph%root%ext_mass_sum = &
    kingraph%root%daughter1%ext_mass_sum + &
    kingraph%root%daughter2%ext_mass_sum
  if (kingraph%root%ext_mass_sum >= feyngraph_set%phs_par%sqrts) then
    kingraph%root%keep = .false.
    kingraph%keep = .false.; call kingraph%tree%final (); return
  end if
  call kingraph%root%subtree%add_entry (kingraph%root)
  kingraph%root%multiplicity &
    = kingraph%root%daughter1%multiplicity &
    + kingraph%root%daughter2%multiplicity
  kingraph%root%n_resonances &
    = kingraph%root%daughter1%n_resonances &
    + kingraph%root%daughter2%n_resonances
  kingraph%root%n_off_shell &
    = kingraph%root%daughter1%n_off_shell &
    + kingraph%root%daughter2%n_off_shell
  kingraph%root%n_log_enhanced &
    = kingraph%root%daughter1%n_log_enhanced &
    + kingraph%root%daughter2%n_log_enhanced
  if (kingraph%root%n_off_shell > feyngraph_set%phs_par%off_shell) then
    kingraph%root%keep = .false.
    kingraph%keep = .false.; call kingraph%tree%final (); return
  else
    kingraph%grove_prop%multiplicity = &
      kingraph%root%multiplicity
    kingraph%grove_prop%n_resonances = &
      kingraph%root%n_resonances
    kingraph%grove_prop%n_off_shell = &
      kingraph%root%n_off_shell
    kingraph%grove_prop%n_log_enhanced = &
      kingraph%root%n_log_enhanced
  end if
  kingraph%tree = kingraph%root%subtree
end if
end subroutine kingraph_assign_mappings_s

```

Compute mappings for the t_line and incoming nodes. This is done recursively using node_compute_t_line.

(*Cascades2: procedures*) +=

```

subroutine kingraph_compute_mappings_t_line (feyngraph, kingraph, feyngraph_set)
  type (feyngraph_t), intent (inout) :: feyngraph
  type (kingraph_t), pointer, intent (inout) :: kingraph
  type (feyngraph_set_t), intent (inout) :: feyngraph_set
  call node_compute_t_line (feyngraph, kingraph, kingraph%root, feyngraph_set)
  if (.not. kingraph%root%keep) then
    kingraph%keep = .false.
    call kingraph%tree%final ()
  end if
end subroutine

```

```

end if
if (kingraph%keep) kingraph%tree = kingraph%root%subtree
end subroutine kingraph_compute_mappings_t_line

```

Perform the kinematical calculations and mapping assignment for a node which is either `incoming` or `t_line`. This is done recursively, going first to the daughter node which has this property. Therefore we first set the pointer `t_node` to this daughter node and `s_node` to the other one. The mapping determination happens again in the same way as in `cascades`.

(*Cascades2: procedures*) \equiv

```

recursive subroutine node_compute_t_line (feyngraph, kingraph, node, feyngraph_set)
  type (feyngraph_t), intent (inout) :: feyngraph
  type (kingraph_t), intent (inout) :: kingraph
  type (k_node_t), intent (inout) :: node
  type (feyngraph_set_t), intent (inout) :: feyngraph_set
  type (k_node_t), pointer :: s_node
  type (k_node_t), pointer :: t_node
  type (k_node_t), pointer :: new_s_node
  if (.not. (node%daughter1%keep .and. node%daughter2%keep)) then
    node%keep = .false.
    return
  end if
  s_node => null ()
  t_node => null ()
  new_s_node => null ()
  if (associated (node%daughter1) .and. associated (node%daughter2)) then
    if (node%daughter1%t_line .or. node%daughter1%incoming) then
      t_node => node%daughter1; s_node => node%daughter2
    else if (node%daughter2%t_line .or. node%daughter2%incoming) then
      t_node => node%daughter2; s_node => node%daughter1
    end if
    if (t_node%t_line) then
      call node_compute_t_line (feyngraph, kingraph, t_node, feyngraph_set)
      if (.not. t_node%keep) then
        node%keep = .false.
        return
      end if
    else if (t_node%incoming) then
      t_node%mapping = EXTERNAL_PRT
      t_node%on_shell = .true.
      t_node%ext_mass_sum = t_node%particle%mass
      if (t_node%particle%mass >= feyngraph_set%phs_par%m_threshold_t) then
        t_node%effective_mass = t_node%particle%mass
      end if
      call t_node%subtree%add_entry (t_node)
    end if
  end if
  !!! root:
  if (.not. node%incoming) then
    if (t_node%incoming) then
      node%ext_mass_sum = s_node%ext_mass_sum
    else
      node%ext_mass_sum &
        = node%daughter1%ext_mass_sum &

```

```

        + node%daughter2%ext_mass_sum
    end if
    if (node%particle%mass > feyngraph_set%phs_par%m_threshold_t) then
        node%effective_mass = max (node%particle%mass, &
            s_node%effective_mass)
    else if (s_node%effective_mass > feyngraph_set%phs_par%m_threshold_t) then
        node%effective_mass = s_node%effective_mass
    else
        node%effective_mass = 0
    end if
    !!! Allowed decay of beam particle
    if (t_node%incoming &
        .and. t_node%particle%mass > s_node%particle%mass &
        + node%particle%mass) then
        call beam_decay (feyngraph_set%fatal_beam_decay)
    !!! Massless splitting
    else if (t_node%effective_mass == 0 &
        .and. s_node%effective_mass < feyngraph_set%phs_par%m_threshold_t &
        .and. node%effective_mass == 0) then
        node%mapping = U_CHANNEL
        node%log_enhanced = .true.
    !!! IR radiation off massive particle
    else if (t_node%effective_mass /= 0 &
        .and. s_node%effective_mass == 0 &
        .and. node%effective_mass /= 0 &
        .and. (t_node%on_shell &
        .or. t_node%mapping == RADIATION) &
        .and. abs (t_node%effective_mass - node%effective_mass) &
        < feyngraph_set%phs_par%m_threshold_t) then
        node%log_enhanced = .true.
        node%mapping = RADIATION
    end if
    node%mapping_assigned = .true.
    call node_assign_bincode (node)
    call node%subtree%add_entry (node)
    call node_count_specific_properties (node)
    if (node%n_off_shell > feyngraph_set%phs_par%off_shell) then
        node%keep = .false.
        kingraph%keep = .false.; call kingraph%tree%final (); return
    else if (node%n_t_channel > feyngraph_set%phs_par%t_channel) then
        node%keep = .false.;
        kingraph%keep = .false.; call kingraph%tree%final (); return
    end if
else
    node%mapping = EXTERNAL_PRT
    node%on_shell = .true.
    node%ext_mass_sum &
        = t_node%ext_mass_sum &
        + s_node%ext_mass_sum
    node%effective_mass = node%particle%mass
    if (.not. (node%ext_mass_sum < feyngraph_set%phs_par%sqrts)) then
        node%keep = .false.
        kingraph%keep = .false.; call kingraph%tree%final (); return
    end if

```

```

if (kingraph%keep) then
  if (t_node%incoming .and. s_node%log_enhanced) then
    call s_node%f_node%k_node_list%add_entry (new_s_node, recycle=.false.)
    new_s_node = s_node
    new_s_node%daughter1 => s_node%daughter1
    new_s_node%daughter2 => s_node%daughter2
    if (s_node%index == node%daughter1%index) then
      node%daughter1 => new_s_node
    else if (s_node%index == node%daughter2%index) then
      node%daughter2 => new_s_node
    end if
    new_s_node%subtree = s_node%subtree
    new_s_node%mapping = NO_MAPPING
    new_s_node%log_enhanced = .false.
    new_s_node%n_log_enhanced &
      = new_s_node%n_log_enhanced - 1
    new_s_node%log_enhanced = .false.
    where (new_s_node%subtree%bc == new_s_node%bincode)
      new_s_node%subtree%mapping = NO_MAPPING
    endwhere
  else if ((t_node%t_line .or. t_node%incoming) .and. &
    t_node%mapping == U_CHANNEL) then
    t_node%mapping = T_CHANNEL
    where (t_node%subtree%bc == t_node%bincode)
      t_node%subtree%mapping = T_CHANNEL
    endwhere
  else if (t_node%incoming .and. &
    .not. associated (s_node%daughter1) .and. &
    .not. associated (s_node%daughter2)) then
    call s_node%f_node%k_node_list%add_entry (new_s_node, recycle=.false.)
    new_s_node = s_node
    new_s_node%mapping = ON_SHELL
    new_s_node%daughter1 => s_node%daughter1
    new_s_node%daughter2 => s_node%daughter2
    new_s_node%subtree = s_node%subtree
    if (s_node%index == node%daughter1%index) then
      node%daughter1 => new_s_node
    else if (s_node%index == node%daughter2%index) then
      node%daughter2 => new_s_node
    end if
    where (new_s_node%subtree%bc == new_s_node%bincode)
      new_s_node%subtree%mapping = ON_SHELL
    endwhere
  end if
end if
call node%subtree%add_entry (node)
node%multiplicity &
  = node%daughter1%multiplicity &
  + node%daughter2%multiplicity
node%n_resonances &
  = node%daughter1%n_resonances &
  + node%daughter2%n_resonances
node%n_off_shell &
  = node%daughter1%n_off_shell &

```

```

        + node%daughter2%n_off_shell
node%n_log_enhanced &
    = node%daughter1%n_log_enhanced &
    + node%daughter2%n_log_enhanced
node%n_t_channel &
    = node%daughter1%n_t_channel &
    + node%daughter2%n_t_channel
if (node%n_off_shell > feyngraph_set%phs_par%off_shell) then
    node%keep = .false.
    kingraph%keep = .false.; call kingraph%tree%final (); return
else if (node%n_t_channel > feyngraph_set%phs_par%t_channel) then
    node%keep = .false.
    kingraph%keep = .false.; call kingraph%tree%final (); return
else
    kingraph%grove_prop%multiplicity = node%multiplicity
    kingraph%grove_prop%n_resonances = node%n_resonances
    kingraph%grove_prop%n_off_shell = node%n_off_shell
    kingraph%grove_prop%n_log_enhanced = node%n_log_enhanced
    kingraph%grove_prop%n_t_channel = node%n_t_channel
end if
end if
end if
contains
subroutine beam_decay (fatal_beam_decay)
    logical, intent(in) :: fatal_beam_decay
    write (msg_buffer, "(1x,A,1x,'->',1x,A,1x,A)") &
        t_node%particle%particle_label, &
        node%particle%particle_label, &
        s_node%particle%particle_label
    call msg_message
    write (msg_buffer, "(1x,'mass(',A,')' =',1x,E17.10)") &
        t_node%particle%particle_label, t_node%particle%mass
    call msg_message
    write (msg_buffer, "(1x,'mass(',A,')' =',1x,E17.10)") &
        node%particle%particle_label, node%particle%mass
    call msg_message
    write (msg_buffer, "(1x,'mass(',A,')' =',1x,E17.10)") &
        s_node%particle%particle_label, s_node%particle%mass
    call msg_message
    if (fatal_beam_decay) then
        call msg_fatal (" Phase space: Initial beam particle can decay")
    else
        call msg_warning (" Phase space: Initial beam particle can decay")
    end if
end subroutine beam_decay
end subroutine node_compute_t_line

```

After all pure s-channel subdiagrams have already been created from the corresponding **f_nodes** and mappings have been determined for their nodes, we complete the calculations here. In a first step, the **kingraphs** have to be created on the basis of the existing **k_nodes**, which means in particular that a **feyngraph** can give rise to several **kingraphs** which will all be attached to the linked list of the **feyngraph**. The calculations which remain are of different

kinds for decay and scattering processes. In a decay process the kinematical calculations have to be done for the `root` node. In a scattering process, after the creation of `kingraphs` in the first step, there will be only `kingraphs` with the first incoming particle as the `root` of the tree. For these graphs the `inverse` variable has the value `.false..` Before performing any calculations on these graphs we make a so-called inverse copy of the graph (see below), which will also be attached to the linked list. Since the s-channel subgraph calculations have already been completed, only the t-line computations remain.

```

<Cascades2: feyngraph: TBP>+≡
  procedure :: make_inverse_kingraphs => feyngraph_make_inverse_kingraphs

<Cascades2: procedures>+≡
  subroutine feyngraph_make_inverse_kingraphs (feyngraph)
    class (feyngraph_t), intent (inout) :: feyngraph
    type (kingraph_t), pointer :: current
    current => feyngraph%kin_first
    do while (associated (current))
      if (current%inverse) exit
      call current%make_inverse_copy (feyngraph)
      current => current%next
    enddo
  end subroutine feyngraph_make_inverse_kingraphs

<Cascades2: feyngraph: TBP>+≡
  procedure :: compute_mappings => feyngraph_compute_mappings

<Cascades2: procedures>+≡
  subroutine feyngraph_compute_mappings (feyngraph, feyngraph_set)
    class (feyngraph_t), intent (inout) :: feyngraph
    type (feyngraph_set_t), intent (inout) :: feyngraph_set
    type (kingraph_t), pointer :: current
    current => feyngraph%kin_first
    do while (associated (current))
      if (feyngraph_set%process_type == DECAY) then
        call kingraph_assign_mappings_s (feyngraph, current, feyngraph_set)
      else if (feyngraph_set%process_type == SCATTERING) then
        call kingraph_compute_mappings_t_line (feyngraph, current, feyngraph_set)
      end if
      current => current%next
    enddo
  end subroutine feyngraph_compute_mappings

```

Here we control the mapping calculations for the nodes of s-channel subgraphs. We start with the nodes with the smallest number of subtree nodes and always increase this number by two because nodes have exactly zero or two daughter nodes. We create the `k_nodes` using the `k_node_list` of each `f_node`. The number of nodes which have to be created depends of the number of existing daughter nodes, which means that we have to create a node for each combination of existing and valid (the ones which we `keep`) daughter nodes. If the node corresponds to an external particle, we create only one node, since there are no daughter nodes. If the particle is not external and the daughter `f_nodes` do not contain any valid `k_nodes`, we do not create a new `k_nodes` either. When

the calculations for all nodes with the same number of subtree nodes have been completed, we compare the valid nodes to eliminate equivalences (see below).

(Cascades2: procedures) +=

```

subroutine f_node_list_compute_mappings_s (feyngraph_set)
  type (feyngraph_set_t), intent (inout) :: feyngraph_set
  type (f_node_ptr_t), dimension(:), allocatable :: set
  type (k_node_ptr_t), dimension(:), allocatable :: k_set
  type (k_node_entry_t), pointer :: k_entry
  type (f_node_entry_t), pointer :: current
  type (k_node_list_t), allocatable :: compare_list
  integer :: n_entries
  integer :: pos
  integer :: i, j, k
  do i = 1, feyngraph_set%f_node_list%max_tree_size - 2, 2
!!! Counter number of f_nodes with subtree size i for s channel calculations
    n_entries = 0
    if (feyngraph_set%use_dag) then
      do j=1, feyngraph_set%dag%n_nodes
        if (allocated (feyngraph_set%dag%node(j)%f_node)) then
          do k=1, size(feyngraph_set%dag%node(j)%f_node)
            if (associated (feyngraph_set%dag%node(j)%f_node(k)%node)) then
              if (.not. (feyngraph_set%dag%node(j)%f_node(k)%node%incoming &
                .or. feyngraph_set%dag%node(j)%f_node(k)%node%t_line) &
                .and. feyngraph_set%dag%node(j)%f_node(k)%node%n_subtree_nodes == i) then
                n_entries = n_entries + 1
              end if
            end if
          enddo
        end if
      enddo
    else
      current => feyngraph_set%f_node_list%first
      do while (associated (current))
        if (.not. (current%node%incoming .or. current%node%t_line) &
          .and. current%node%n_subtree_nodes == i) then
          n_entries = n_entries + 1
        end if
        current => current%next
      enddo
    end if
    if (n_entries == 0) exit
!!! Create a temporary k node list for comparison
    allocate (set(n_entries))
    pos = 0
    if (feyngraph_set%use_dag) then
      do j=1, feyngraph_set%dag%n_nodes
        if (allocated (feyngraph_set%dag%node(j)%f_node)) then
          do k=1, size(feyngraph_set%dag%node(j)%f_node)
            if (associated (feyngraph_set%dag%node(j)%f_node(k)%node)) then
              if (.not. (feyngraph_set%dag%node(j)%f_node(k)%node%incoming &
                .or. feyngraph_set%dag%node(j)%f_node(k)%node%t_line) &
                .and. feyngraph_set%dag%node(j)%f_node(k)%node%n_subtree_nodes == i) then
                pos = pos + 1
                set(pos)%node => feyngraph_set%dag%node(j)%f_node(k)%node
              end if
            end if
          enddo
        end if
      enddo
    else
      current => feyngraph_set%f_node_list%first
      do while (associated (current))
        if (.not. (current%node%incoming .or. current%node%t_line) &
          .and. current%node%n_subtree_nodes == i) then
          pos = pos + 1
          set(pos)%node => current%node
        end if
        current => current%next
      enddo
    end if
  enddo
end subroutine f_node_list_compute_mappings_s

```



```

                                end if
                                end if
                                enddo
                                end if
                                enddo
else
    current => feyngraph_set%f_node_list%first
    do while (associated (current))
        if (.not. (current%node%incoming .or. current%node%t_line) &
            .and. current%node%n_subtree_nodes == i) then
            pos = pos + 1
            set(pos)%node => current%node
        end if
        current => current%next
    enddo
end if
allocate (compare_list)
compare_list%observer = .true.
do j = 1, n_entries
    call k_node_init_from_f_node (set(j)%node, k_set, &
        feyngraph_set)
    if (allocated (k_set)) deallocate (k_set)
enddo
!$OMP PARALLEL DO PRIVATE (k_entry)
do j = 1, n_entries
    k_entry => set(j)%node%k_node_list%first
    do while (associated (k_entry))
        call node_assign_mapping_s(feyngraph_set%first, k_entry%node, feyngraph_set)
        k_entry => k_entry%next
    enddo
enddo
!$OMP END PARALLEL DO
do j = 1, size (set)
    k_entry => set(j)%node%k_node_list%first
    do while (associated (k_entry))
        if (k_entry%node%keep) then
            if (k_entry%node%mapping == NO_MAPPING .or. k_entry%node%mapping == NONRESONANT) t
                call compare_list%add_pointer (k_entry%node)
            end if
        end if
        k_entry => k_entry%next
    enddo
enddo
deallocate (set)
call compare_list%check_subtree_equivalences(feyngraph_set%model)
call compare_list%final
deallocate (compare_list)
enddo
end subroutine f_node_list_compute_mappings_s

```

19.14.14 Fill the grove list

Find the `grove` within the `grove_list` for a `kingraph` for which the kinematical calculations and mapping assignments have been completed. The `groves` are defined by the `grove_prop` entries and the value of the resonance hash (`res_hash`). Whenever a matching grove does not exist, we create one. In a first step we consider only part of the grove properties (see `grove_prop_match`) and the resonance hash is ignored, which leads to a preliminary grove list. In the end all numbers in `grove_prop` as well as the resonance hash are compared, i.e. we create a new `grove_list`.

```

(Cascades2: grove list: TBP)+≡
  procedure :: get_grove => grove_list_get_grove

(Cascades2: procedures)+≡
  subroutine grove_list_get_grove (grove_list, kingraph, return_grove, preliminary)
    class (grove_list_t), intent (inout) :: grove_list
    type (kingraph_t), intent (in), pointer :: kingraph
    type (grove_t), intent (inout), pointer :: return_grove
    logical, intent (in) :: preliminary
    type (grove_t), pointer :: current_grove
    return_grove => null ()
    if (.not. associated(grove_list%first)) then
      allocate (grove_list%first)
      grove_list%first%grove_prop = kingraph%grove_prop
      return_grove => grove_list%first
      return
    end if
    current_grove => grove_list%first
    do while (associated (current_grove))
      if ((preliminary .and. (current_grove%grove_prop .match. kingraph%grove_prop)) .or. &
        (.not. preliminary .and. current_grove%grove_prop == kingraph%grove_prop)) then
        return_grove => current_grove
        exit
      else if (.not. associated (current_grove%next)) then
        allocate (current_grove%next)
        current_grove%next%grove_prop = kingraph%grove_prop
        if (size (kingraph%tree%bc) < 9) &
          current_grove%compare_tree%depth = 1
        return_grove => current_grove%next
        exit
      end if
      if (associated (current_grove%next)) then
        current_grove => current_grove%next
      end if
    enddo
  end subroutine grove_list_get_grove

```

Add a valid `kingraph` to a `grove_list`. We first look for the `grove` which has the grove properties of the `kingraph`. If no such `grove` exists so far, it is created.

```

(Cascades2: grove list: TBP)+≡
  procedure :: add_kingraph => grove_list_add_kingraph

(Cascades2: procedures)+≡
  subroutine grove_list_add_kingraph (grove_list, kingraph, preliminary, check, model)

```

```

class (grove_list_t), intent (inout) :: grove_list
type (kingraph_t), pointer, intent (inout) :: kingraph
logical, intent (in) :: preliminary
logical, intent (in) :: check
type (model_data_t), optional, intent (in) :: model
type (grove_t), pointer :: grove
type (kingraph_t), pointer :: current
integer, save :: index = 0
grove => null ()
current => null ()
if (preliminary) then
  if (kingraph%index == 0) then
    index = index + 1
    kingraph%index = index
  end if
end if
call grove_list%get_grove (kingraph, grove, preliminary)
if (check) then
  call grove%compare_tree%check_kingraph (kingraph, model, preliminary)
end if
if (kingraph%keep) then
  if (associated (grove%first)) then
    grove%last%grove_next => kingraph
    grove%last => kingraph
  else
    grove%first => kingraph
    grove%last => kingraph
  end if
end if
end subroutine grove_list_add_kingraph

```

For a given feyngraph we store all valid kingraphs in the grove_list.

```

<Cascades2: grove list: TBP>+≡
  procedure :: add_feyngraph => grove_list_add_feyngraph

<Cascades2: procedures>+≡
  subroutine grove_list_add_feyngraph (grove_list, feyngraph, model)
    class (grove_list_t), intent (inout) :: grove_list
    type (feyngraph_t), intent (inout) :: feyngraph
    type (model_data_t), intent (in) :: model
    type (kingraph_t), pointer :: current_kingraph, add_kingraph
    do while (associated (feyngraph%kin_first))
      if (feyngraph%kin_first%keep) then
        add_kingraph => feyngraph%kin_first
        feyngraph%kin_first => feyngraph%kin_first%next
        add_kingraph%next => null ()
        call grove_list%add_kingraph (kingraph=add_kingraph, &
          preliminary=.true., check=.true., model=model)
      else
        exit
      end if
    enddo
    if (associated (feyngraph%kin_first)) then
      current_kingraph => feyngraph%kin_first
    end if
  end subroutine

```

```

do while (associated (current_kingraph%next))
  if (current_kingraph%next%keep) then
    add_kingraph => current_kingraph%next
    current_kingraph%next => current_kingraph%next%next
    add_kingraph%next => null ()
    call grove_list%add_kingraph (kingraph=add_kingraph, &
      preliminary=.true., check=.true., model=model)
  else
    current_kingraph => current_kingraph%next
  end if
enddo
end if
end subroutine grove_list_add_feyngraph

```

Compare two `grove_prop` objects. The `.match.` operator is used for preliminary groves in which the `kingraphs` share only the 3 numbers `n_resonances`, `n_log_enhanced` and `n_t_channel`. These groves are only used for comparing the kingraphs, because only graphs within these preliminary groves can be equivalent (the numbers which are compared here are unambiguously fixed by the combination of mappings in these channels).

```

<Cascades2: interfaces>+≡
  interface operator (.match.)
    module procedure grove_prop_match
  end interface operator (.match.)

<Cascades2: procedures>+≡
  function grove_prop_match (grove_prop1, grove_prop2) result (gp_match)
    type (grove_prop_t), intent (in) :: grove_prop1
    type (grove_prop_t), intent (in) :: grove_prop2
    logical :: gp_match
    gp_match = (grove_prop1%n_resonances == grove_prop2%n_resonances) &
      .and. (grove_prop1%n_log_enhanced == grove_prop2%n_log_enhanced) &
      .and. (grove_prop1%n_t_channel == grove_prop2%n_t_channel)
  end function grove_prop_match

```

The equal operator on the other hand will be used when all valid `kingraphs` have been created and mappings have been determined, to split up the existing (preliminary) grove list, i.e. to create new groves which are determined by all entries in `grove_prop_t`.

```

<Cascades2: interfaces>+≡
  interface operator (==)
    module procedure grove_prop_equal
  end interface operator (==)

<Cascades2: procedures>+≡
  function grove_prop_equal (grove_prop1, grove_prop2) result (gp_equal)
    type (grove_prop_t), intent (in) :: grove_prop1
    type (grove_prop_t), intent (in) :: grove_prop2
    logical :: gp_equal
    gp_equal = (grove_prop1%res_hash == grove_prop2%res_hash) &
      .and. (grove_prop1%n_resonances == grove_prop2%n_resonances) &
      .and. (grove_prop1%n_log_enhanced == grove_prop2%n_log_enhanced) &
      .and. (grove_prop1%n_off_shell == grove_prop2%n_off_shell) &

```

```

        .and. (grove_prop1%multiplicity == grove_prop2%multiplicity) &
        .and. (grove_prop1%n_t_channel == grove_prop2%n_t_channel)
    end function grove_prop_equal

```

19.14.15 Remove equivalent channels

Here we define the equivalence condition for completed **kingraphs**. The aim is to keep those **kingraphs** which describe the strongest peaks of the amplitude. The **bincodes** and **mappings** have to be the same for an equivalence, but the **pdgs** can be different. At the same time we check if the trees are exactly the same (up to the sign of pdg codes) in which case we do not keep both of them. This can be the case when the incoming particles are the same or their mutual anti-particles and there are no t-channel lines in the Feynman diagram to which the kingraph belongs.

```

<Cascades2: parameters>+=
    integer, parameter :: EMPTY = -999

<Cascades2: procedures>+=
    function kingraph_eqv (kingraph1, kingraph2) result (eqv)
        type (kingraph_t), intent (in) :: kingraph1
        type (kingraph_t), intent (inout) :: kingraph2
        logical :: eqv
        integer :: i
        logical :: equal
        eqv = .false.
        do i = kingraph1%tree%n_entries, 1, -1
            if (kingraph1%tree%bc(i) /= kingraph2%tree%bc(i)) return
        enddo
        do i = kingraph1%tree%n_entries, 1, -1
            if ( .not. (kingraph1%tree%mapping(i) == kingraph2%tree%mapping(i) &
                .or. ((kingraph1%tree%mapping(i) == NO_MAPPING .or. &
                    kingraph1%tree%mapping(i) == NONRESONANT) .and. &
                    (kingraph2%tree%mapping(i) == NO_MAPPING .or. &
                    kingraph2%tree%mapping(i) == NONRESONANT)))) return
        enddo
        equal = .true.
        do i = kingraph1%tree%n_entries, 1, -1
            if (abs(kingraph1%tree%pdg(i)) /= abs(kingraph2%tree%pdg(i))) then
                equal = .false.;
                select case (kingraph1%tree%mapping(i))
                case (S_CHANNEL, RADIATION)
                    select case (kingraph2%tree%mapping(i))
                    case (S_CHANNEL, RADIATION)
                        return
                    end select
                end select
            end if
        enddo
        if (equal) then
            kingraph2%keep = .false.
            call kingraph2%tree%final ()
        else

```

```

        eqv = .true.
    end if
end function kingraph_eqv

```

Select between two **kingraphs** which fulfill the equivalence condition above. This is done by comparing the **pdg** values of the **tree** for increasing bincode. If the particles are different at some place, we usually choose the one which would be returned first by the subroutine **match_vertex** of the model for the daughter **pdg** codes. Since we work here only on the basis of the **trees** of the completed **kingraphs**, we have to use the **bc** array to determine the positions of the daughter nodes' entries in the array. The graph which has to be kept should correspond to the stronger peak at the place which is compared.

(*Cascades2: procedures*)+≡

```

subroutine kingraph_select (kingraph1, kingraph2, model, preliminary)
    type (kingraph_t), intent (inout) :: kingraph1
    type (kingraph_t), intent (inout) :: kingraph2
    type (model_data_t), intent (in) :: model
    logical, intent (in) :: preliminary
    integer(TC), dimension(:), allocatable :: tmp_bc, daughter_bc
    integer, dimension(:), allocatable :: tmp_pdg, daughter_pdg
    integer, dimension(:), allocatable :: pdg_match
    integer :: i, j
    integer :: n_ext1, n_ext2
    if (kingraph_eqv (kingraph1, kingraph2)) then
        if (.not. preliminary) then
            kingraph2%keep = .false.; call kingraph2%tree%final ()
            return
        end if
        do i=1, size (kingraph1%tree%bc)
            if (abs(kingraph1%tree%pdg(i)) /= abs(kingraph2%tree%pdg(i))) then
                if (kingraph1%tree%mapping(i) /= EXTERNAL_PRT) then
                    n_ext1 = popcnt (kingraph1%tree%bc(i))
                    n_ext2 = n_ext1
                    do j=i+1, size (kingraph1%tree%bc)
                        if (abs(kingraph1%tree%pdg(j)) /= abs(kingraph2%tree%pdg(j))) then
                            n_ext2 = popcnt (kingraph1%tree%bc(j))
                            if (n_ext2 < n_ext1) exit
                        end if
                    enddo
                    if (n_ext2 < n_ext1) cycle
                    allocate (tmp_bc(i-1))
                    tmp_bc = kingraph1%tree%bc(:i-1)
                    allocate (tmp_pdg(i-1))
                    tmp_pdg = kingraph1%tree%pdg(:i-1)
                    do j=i-1, 1, - 1
                        where (iand (tmp_bc(:j-1),tmp_bc(j)) /= 0 &
                             .or. iand(tmp_bc(:j-1),kingraph1%tree%bc(i)) == 0)
                            tmp_bc(:j-1) = 0
                            tmp_pdg(:j-1) = 0
                        endwhere
                    enddo
                    allocate (daughter_bc(size(pack(tmp_bc, tmp_bc /= 0))))
                    daughter_bc = pack (tmp_bc, tmp_bc /= 0)

```

```

allocate (daughter_pdg(size(pack(tmp_pdg, tmp_pdg /= 0)))
daughter_pdg = pack (tmp_pdg, tmp_pdg /= 0)
if (size (daughter_pdg) == 2) then
    call model%match_vertex(daughter_pdg(1), daughter_pdg(2), pdg_match)
end if
do j=1, size (pdg_match)
    if (abs(pdg_match(j)) == abs(kinggraph1%tree%pdg(i))) then
        kinggraph2%keep = .false.; call kinggraph2%tree%final ()
        exit
    else if (abs(pdg_match(j)) == abs(kinggraph2%tree%pdg(i))) then
        kinggraph1%keep = .false.; call kinggraph1%tree%final ()
        exit
    end if
enddo
deallocate (tmp_bc, tmp_pdg, daughter_bc, daughter_pdg, pdg_match)
if (.not. (kinggraph1%keep .and. kinggraph2%keep)) exit
end if
end if
enddo
end if
end subroutine kinggraph_select

```

At the beginning we do not care about the resonance hash, but only about part of the grove properties, which is defined in `grove_prop_match`. In these resulting preliminary groves the kingraphs can be equivalent, i.e. we do not have to compare all graphs with each other but only all graphs within each of these preliminary groves. In the end we create a new grove list where the grove properties of the `kingraphs` within a `grove` have to be exactly the same and in addition the groves are distinguished by the resonance hash values. Here the kingraphs are not compared any more, which means that the number of channels is not reduced any more.

<Cascades2: grove list: TBP>+≡

```

procedure :: merge => grove_list_merge

```

<Cascades2: procedures>+≡

```

subroutine grove_list_merge (target_list, grove_list, model, prc_component)
    class (grove_list_t), intent (inout) :: target_list
    type (grove_list_t), intent (inout) :: grove_list
    type (model_data_t), intent (in) :: model
    integer, intent (in) :: prc_component
    type (grove_t), pointer :: current_grove
    type (kingraph_t), pointer :: current_graph
    current_grove => grove_list%first
    do while (associated (current_grove))
        do while (associated (current_grove%first))
            current_graph => current_grove%first
            current_grove%first => current_grove%first%grove_next
            current_graph%grove_next => null ()
            if (current_graph%keep) then
                current_graph%prc_component = prc_component
                call target_list%add_kingraph(kingraph=current_graph, &
                    preliminary=.false., check=.true., model=model)
            else

```

```

        call current_graph%final ()
        deallocate (current_graph)
    end if
enddo
current_grove => current_grove%next
enddo
end subroutine grove_list_merge

```

Recreate a grove list where we have different groves for different resonance hashes.

```

<Cascades2: grove list: TBP>+≡
    procedure :: rebuild => grove_list_rebuild

<Cascades2: procedures>+≡
    subroutine grove_list_rebuild (grove_list)
        class (grove_list_t), intent (inout) :: grove_list
        type (grove_list_t) :: tmp_list
        type (grove_t), pointer :: current_grove
        type (grove_t), pointer :: remove_grove
        type (kingraph_t), pointer :: current_graph
        type (kingraph_t), pointer :: next_graph
        tmp_list%first => grove_list%first
        grove_list%first => null ()
        current_grove => tmp_list%first
        do while (associated (current_grove))
            current_graph => current_grove%first
            do while (associated (current_graph))
                call current_graph%assign_resonance_hash ()
                next_graph => current_graph%grove_next
                current_graph%grove_next => null ()
                if (current_graph%keep) then
                    call grove_list%add_kingraph (kingraph=current_graph, &
                        preliminary=.false., check=.false.)
                end if
                current_graph => next_graph
            enddo
            current_grove => current_grove%next
        enddo
        call tmp_list%final
    end subroutine grove_list_rebuild

```

19.14.16 Write the phase-space file

The phase-space file is written from the graphs which survive the calculations and equivalence checks and are in the grove list. It is written grove by grove. The output should be the same as in the corresponding procedure `cascade_set_write_file_format` of `cascades`, up to the order of groves and channels.

```

<Cascades2: public>+≡
    public :: feyngraph_set_write_file_format

```



```

<Cascades2: procedures>+≡
  subroutine feyngraph_set_write_file_format (feyngraph_set, u)
    type (feyngraph_set_t), intent (in) :: feyngraph_set
    integer, intent (in) :: u
    type (grove_t), pointer :: grove
    integer :: channel_number
    integer :: grove_number
    channel_number = 0
    grove_number = 0
    grove => feyngraph_set%grove_list%first
    do while (associated (grove))
      grove_number = grove_number + 1
      call grove%write_file_format (feyngraph_set, grove_number, channel_number, u)
      grove => grove%next
    enddo
  end subroutine feyngraph_set_write_file_format

```

Write the relevant information of the kingraphs of a grove and the grove properties in the file format.

```

<Cascades2: grove: TBP>+≡
  procedure :: write_file_format => grove_write_file_format

<Cascades2: procedures>+≡
  recursive subroutine grove_write_file_format (grove, feyngraph_set, gr_number, ch_number, u)
    class (grove_t), intent (in) :: grove
    type (feyngraph_set_t), intent (in) :: feyngraph_set
    integer, intent (in) :: u
    integer, intent (inout) :: gr_number
    integer, intent (inout) :: ch_number
    type (kingraph_t), pointer :: current
1  format(3x,A,1x,40(1x,I4))
    write (u, "(A)")
    write (u, "(1x,'!',1x,A,1x,I0,A)", advance='no') &
      'Multiplicity =', grove%grove_prop%multiplicity, ","
    select case (grove%grove_prop%n_resonances)
    case (0)
      write (u, '(1x,A)', advance='no') 'no resonances, '
    case (1)
      write (u, '(1x,A)', advance='no') '1 resonance, '
    case default
      write (u, '(1x,I0,1x,A)', advance='no') &
        grove%grove_prop%n_resonances, 'resonances, '
    end select
    write (u, '(1x,I0,1x,A)', advance='no') &
      grove%grove_prop%n_log_enhanced, 'logs, '
    write (u, '(1x,I0,1x,A)', advance='no') &
      grove%grove_prop%n_off_shell, 'off-shell, '
    select case (grove%grove_prop%n_t_channel)
    case (0); write (u, '(1x,A)') 's-channel graph'
    case (1); write (u, '(1x,A)') '1 t-channel line'
    case default
      write(u,'(1x,I0,1x,A)') &
        grove%grove_prop%n_t_channel, 't-channel lines'
    end select

```

```

write (u, '(1X,A,I0)') 'grove #', gr_number
current => grove%first
do while (associated (current))
  if (current%keep) then
    ch_number = ch_number + 1
    call current%write_file_format (feyngraph_set, ch_number, u)
  end if
  current => current%grove_next
enddo
end subroutine grove_write_file_format

```

Write the relevant information of a valid kingraph in the file format. The information is extracted from the tree.

<Cascades2: kingraph: TBP>+≡

```

  procedure :: write_file_format => kingraph_write_file_format

```

<Cascades2: procedures>+≡

```

  subroutine kingraph_write_file_format (kingraph, feyngraph_set, ch_number, u)
    class (kingraph_t), intent (in) :: kingraph
    type (feyngraph_set_t), intent (in) :: feyngraph_set
    integer, intent (in) :: ch_number
    integer, intent (in) :: u
    integer :: i
    integer(TC) :: bincode_incoming
2   format(3X,'map',1X,I3,1X,A,1X,I9,1X,'!',1X,A)
!!! determine bincode of incoming particle from tree
    bincode_incoming = maxval (kingraph%tree%bc)
    write (unit=u, fmt='(1X,A,I0)') '! Channel #', ch_number
    write (unit=u, fmt='(3X,A,1X)', advance='no') 'tree'
    do i=1, size (kingraph%tree%bc)
      if (kingraph%tree%mapping(i) >=0 .or. kingraph%tree%mapping(i) == NONRESONANT &
        .or. (kingraph%tree%bc(i) == bincode_incoming &
        .and. feyngraph_set%process_type == DECAY)) then
        write (unit=u, fmt='(1X,I0)', advance='no') kingraph%tree%bc(i)
      end if
    enddo
    write (unit=u, fmt='(A)', advance='yes')
    do i=1, size(kingraph%tree%bc)
      select case (kingraph%tree%mapping(i))
      case (NO_MAPPING, NONRESONANT, EXTERNAL_PRT)
      case (S_CHANNEL)
        write (unit=u, fmt=2) kingraph%tree%bc(i), 's_channel', &
          kingraph%tree%pdg(i), &
          trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
      case (T_CHANNEL)
        write (unit=u, fmt=2) kingraph%tree%bc(i), 't_channel', &
          abs (kingraph%tree%pdg(i)), &
          trim(get_particle_name (feyngraph_set, abs(kingraph%tree%pdg(i))))
      case (U_CHANNEL)
        write (unit=u, fmt=2) kingraph%tree%bc(i), 'u_channel', &
          abs (kingraph%tree%pdg(i)), &
          trim(get_particle_name (feyngraph_set, abs(kingraph%tree%pdg(i))))
      case (RADIATION)
        write (unit=u, fmt=2) kingraph%tree%bc(i), 'radiation', &

```

```

        kingraph%tree%pdg(i), &
        trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
case (COLLINEAR)
    write (unit=u, fmt=2) kingraph%tree%bc(i), 'collinear', &
        kingraph%tree%pdg(i), &
        trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
case (INFRARED)
    write (unit=u, fmt=2) kingraph%tree%bc(i), 'infrared ', &
        kingraph%tree%pdg(i), &
        trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
case (ON_SHELL)
    write (unit=u, fmt=2) kingraph%tree%bc(i), 'on_shell ', &
        kingraph%tree%pdg(i), &
        trim(get_particle_name (feyngraph_set, kingraph%tree%pdg(i)))
case default
    call msg_bug (" Impossible mapping mode encountered")
end select
enddo
end subroutine kingraph_write_file_format

```

Get the particle name from the particle array of the `feyngraph_set`. This is needed for the phs file creation.

```

<Cascades2: procedures> +=
function get_particle_name (feyngraph_set, pdg) result (particle_name)
    type (feyngraph_set_t), intent (in) :: feyngraph_set
    integer, intent (in) :: pdg
    character (len=LABEL_LEN) :: particle_name
    integer :: i
    do i=1, size (feyngraph_set%particle)
        if (feyngraph_set%particle(i)%pdg == pdg) then
            particle_name = feyngraph_set%particle(i)%particle_label
            exit
        end if
    enddo
end function get_particle_name

```

19.14.17 Invert a graph

All Feynman diagrams given by O'Mega look like a decay. The `feyngraph` which is constructed from this output also looks like a decay, where one of the incoming particles is the decaying particle (or the root of the tree). The calculations can in principle be done on this data structure. However, it is also performed with the other incoming particle as the root. The first part of the calculation is the same for both cases. For the second part we need to transform/turn the graphs such that the other incoming particle becomes the root. This is done by identifying the incoming particles from the O'Mega output (the first one is simply the root of the existing tree, the second contains [2] in the `particle_label`) and the nodes/particles which connect both incoming particles (here we set `t.line = .true.`). At the same time we set the pointers `inverse_daughter1` and `inverse_daughter2` for the corresponding node, which

point to the mother node and the other daughter of the mother node; these will be the daughters of the node in the inverted feyngraph.

```

<Cascades2: feyngraph: TBP>+≡
  procedure :: make_invertible => feyngraph_make_invertible

<Cascades2: procedures>+≡
  subroutine feyngraph_make_invertible (feyngraph)
    class (feyngraph_t), intent (inout) :: feyngraph
    logical :: t_line_found
    feyngraph%root%incoming = .true.
    t_line_found = .false.
    if (associated (feyngraph%root%daughter1)) then
      call f_node_t_line_check (feyngraph%root%daughter1, t_line_found)
      if (.not. t_line_found) then
        if (associated (feyngraph%root%daughter2)) then
          call f_node_t_line_check (feyngraph%root%daughter2, t_line_found)
        end if
      end if
    end if
  end if

  contains

  <k node t line check>
    end subroutine feyngraph_make_invertible

```

Check if a node has to be t_line or incoming and assign inverse daughter pointers.

```

<k node t line check>≡
  recursive subroutine f_node_t_line_check (node, t_line_found)
    type (f_node_t), target, intent (inout) :: node
    integer :: pos
    logical, intent (inout) :: t_line_found
    if (associated (node%daughter1)) then
      call f_node_t_line_check (node%daughter1, t_line_found)
      if (node%daughter1%incoming .or. node%daughter1%t_line) then
        node%t_line = .true.
      else if (associated (node%daughter2)) then
        call f_node_t_line_check (node%daughter2, t_line_found)
        if (node%daughter2%incoming .or. node%daughter2%t_line) then
          node%t_line = .true.
        end if
      end if
    else
      pos = index (node%particle_label, '[') + 1
      if (node%particle_label(pos:pos) == '2') then
        node%incoming = .true.
        t_line_found = .true.
      end if
    end if
  end if
end subroutine f_node_t_line_check

```

Make an inverted copy of a kingraph using the inverse daughter pointers.

```

<Cascades2: kingraph: TBP>+≡

```

```

procedure :: make_inverse_copy => kingraph_make_inverse_copy
<Cascades2: procedures>+=
  subroutine kingraph_make_inverse_copy (original_kingraph, feyngraph)
    class (kingraph_t), intent (inout) :: original_kingraph
    type (feyngraph_t), intent (inout) :: feyngraph
    type (kingraph_t), pointer :: kingraph_copy
    type (k_node_t), pointer :: potential_root
    allocate (kingraph_copy)
    if (associated (feyngraph%kin_last)) then
      allocate (feyngraph%kin_last%next)
      feyngraph%kin_last => feyngraph%kin_last%next
    else
      allocate (feyngraph%kin_first)
      feyngraph%kin_last => feyngraph%kin_first
    end if
    kingraph_copy => feyngraph%kin_last
    call kingraph_set_inverse_daughters (original_kingraph)
    kingraph_copy%inverse = .true.
    kingraph_copy%n_nodes = original_kingraph%n_nodes
    kingraph_copy%keep = original_kingraph%keep
    potential_root => original_kingraph%root
    do while (.not. potential_root%incoming .or. &
      (associated (potential_root%daughter1) .and. associated (potential_root%daughter2)))
      if (potential_root%daughter1%incoming .or. potential_root%daughter1%t_line) then
        potential_root => potential_root%daughter1
      else if (potential_root%daughter2%incoming .or. potential_root%daughter2%t_line) then
        potential_root => potential_root%daughter2
      end if
    enddo
    call node_inverse_deep_copy (potential_root, kingraph_copy%root)
  end subroutine kingraph_make_inverse_copy

```

Recursively deep-copy nodes, but along the t-line the inverse daughters become the new daughters. We need a deep copy only for the `incoming` or `t_line` nodes. For the other nodes (of s-channel subgraphs) we set only pointers to the existing nodes of the non-inverted graph.

```

<Cascades2: procedures>+=
  recursive subroutine node_inverse_deep_copy (original_node, node_copy)
    type (k_node_t), intent (in) :: original_node
    type (k_node_t), pointer, intent (out) :: node_copy
    call original_node%f_node%k_node_list%add_entry(node_copy, recycle=.false.)
    node_copy = original_node
    if (node_copy%t_line .or. node_copy%incoming) then
      node_copy%particle => original_node%particle%anti
    else
      node_copy%particle => original_node%particle
    end if
    if (associated (original_node%inverse_daughter1) .and. associated (original_node%inverse_daughter2)) then
      if (original_node%inverse_daughter1%incoming .or. original_node%inverse_daughter1%t_line) then
        node_copy%daughter2 => original_node%inverse_daughter2
        call node_inverse_deep_copy (original_node%inverse_daughter1, &
          node_copy%daughter1)
      else if (original_node%inverse_daughter2%incoming .or. original_node%inverse_daughter2%t_line) then
        node_copy%daughter1 => original_node%inverse_daughter1
        call node_inverse_deep_copy (original_node%inverse_daughter2, &
          node_copy%daughter2)
      end if
    end if
  end recursive subroutine node_inverse_deep_copy

```

```

        node_copy%daughter1 => original_node%inverse_daughter1
        call node_inverse_deep_copy (original_node%inverse_daughter2, &
            node_copy%daughter2)
    end if
end if
end subroutine node_inverse_deep_copy

```

19.14.18 Find phase-space parametrizations

Perform all mapping calculations for a single process and store valid **kingraphs** (channels) into the grove list, without caring for instance about the resonance hash values.

```

<Cascades2: public>+≡
    public :: feyngraph_set_generate_single

<Cascades2: procedures>+≡
    subroutine feyngraph_set_generate_single (feyngraph_set, model, n_in, n_out, &
        phs_par, fatal_beam_decay, u_in)
        type(feyngraph_set_t), intent(inout) :: feyngraph_set
        type(model_data_t), target, intent(in) :: model
        integer, intent(in) :: n_in, n_out
        type(phs_parameters_t), intent(in) :: phs_par
        logical, intent(in) :: fatal_beam_decay
        integer, intent(in) :: u_in
        feyngraph_set%n_in = n_in
        feyngraph_set%n_out = n_out
        feyngraph_set%process_type = n_in
        feyngraph_set%phs_par = phs_par
        feyngraph_set%model => model
        if (debug_on) call msg_debug (D_PHASESPACE, "Construct relevant Feynman diagrams from Omega ou
        call feyngraph_set%build (u_in)
        if (debug_on) call msg_debug (D_PHASESPACE, "Find phase-space parametrizations")
        call feyngraph_set_find_phs_parametrizations(feyngraph_set)
    end subroutine feyngraph_set_generate_single

```

Find the phase space parametrizations. We start with the computation of pure s-channel subtrees, i.e. we determine mappings and compare subtrees in order to reduce the number of channels. This can be parallelized easily. When all s-channel **k_nodes** exist, the possible **kingraphs** are created using these nodes and we determine mappings for t-channel nodes.

```

<Cascades2: procedures>+≡
    subroutine feyngraph_set_find_phs_parametrizations (feyngraph_set)
        class (feyngraph_set_t), intent (inout) :: feyngraph_set
        type (feyngraph_t), pointer :: current => null ()
        type (feyngraph_ptr_t), dimension (:), allocatable :: set
        integer :: pos
        integer :: i
        allocate (set (feyngraph_set%n_graphs))
        pos = 0
        current => feyngraph_set%first
        do while (associated (current))
            pos = pos + 1

```

```

        set(pos)%graph => current
        current => current%next
    enddo
    if (feyngraph_set%process_type == SCATTERING) then
        !$OMP PARALLEL DO
        do i=1, feyngraph_set%n_graphs
            if (set(i)%graph%keep) then
                call set(i)%graph%make_invertible ()
            end if
        enddo
        !$OMP END PARALLEL DO
    end if
    call f_node_list_compute_mappings_s (feyngraph_set)
    do i=1, feyngraph_set%n_graphs
        if (set(i)%graph%keep) then
            call set(i)%graph%make_kingraphs (feyngraph_set)
        end if
    enddo
    if (feyngraph_set%process_type == SCATTERING) then
        do i=1, feyngraph_set%n_graphs
            if (set(i)%graph%keep) then
                call set(i)%graph%make_inverse_kingraphs ()
            end if
        enddo
    end if
    do i=1, feyngraph_set%n_graphs
        if (set(i)%graph%keep) then
            call set(i)%graph%compute_mappings (feyngraph_set)
        end if
    enddo
    do i=1, feyngraph_set%n_graphs
        if (set(i)%graph%keep) then
            call feyngraph_set%grove_list%add_feyngraph (set(i)%graph, &
                feyngraph_set%model)
        end if
    enddo
enddo
end subroutine feyngraph_set_find_phs_parametrizations

```

Compare objects of type `tree_t`.

```

<Cascades2: interfaces>+≡
    interface operator (==)
        module procedure tree_equal
    end interface operator (==)

<Cascades2: procedures>+≡
    elemental function tree_equal (tree1, tree2) result (flag)
        type (tree_t), intent (in) :: tree1, tree2
        logical :: flag
        if (tree1%n_entries == tree2%n_entries) then
            if (tree1%bc(size(tree1%bc)) == tree2%bc(size(tree2%bc))) then
                flag = all (tree1%mapping == tree2%mapping) .and. &
                    all (tree1%bc == tree2%bc) .and. &
                    all (abs(tree1%pdg) == abs(tree2%pdg))
            else

```

```

        flag = .false.
    end if
else
    flag = .false.
end if
end function tree_equal

```

Select between equivalent subtrees (type `tree_t`). This is similar to `kingraph_select`, but we compare only positions with mappings `NONRESONANT` and `NO_MAPPING`.

```

<Cascades2: interfaces>+≡
interface operator (.eqv.)
    module procedure subtree_eqv
end interface operator (.eqv.)

<Cascades2: procedures>+≡
pure function subtree_eqv (subtree1, subtree2) result (eqv)
    type (tree_t), intent (in) :: subtree1, subtree2
    logical :: eqv
    integer :: root_pos
    integer :: i
    logical :: equal
    eqv = .false.
    if (subtree1%n_entries /= subtree2%n_entries) return
    root_pos = subtree1%n_entries
    if (subtree1%mapping(root_pos) == NONRESONANT .or. &
        subtree2%mapping(root_pos) == NONRESONANT .or. &
        (subtree1%mapping(root_pos) == NO_MAPPING .and. &
         subtree2%mapping(root_pos) == NO_MAPPING .and. &
         abs(subtree1%pdg(root_pos)) == abs(subtree2%pdg(root_pos)))) then
        do i = subtree1%n_entries, 1, -1
            if (subtree1%bc(i) /= subtree2%bc(i)) return
        enddo
        equal = .true.
        do i = subtree1%n_entries, 1, -1
            if (abs(subtree1%pdg(i)) /= abs(subtree2%pdg(i))) then
                select case (subtree1%mapping(i))
                case (NO_MAPPING, NONRESONANT)
                    select case (subtree2%mapping(i))
                    case (NO_MAPPING, NONRESONANT)
                        equal = .false.
                    case default
                        return
                    end select
                case default
                    return
                end select
            end if
        enddo
        do i = subtree1%n_entries, 1, -1
            if (subtree1%mapping(i) /= subtree2%mapping(i)) then
                select case (subtree1%mapping(i))
                case (NO_MAPPING, NONRESONANT)
                    select case (subtree2%mapping(i))
                    case (NO_MAPPING, NONRESONANT)

```



```

        case default
            return
        end select
    case default
        return
    end select
end if
enddo
if (.not. equal) eqv = .true.
end if
end function subtree_eqv

```

(*Cascades2: procedures*) +=

```

subroutine subtree_select (subtree1, subtree2, model)
    type (tree_t), intent (inout) :: subtree1, subtree2
    type (model_data_t), intent (in) :: model
    integer :: j, k
    integer(TC), dimension(:), allocatable :: tmp_bc, daughter_bc
    integer, dimension(:), allocatable :: tmp_pdg, daughter_pdg
    integer, dimension(:), allocatable :: pdg_match
    if (subtree1 .eqv. subtree2) then
        do j=1, subtree1%n_entries
            if (abs(subtree1%pdg(j)) /= abs(subtree2%pdg(j))) then
                tmp_bc = subtree1%bc(:j-1); tmp_pdg = subtree1%pdg(:j-1)
                do k=j-1, 1, - 1
                    where (iand (tmp_bc(:k-1),tmp_bc(k)) /= 0 &
                        .or. iand(tmp_bc(:k-1),subtree1%bc(j)) == 0)
                        tmp_bc(:k-1) = 0
                        tmp_pdg(:k-1) = 0
                    endwhile
                enddo
                daughter_bc = pack (tmp_bc, tmp_bc /= 0)
                daughter_pdg = pack (tmp_pdg, tmp_pdg /= 0)
                if (size (daughter_pdg) == 2) then
                    call model%match_vertex(daughter_pdg(1), daughter_pdg(2), pdg_match)
                    if (.not. allocated (pdg_match)) then
                        !!! Relevant if tree contains only abs (pdg). In this case, changing the
                        !!! sign of one of the pdg codes should give a result.
                        call model%match_vertex(-daughter_pdg(1), daughter_pdg(2), pdg_match)
                    end if
                end if
                do k=1, size (pdg_match)
                    if (abs(pdg_match(k)) == abs(subtree1%pdg(j))) then
                        if (subtree1%keep) subtree2%keep = .false.
                        exit
                    else if (abs(pdg_match(k)) == abs(subtree2%pdg(j))) then
                        if (subtree2%keep) subtree1%keep = .false.
                        exit
                    end if
                enddo
                deallocate (tmp_bc, tmp_pdg, daughter_bc, daughter_pdg, pdg_match)
                if (.not. (subtree1%keep .and. subtree2%keep)) exit
            end if
        enddo
    enddo
enddo

```

```

        end if
    end subroutine subtree_select

```

Assign a resonance hash value to a kingraph, like in cascades, but here without the array `tree_resonant`.

```

<Cascades2: kingraph: TBP>+≡
    procedure :: assign_resonance_hash => kingraph_assign_resonance_hash

<Cascades2: procedures>+≡
    subroutine kingraph_assign_resonance_hash (kingraph)
        class (kingraph_t), intent (inout) :: kingraph
        logical, dimension (:), allocatable :: tree_resonant
        integer(i8), dimension(1) :: mold
        allocate (tree_resonant (kingraph%tree%n_entries))
        tree_resonant = (kingraph%tree%mapping == S_CHANNEL)
        kingraph%grove_prop%res_hash = hash (transfer &
            ([sort (pack (kingraph%tree%pdg, tree_resonant)), &
                sort (pack (abs (kingraph%tree%pdg), &
                    kingraph%tree%mapping == T_CHANNEL .or. &
                    kingraph%tree%mapping == U_CHANNEL))], mold))
        deallocate (tree_resonant)
    end subroutine kingraph_assign_resonance_hash

```

Write the process in the bincode format. This is again a copy of the corresponding procedure in cascades, using `feyngraph_set` instead of `cascade_set` as an argument.

```

<Cascades2: public>+≡
    public :: feyngraph_set_write_process_bincode_format

<Cascades2: procedures>+≡
    subroutine feyngraph_set_write_process_bincode_format (feyngraph_set, unit)
        type(feyngraph_set_t), intent(in), target :: feyngraph_set
        integer, intent(in), optional :: unit
        integer, dimension(:), allocatable :: bincode, field_width
        integer :: n_in, n_out, n_tot, n_flv
        integer :: u, f, i, bc
        character(20) :: str
        type(string_t) :: fmt_head
        type(string_t), dimension(:), allocatable :: fmt_proc
        u = given_output_unit (unit); if (u < 0) return
        if (.not. allocated (feyngraph_set%flv)) return
        write (u, "('!',1x,A)") "List of subprocesses with particle bincodes:"
        n_in = feyngraph_set%n_in
        n_out = feyngraph_set%n_out
        n_tot = n_in + n_out
        n_flv = size (feyngraph_set%flv, 2)
        allocate (bincode (n_tot), field_width (n_tot), fmt_proc (n_tot))
        bc = 1
        do i = 1, n_out
            bincode(n_in + i) = bc
            bc = 2 * bc
        end do
        do i = n_in, 1, -1
            bincode(i) = bc

```

```

        bc = 2 * bc
    end do
    do i = 1, n_tot
        write (str, "(I0)")  bincode(i)
        field_width(i) = len_trim (str)
        do f = 1, n_flv
            field_width(i) = max (field_width(i), &
                len (feyngraph_set%flv(i,f)%get_name ()))
        end do
    end do
    fmt_head = "('!'"
    do i = 1, n_tot
        fmt_head = fmt_head // ",1x,"
        fmt_proc(i) = "(1x,"
        write (str, "(I0)")  field_width(i)
        fmt_head = fmt_head // "I" // trim(str)
        fmt_proc(i) = fmt_proc(i) // "A" // trim(str)
        if (i == n_in) then
            fmt_head = fmt_head // ",1x,' '"
        end if
    end do
    do i = 1, n_tot
        fmt_proc(i) = fmt_proc(i) // ")"
    end do
    fmt_head = fmt_head // ")"
    write (u, char (fmt_head))  bincode
    do f = 1, n_flv
        write (u, "('!'"", advance="no")
        do i = 1, n_tot
            write (u, char (fmt_proc(i)), advance="no") &
                char (feyngraph_set%flv(i,f)%get_name ())
            if (i == n_in) write (u, "(1x,'=>'", advance="no")
        end do
        write (u, *)
    end do
    write (u, char (fmt_head))  bincode
end subroutine feyngraph_set_write_process_bincode_format

```

Write tex file for graphical display of channels.

<Cascades2: public>+≡

public :: feyngraph_set_write_graph_format

<Cascades2: procedures>+≡

```

subroutine feyngraph_set_write_graph_format (feyngraph_set, filename, process_id, unit)
    type(feyngraph_set_t), intent(in), target :: feyngraph_set
    type(string_t), intent(in) :: filename, process_id
    integer, intent(in), optional :: unit
    type(kingraph_t), pointer :: kingraph
    type(grove_t), pointer :: grove
    integer :: u, n_grove, count, pgcount
    logical :: first_in_grove
    u = given_output_unit (unit); if (u < 0) return
    write (u, '(A)') "\documentclass[10pt]{article}"
    write (u, '(A)') "\usepackage{amsmath}"

```

```

write (u, '(A)') "\usepackage{feynmp}"
write (u, '(A)') "\usepackage{url}"
write (u, '(A)') "\usepackage{color}"
write (u, *)
write (u, '(A)') "\textwidth 18.5cm"
write (u, '(A)') "\evensidemargin -1.5cm"
write (u, '(A)') "\oddsidemargin -1.5cm"
write (u, *)
write (u, '(A)') "\newcommand{\blue}{\color{blue}}"
write (u, '(A)') "\newcommand{\green}{\color{green}}"
write (u, '(A)') "\newcommand{\red}{\color{red}}"
write (u, '(A)') "\newcommand{\magenta}{\color{magenta}}"
write (u, '(A)') "\newcommand{\cyan}{\color{cyan}}"
write (u, '(A)') "\newcommand{\sm}{\footnotesize}"
write (u, '(A)') "\setlength{\parindent}{0pt}"
write (u, '(A)') "\setlength{\parsep}{20pt}"
write (u, *)
write (u, '(A)') "\begin{document}"
write (u, '(A)') "\begin{fmffile}{ " // char (filename) // "}"
write (u, '(A)') "\fmfcmd{color magenta; magenta = red + blue;}"
write (u, '(A)') "\fmfcmd{color cyan; cyan = green + blue;}"
write (u, '(A)') "\begin{fmfshrink}{0.5}"
write (u, '(A)') "\begin{flushleft}"
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{\large\texttt{WHIZARD}} phase space channels}" // &
& "\hfill\today"
write (u, *)
write (u, '(A)') "\vspace{10pt}"
write (u, '(A)') "\noindent" // &
& "\textbf{Process:} \url{ " // char (process_id) // "}"
call feyngraph_set_write_process_tex_format (feyngraph_set, u)
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{Note:} These are pseudo Feynman graphs that "
write (u, '(A)') "visualize phase-space parameterizations " // &
& ("integration channels"). "
write (u, '(A)') "They do \emph{not} indicate Feynman graphs used for the " // &
& "matrix element."
write (u, *)
write (u, '(A)') "\textbf{Color code:} " // &
& "{\blue resonance,} " // &
& "{\cyan t-channel,} " // &
& "{\green radiation,} "
write (u, '(A)') "{\red infrared,} " // &
& "{\magenta collinear,} " // &
& "external/off-shell"
write (u, *)
write (u, '(A)') "\noindent" // &
& "\textbf{Black square:} Keystone, indicates ordering of " // &
& "phase space parameters."
write (u, *)
write (u, '(A)') "\vspace{-20pt}"
count = 0

```

```

pgcount = 0
n_grove = 0
grove => feyngraph_set%grove_list%first
do while (associated (grove))
  n_grove = n_grove + 1
  write (u, *)
  write (u, '(A)') "\vspace{20pt}"
  write (u, '(A)') "\begin{tabular}{l}"
  write (u, '(A,I5,A)') &
    & "\fbox{\bf Grove \boldmath$, n_grove, "$} \\[10pt]"
  write (u, '(A,I1,A)') "Multiplicity: ", &
    grove%grove_prop%multiplicity, "\\"
  write (u, '(A,I1,A)') "Resonances: ", &
    grove%grove_prop%n_resonances, "\\"
  write (u, '(A,I1,A)') "Log-enhanced: ", &
    grove%grove_prop%n_log_enhanced, "\\"
  write (u, '(A,I1,A)') "Off-shell: ", &
    grove%grove_prop%n_off_shell, "\\"
  write (u, '(A,I1,A)') "t-channel: ", &
    grove%grove_prop%n_t_channel, ""
  write (u, '(A)') "\end{tabular}"
  kingraph => grove%first
  do while (associated (kingraph))
    count = count + 1
    call kingraph_write_graph_format (kingraph, count, unit)
    kingraph => kingraph%grove_next
  enddo
  grove => grove%next
enddo
write (u, '(A)') "\end{flushleft}"
write (u, '(A)') "\end{fmfshrink}"
write (u, '(A)') "\end{fmffile}"
write (u, '(A)') "\end{document}"
end subroutine feyngraph_set_write_graph_format

```

Write the process as a L^AT_EX expression. This is a slightly modified copy of `cascade_set_write_process_tex_format` which has only been adapted to the types which are used here.

```

<Cascades2: procedures>+≡
subroutine feyngraph_set_write_process_tex_format (feyngraph_set, unit)
  type(feyngraph_set_t), intent(in), target :: feyngraph_set
  integer, intent(in), optional :: unit
  integer :: n_tot
  integer :: u, f, i
  n_tot = feyngraph_set%n_in + feyngraph_set%n_out
  u = given_output_unit (unit); if (u < 0) return
  if (.not. allocated (feyngraph_set%flv)) return
  write (u, "(A)") "\begin{align*}"
  do f = 1, size (feyngraph_set%flv, 2)
    do i = 1, feyngraph_set%n_in
      if (i > 1) write (u, "(A)", advance="no") "\quad "
      write (u, "(A)", advance="no") &
        char (feyngraph_set%flv(i,f)%get_tex_name ())
    enddo
  enddo
end subroutine

```

```

end do
write (u, "(A)", advance="no") "\quad &\to\quad "
do i = feyngraph_set%n_in + 1, n_tot
  if (i > feyngraph_set%n_in + 1) write (u, "(A)", advance="no") "\quad "
  write (u, "(A)", advance="no") &
    char (feyngraph_set%flv(i,f)%get_tex_name ())
end do
if (f < size (feyngraph_set%flv, 2)) then
  write (u, "(A)") "\\ "
else
  write (u, "(A)") ""
end if
end do
write (u, "(A)") "\end{align*}"
end subroutine feyngraph_set_write_process_tex_format

```

This creates metapost source for graphical display for a given `kingraph`. It is the analogon to `cascade_write_graph_format` (a modified copy).

```

<Cascades2: procedures>+≡
subroutine kingraph_write_graph_format (kingraph, count, unit)
  type(kingraph_t), intent(in) :: kingraph
  integer, intent(in) :: count
  integer, intent(in), optional :: unit
  integer :: u
  type(string_t) :: left_str, right_str
  u = given_output_unit (unit); if (u < 0) return
  left_str = ""
  right_str = ""
  write (u, '(A)') "\begin{minipage}{105pt}"
  write (u, '(A)') "\vspace{30pt}"
  write (u, '(A)') "\begin{center}"
  write (u, '(A)') "\begin{fmfgraph*}(55,55)"
  call graph_write_node (kingraph%root)
  write (u, '(A)') "\fmfleft{" // char (extract (left_str, 2)) // "}"
  write (u, '(A)') "\fmfright{" // char (extract (right_str, 2)) // "}"
  write (u, '(A)') "\end{fmfgraph*}\\ "
  write (u, '(A,I5,A)') "\fbox{$", count, "$}"
  write (u, '(A)') "\end{center}"
  write (u, '(A)') "\end{minipage}"
  write (u, '(A)') "%"
contains
  recursive subroutine graph_write_node (node)
    type(k_node_t), intent(in) :: node
    if (associated (node%daughter1) .or. associated (node%daughter2)) then
      if (node%daughter2%t_line .or. node%daughter2%incoming) then
        call vertex_write (node, node%daughter2)
        call vertex_write (node, node%daughter1)
      else
        call vertex_write (node, node%daughter1)
        call vertex_write (node, node%daughter2)
      end if
    if (node%mapping == EXTERNAL_PRT) then
      call line_write (node%bincode, 0, node%particle)
    end if
  end subroutine graph_write_node

```

```

        call external_write (node%bincode, node%particle%tex_name, &
            left_str)
        write (u, '(A,I0,A)') "\fmfv{d.shape=square}{v0}"
    end if
else
    if (node%incoming) then
        call external_write (node%bincode, node%particle%anti%tex_name, &
            left_str)
    else
        call external_write (node%bincode, node%particle%tex_name, &
            right_str)
    end if
end if
end subroutine graph_write_node
recursive subroutine vertex_write (node, daughter)
    type(k_node_t), intent(in) :: node, daughter
    integer :: bincode
    if (associated (node%daughter1) .and. associated (node%daughter2) &
        .and. node%mapping == EXTERNAL_PRT) then
        bincode = 0
    else
        bincode = node%bincode
    end if
    call graph_write_node (daughter)
    if (associated (node%daughter1) .or. associated (node%daughter2)) then
        call line_write (bincode, daughter%bincode, daughter%particle, &
            mapping=daughter%mapping)
    else
        call line_write (bincode, daughter%bincode, daughter%particle)
    end if
end subroutine vertex_write
subroutine line_write (i1, i2, particle, mapping)
    integer(TC), intent(in) :: i1, i2
    type(part_prop_t), intent(in) :: particle
    integer, intent(in), optional :: mapping
    integer :: k1, k2
    type(string_t) :: prt_type
    select case (particle%spin_type)
    case (SCALAR);      prt_type = "plain"
    case (SPINOR);      prt_type = "fermion"
    case (VECTOR);      prt_type = "boson"
    case (VECTORSPINOR); prt_type = "fermion"
    case (TENSOR);      prt_type = "dbl_wiggly"
    case default;       prt_type = "dashes"
    end select
    if (particle%pdg < 0) then
!!! anti-particle
        k1 = i2; k2 = i1
    else
        k1 = i1; k2 = i2
    end if
    if (present (mapping)) then
        select case (mapping)
        case (S_CHANNEL)

```

```

        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=blue,lab=\sm\blue$" // &
        & char (particle%tex_name) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    case (T_CHANNEL, U_CHANNEL)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=cyan,lab=\sm\cyan$" // &
        & char (particle%tex_name) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    case (RADIATION)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=green,lab=\sm\green$" // &
        & char (particle%tex_name) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    case (COLLINEAR)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=magenta,lab=\sm\magenta$" // &
        & char (particle%tex_name) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    case (INFRARED)
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=red,lab=\sm\red$" // &
        & char (particle%tex_name) // "$}" // &
        & "{v", k1, ",v", k2, "}"
    case default
        write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
        & ",f=black}" // &
        & "{v", k1, ",v", k2, "}"
    end select
else
    write (u, '(A,I0,A,I0,A)') "\fmf{" // char (prt_type) // &
    & "}" // &
    & "{v", k1, ",v", k2, "}"
end if
end subroutine line_write
subroutine external_write (bincode, name, ext_str)
    integer(TC), intent(in) :: bincode
    type(string_t), intent(in) :: name
    type(string_t), intent(inout) :: ext_str
    character(len=20) :: str
    write (str, '(A2,I0)') ",v", bincode
    ext_str = ext_str // trim (str)
    write (u, '(A,I0,A,I0,A)') "\fmflabel{\sm$" &
    // char (name) &
    // "\",(" , bincode, ")" &
    // "$}{v", bincode, "}"
end subroutine external_write
end subroutine kingraph_write_graph_format

```

Generate a `feyngraph_set` for several subprocesses. Mapping calculations are performed separately, but the final grove list is shared between the subsets `fset` of the `feyngraph_set`.

(Cascades2: public)+≡


```

public :: feyngraph_set_generate
<Cascades2: procedures>+≡
subroutine feyngraph_set_generate &
  (feyngraph_set, model, n_in, n_out, flv, phs_par, fatal_beam_decay, &
   u_in, vis_channels, use_dag)
  type(feyngraph_set_t), intent(out) :: feyngraph_set
  class(model_data_t), intent(in), target :: model
  integer, intent(in) :: n_in, n_out
  type(flavor_t), dimension(:,:), intent(in) :: flv
  type(phs_parameters_t), intent(in) :: phs_par
  logical, intent(in) :: fatal_beam_decay
  integer, intent(in) :: u_in
  logical, intent(in) :: vis_channels
  logical, optional, intent(in) :: use_dag
  type(grove_t), pointer :: grove
  integer :: i, j
  type(kingraph_t), pointer :: kingraph
  if (phase_space_vanishes (phs_par%sqrts, n_in, flv)) return
  if (present (use_dag)) feyngraph_set%use_dag = use_dag
  feyngraph_set%process_type = n_in
  feyngraph_set%n_in = n_in
  feyngraph_set%n_out = n_out
  allocate (feyngraph_set%flv (size (flv, 1), size (flv, 2)))
  do i = 1, size (flv, 2)
    do j = 1, size (flv, 1)
      call feyngraph_set%flv(j,i)%init (flv(j,i)%get_pdg (), model)
    end do
  end do
  allocate (feyngraph_set%particle (PRT_ARRAY_SIZE))
  allocate (feyngraph_set%grove_list)
  allocate (feyngraph_set%fset (size (flv, 2)))
  do i = 1, size (feyngraph_set%fset)
    feyngraph_set%fset(i)%use_dag = feyngraph_set%use_dag
    allocate (feyngraph_set%fset(i)%flv(size (flv,1),1))
    feyngraph_set%fset(i)%flv(:,1) = flv(:,i)
    feyngraph_set%fset(i)%particle => feyngraph_set%particle
    allocate (feyngraph_set%fset(i)%grove_list)
    call feyngraph_set_generate_single (feyngraph_set%fset(i), &
      model, n_in, n_out, phs_par, fatal_beam_decay, u_in)
    call feyngraph_set%grove_list%merge (feyngraph_set%fset(i)%grove_list, model, i)
    if (.not. vis_channels) call feyngraph_set%fset(i)%final()
  enddo
  call feyngraph_set%grove_list%rebuild ()
end subroutine feyngraph_set_generate

```

Check whether the `grove_list` of the `feyngraph_set` contains any kingraphs which are valid, i.e. where the `keep` variable has the value `.true.`. This is necessary to write a non-empty phase-space file. The function is the pendant to `cascade_set_is_valid`.

```

<Cascades2: public>+≡
public :: feyngraph_set_is_valid
<Cascades2: procedures>+≡

```

```

function feyngraph_set_is_valid (feyngraph_set) result (flag)
  class (feyngraph_set_t), intent(in) :: feyngraph_set
  type (kingraph_t), pointer :: kingraph
  type (grove_t), pointer :: grove
  logical :: flag
  flag = .false.
  if (associated (feyngraph_set%grove_list)) then
    grove => feyngraph_set%grove_list%first
    do while (associated (grove))
      kingraph => grove%first
      do while (associated (kingraph))
        if (kingraph%keep) then
          flag = .true.
          return
        end if
        kingraph => kingraph%next
      enddo
      grove => grove%next
    enddo
  end if
end function feyngraph_set_is_valid

```

19.14.19 Return the resonance histories for subtraction

The following procedures are copies of corresponding procedures in `cascades`, which only have been adapted to the new types used in this module. Extract the resonance set from a valid `kingraph` which is kept in the final grove list.

<Cascades2: kingraph: TBP>+≡

```

  procedure :: extract_resonance_history => kingraph_extract_resonance_history

```

<Cascades2: procedures>+≡

```

  subroutine kingraph_extract_resonance_history &
    (kingraph, res_hist, model, n_out)
    class(kingraph_t), intent(in), target :: kingraph
    type(resonance_history_t), intent(out) :: res_hist
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: n_out
    type(resonance_info_t) :: resonance
    integer :: i, mom_id, pdg
    if (debug_on) call msg_debug2 (D_PHASESPACE, "kingraph_extract_resonance_history")
    if (kingraph%grove_prop%n_resonances > 0) then
      if (associated (kingraph%root%daughter1) .or. &
        associated (kingraph%root%daughter2)) then
        if (debug_on) call msg_debug2 (D_PHASESPACE, "kingraph has resonances, root has children")
        do i = 1, kingraph%tree%n_entries
          if (kingraph%tree%mapping(i) == S_CHANNEL) then
            mom_id = kingraph%tree%bc (i)
            pdg = kingraph%tree%pdg (i)
            call resonance%init (mom_id, pdg, model, n_out)
            if (debug2_active (D_PHASESPACE)) then
              print *, 'D: Adding resonance'
              call resonance%write ()
            end if
          end if
        enddo
      end if
    end if
  end subroutine

```

```

        end if
        call res_hist%add_resonance (resonance)
    end if
end do
end if
end if
end if
end subroutine kingraph_extract_resonance_history

```

Determine the number of valid kingraphs in grove_list.

```

<Cascades2: public>+≡
    public :: grove_list_get_n_trees

<Cascades2: procedures>+≡
    function grove_list_get_n_trees (grove_list) result (n)
        class (grove_list_t), intent (in) :: grove_list
        integer :: n
        type(kingraph_t), pointer :: kingraph
        type(grove_t), pointer :: grove
        if (debug_on) call msg_debug (D_PHASESPACE, "grove_list_get_n_trees")
        n = 0
        grove => grove_list%first
        do while (associated (grove))
            kingraph => grove%first
            do while (associated (kingraph))
                if (kingraph%keep) n = n + 1
                kingraph => kingraph%grove_next
            enddo
            grove => grove%next
        enddo
        if (debug_on) call msg_debug (D_PHASESPACE, "n", n)
    end function grove_list_get_n_trees

```

Extract the resonance histories from the feyngraph_set, in complete analogy to cascade_set_get_resonance_histories

```

<Cascades2: public>+≡
    public :: feyngraph_set_get_resonance_histories

<Cascades2: procedures>+≡
    subroutine feyngraph_set_get_resonance_histories (feyngraph_set, n_filter, res_hists)
        type(feyngraph_set_t), intent(in), target :: feyngraph_set
        integer, intent(in), optional :: n_filter
        type(resonance_history_t), dimension(:), allocatable, intent(out) :: res_hists
        type(kingraph_t), pointer :: kingraph
        type(grove_t), pointer :: grove
        type(resonance_history_t) :: res_hist
        type(resonance_history_set_t) :: res_hist_set
        integer :: i_grove
        if (debug_on) call msg_debug (D_PHASESPACE, "grove_list_get_resonance_histories")
        call res_hist_set%init (n_filter = n_filter)
        grove => feyngraph_set%grove_list%first
        i_grove = 0
        do while (associated (grove))
            i_grove = i_grove + 1
            kingraph => grove%first

```

```

do while (associated (kingraph))
  if (kingraph%keep) then
    if (debug_on) call msg_debug2 (D_PHASESPACE, "grove", i_grove)
    call kingraph%extract_resonance_history &
      (res_hist, feyngraph_set%model, feyngraph_set%n_out)
    call res_hist_set%enter (res_hist)
  end if
  kingraph => kingraph%grove_next
end do
end do
call res_hist_set%freeze ()
call res_hist_set%to_array (res_hists)
end subroutine feyngraph_set_get_resonance_histories

<cascades2.ut.f90>≡
<File header>

module cascades2_ut
  use unit_tests
  use cascades2_util

<Standard module head>

<Cascades2: public test>

contains

<Cascades2: test driver>

end module cascades2_ut

<cascades2_util.f90>≡
<File header>

module cascades2_util

<Use kinds>
<Use strings>
  use numeric_utils

  use cascades2
  use flavors
  use pbs_forests, only: pbs_parameters_t
  use model_data

<Standard module head>

<Cascades2: test declarations>

contains

<Cascades2: tests>

end module cascades2_util

```

API: driver for the unit tests below.

```

<Cascades2: public test>≡
  public :: cascades2_test

<Cascades2: test driver>≡
  subroutine cascades2_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Cascades2: execute tests>
  end subroutine cascades2_test

<Cascades2: execute tests>≡
  call test (cascades2_1, "cascades2_1", &
    "make phase-space", u, results)
  call test (cascades2_2, "cascades2_2", &
    "make phase-space (scattering)", u, results)

<Cascades2: test declarations>≡
  public :: cascades2_1

<Cascades2: tests>≡
  subroutine cascades2_1 (u)
    integer, intent(in) :: u
    type (feyngraph_set_t) :: feyngraph_set
    type (model_data_t) :: model
    integer :: n_in = 1
    integer :: n_out = 6
    type(flavor_t), dimension(7,1) :: flv
    type (phs_parameters_t) :: phs_par
    logical :: fatal_beam_decay = .true.
    integer :: u_in = 8

    write (u, "(A)")  "* Test output: cascades2_1"
    write (u, "(A)")  "* Purpose: create a test phs file (decay) with the forest"
    write (u, "(A)")  "* output of 0'Mega"
    write (u, "(A)")

    write (u, "(A)")  "* Initializing"
    write (u, "(A)")

    call init_sm_full_test (model)

    call flv(1,1)%init (6, model)
    call flv(2,1)%init (5, model)
    call flv(3,1)%init (-11, model)
    call flv(4,1)%init (12, model)
    call flv(5,1)%init (21, model)
    call flv(6,1)%init (22, model)
    call flv(7,1)%init (21, model)

    phs_par%sqrts = 173.1_default
    phs_par%m_threshold_s = 50._default
    phs_par%m_threshold_t = 100._default
    phs_par%keep_nonresonant = .true.
    phs_par%off_shell = 2

```

```

open (unit=u_in, file="cascades2_1.fds", status='old', action='read')

write (u, "(A)")
write (u, "(A)")  "* Generating phase-space parametrizations"
write (u, "(A)")

call feyngraph_set_generate (feyngraph_set, model, n_in, n_out, &
    flv, phs_par, fatal_beam_decay, u_in, use_dag = .false., &
    vis_channels = .false.)
call feyngraph_set_write_process_bincode_format (feyngraph_set, u)
call feyngraph_set_write_file_format (feyngraph_set, u)

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

close (u_in)
call feyngraph_set%final ()
call model%final ()

write (u, *)
write (u, "(A)")  "* Test output end: cascades2_1"
end subroutine cascades2_1

```

<Cascades2: test declarations>+≡

```
public :: cascades2_2
```

<Cascades2: tests>+≡

```

subroutine cascades2_2 (u)
    integer, intent(in) :: u
    type (feyngraph_set_t) :: feyngraph_set
    type (model_data_t) :: model
    integer :: n_in = 2
    integer :: n_out = 5
    type(flavor_t), dimension(7,1) :: flv
    type (phs_parameters_t) :: phs_par
    logical :: fatal_beam_decay = .true.
    integer :: u_in = 8

    write (u, "(A)")  "* Test output: cascades2_2"
    write (u, "(A)")  "*   Purpose: create a test phs file (scattering) with the"
    write (u, "(A)")  "*                   parsable DAG output of 0'Mega"
    write (u, "(A)")

    write (u, "(A)")  "* Initializing"
    write (u, "(A)")

    call init_sm_full_test (model)

    call flv(1,1)%init (-11, model)
    call flv(2,1)%init (11, model)
    call flv(3,1)%init (-11, model)
    call flv(4,1)%init (12, model)
    call flv(5,1)%init (1, model)

```

```

call flv(6,1)%init (-2, model)
call flv(7,1)%init (22, model)

phs_par%sqrts = 500._default
phs_par%m_threshold_s = 50._default
phs_par%m_threshold_t = 100._default
phs_par%keep_nonresonant = .true.
phs_par%off_shell = 2
phs_par%t_channel = 6

open (unit=u_in, file="cascades2_2.fds", &
      status='old', action='read')

write (u, "(A)")
write (u, "(A)")  "* Generating phase-space parametrizations"
write (u, "(A)")

call feyngraph_set_generate (feyngraph_set, model, n_in, n_out, &
                             flv, phs_par, fatal_beam_decay, u_in, use_dag = .true., &
                             vis_channels = .false.)
call feyngraph_set_write_process_bincode_format (feyngraph_set, u)
call feyngraph_set_write_file_format (feyngraph_set, u)

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

close (u_in)
call feyngraph_set%final ()
call model%final ()

write (u, *)
write (u, "(A)")  "* Test output end: cascades2_2"
end subroutine cascades2_2

```

Chapter 20

VEGAS Integration

The backbone integrator of WHIZARD is a object-oriented implemetation of the VEGAS algorithm.

```
<vegas.f90>≡  
  <File header>  
  
  module vegas  
    <Use kinds>  
  
    <vegas: modules>  
  
    <Standard module head>  
  
    <vegas: public>  
  
    <vegas: parameters>  
  
    <vegas: types>  
  
    <vegas: interfaces>  
  
    contains  
  
    <vegas: procedures>  
  
  end module vegas  
<vegas: modules>≡  
  use diagnostics  
  use io_units  
  use format_utils, only: write_indent  
  use format_defs, only: FMT_17  
  use rng_base, only: rng_t  
  use rng_stream, only: rng_stream_t  
  
MPI Module.  
<MPI: vegas: modules>≡  
  use request_callback, only: request_handler_t  
  use mpi_f08 !NODEP!
```


20.1 Integration modes

VEGAS operates in three different modes: `vegas_mode_importance_only`, `vegas_mode_importance` or `vegas_mode_stratified`. The default mode is `vegas_mode_importance`, where the algorithm decides whether if it is possible to use importance sampling or stratified sampling. In low dimensions VEGAS uses strict stratified sampling.

```
<vegas: parameters>≡  
  integer, parameter, public :: VEGAS_MODE_IMPORTANCE = 0, &  
    & VEGAS_MODE_STRATIFIED = 1, VEGAS_MODE_IMPORTANCE_ONLY = 2
```

20.2 Type: `vegas_func_t`

We define a abstract `func` type which only gives an interface to an `evaluate` procedure. The inside of implementation and also the optimization of are not a concern of the `vegas` implementation.

```
<vegas: public>≡  
  public :: vegas_func_t  
<vegas: types>≡  
  type, abstract :: vegas_func_t  
    !  
    contains  
    procedure(vegas_func_evaluate), deferred, pass, public :: evaluate  
  end type vegas_func_t
```

The only procedure called in `vegas` is `vegas_func_evaluate`. It takes a real value `x` and returns a real value `f`.

```
<vegas: interfaces>≡  
  abstract interface  
    real(default) function vegas_func_evaluate (self, x) result (f)  
      import :: default, vegas_func_t  
      class(vegas_func_t), intent(inout) :: self  
      real(default), dimension(:), intent(in) :: x  
    end function vegas_func_evaluate  
  end interface
```

20.3 Type: `vegas_config_t`

We store the complete configuration in a transparent container. The `vegas_config_t` object inside VEGAS must not be directly accesible. We provide a `get` method which returns a copy of the `vegas_config_t` object.

Apart from the options which can be set by the constructor of `vegas_t` object, we store the run-time configuration `n_calls`, `calls_per_box`, `n_bins` and `n_boxes`. Those are calculated and set accordingly by VEGAS.

```
<vegas: public>+≡  
  public :: vegas_config_t
```

```

<vegas: types>+≡
  type :: vegas_config_t
    integer :: n_dim = 0
    real(default) :: alpha = 1.5
    integer :: n_bins_max = 50
    integer :: iterations = 5
    integer :: mode = VEGAS_MODE_STRATIFIED
    integer :: calls_per_box = 0
    integer :: n_calls = 0
    integer :: n_calls_min = 20
    integer :: n_boxes = 1
    integer :: n_bins = 1
  contains
    <vegas: vegas config: TBP>
  end type vegas_config_t

```

Write out the configuration of the grid.

```

<vegas: vegas config: TBP>≡
  procedure, public :: write => vegas_config_write

<vegas: procedures>≡
  subroutine vegas_config_write (self, unit, indent)
    class(vegas_config_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") &
      & "Number of dimensions" = ", self%n_dim
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
      & "Adaption power (alpha)" = ", self%alpha
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") &
      & "Max. number of bins (per dim.)" = ", self%n_bins_max
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") &
      & "Number of iterations" = ", self%iterations
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") &
      & "Mode (stratified or importance)" = ", self%mode
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") &
      & "Calls per box" = ", self%calls_per_box
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") &
      & "Number of calls" = ", self%n_calls
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") &
      & "Min. number of calls" = ", self%n_calls_min
    call write_indent (u, ind)
    write (u, "(2x,A,I0)") &

```

```

        & "Number of bins" = ", self%n_bins
    call write_indent (u, ind)
    write (u, "(2x,A,I0)" &
        & "Number of boxes" = ", self%n_boxes
end subroutine vegas_config_write

```

20.4 Type: vegas_grid_t

We provide a simple and transparent grid container. The container can then later be used, to export the actual grid.

```

<vegas: public>+≡
    public :: vegas_grid_t

<vegas: types>+≡
    type :: vegas_grid_t
        integer :: n_dim = 1
        integer :: n_bins = 1
        real(default), dimension(:), allocatable :: x_lower
        real(default), dimension(:), allocatable :: x_upper
        real(default), dimension(:), allocatable :: delta_x
        real(default), dimension(:,,:), allocatable :: xi
    contains
        <vegas: vegas_grid: TBP>
    end type vegas_grid_t

```

Initialise grid.

```

<vegas: interfaces>+≡
    interface vegas_grid_t
        module procedure vegas_grid_init
    end interface vegas_grid_t

<vegas: procedures>+≡
    type(vegas_grid_t) function vegas_grid_init (n_dim, n_bins_max) result (self)
        integer, intent(in) :: n_dim
        integer, intent(in) :: n_bins_max
        self%n_dim = n_dim
        self%n_bins = 1
        allocate (self%x_upper(n_dim), source=1.0_default)
        allocate (self%x_lower(n_dim), source=0.0_default)
        allocate (self%delta_x(n_dim), source=1.0_default)
        allocate (self%xi((n_bins_max + 1), n_dim), source=0.0_default)
    end function vegas_grid_init

```

Output.

```

<vegas: vegas_grid: TBP>≡
    procedure, public :: write => vegas_grid_write

<vegas: procedures>+≡
    subroutine vegas_grid_write (self, unit, pacify)
        class(vegas_grid_t), intent(in) :: self

```

```

integer, intent(in), optional :: unit
logical, intent(in), optional :: pacify
logical :: pac
integer :: u, i, j
pac = .false.; if (present (pacify)) pac = pacify
u = given_output_unit (unit)
write (u, descr_fmt) "begin vegas_grid_t"
write (u, integer_fmt) "n_dim = ", self%n_dim
write (u, integer_fmt) "n_bins = ", self%n_bins
write (u, descr_fmt) "begin x_lower"
do j = 1, self%n_dim
  if (pac) then
    write (u, double_array_pac_fmt) j, self%x_lower(j)
  else
    write (u, double_array_fmt) j, self%x_lower(j)
  end if
end do
write (u, descr_fmt) "end x_lower"
write (u, descr_fmt) "begin x_upper"
do j = 1, self%n_dim
  if (pac) then
    write (u, double_array_pac_fmt) j, self%x_upper(j)
  else
    write (u, double_array_fmt) j, self%x_upper(j)
  end if
end do
write (u, descr_fmt) "end x_upper"
write (u, descr_fmt) "begin delta_x"
do j = 1, self%n_dim
  if (pac) then
    write (u, double_array_pac_fmt) j, self%delta_x(j)
  else
    write (u, double_array_fmt) j, self%delta_x(j)
  end if
end do
write (u, descr_fmt) "end delta_x"
write (u, descr_fmt) "begin xi"
do j = 1, self%n_dim
  do i = 1, self%n_bins + 1
    if (pac) then
      write (u, double_array2_pac_fmt) i, j, self%xi(i, j)
    else
      write (u, double_array2_fmt) i, j, self%xi(i, j)
    end if
  end do
end do
write (u, descr_fmt) "end xi"
write (u, descr_fmt) "end vegas_grid_t"
end subroutine vegas_grid_write

```

Compare two grids, if they match up to an given precision.

```

<vegas: public>+≡
public :: operator (==)

```

```

<vegas: interfaces> +=
  interface operator (==)
    module procedure vegas_grid_equal
  end interface operator (==)

<vegas: procedures> +=
  logical function vegas_grid_equal (grid_a, grid_b) result (yorn)
    type(vegas_grid_t), intent(in) :: grid_a, grid_b
    yorn = .true.
    yorn = yorn .and. (grid_a%n_dim == grid_b%n_dim)
    yorn = yorn .and. (grid_a%n_bins == grid_b%n_bins)
    yorn = yorn .and. all (grid_a%x_lower == grid_b%x_lower)
    yorn = yorn .and. all (grid_a%x_upper == grid_b%x_upper)
    yorn = yorn .and. all (grid_a%delta_x == grid_b%delta_x)
    yorn = yorn .and. all (grid_a%xi == grid_b%xi)
  end function vegas_grid_equal

```

Resize each bin accordingly to its corresponding weight w . Can be used to resize the grid to a new size of bins or refinement.

The procedure expects two arguments, firstly, `n_bins` and, secondly, the refinement weights w . If `n_bins` differs from the internally stored one, we resize the grid under consideration of w . If each element of w equals one, then the bins are resized preserving their original bin density.

Anytime else, we refine the grid accordingly to w .

```

<vegas: vegas_grid: TBP> +=
  procedure, private :: resize => vegas_grid_resize

<vegas: procedures> +=
  subroutine vegas_grid_resize (self, n_bins, w)
    class(vegas_grid_t), intent(inout) :: self
    integer, intent(in) :: n_bins
    real(default), dimension(:, :), intent(in) :: w
    real(default), dimension(size(self%xi)) :: xi_new
    integer :: i, j, k
    real(default) :: pts_per_bin
    real(default) :: d_width
    do j = 1, self%n_dim
      if (self%n_bins /= n_bins) then
        pts_per_bin = real(self%n_bins, default) / real(n_bins, default)
        self%n_bins = n_bins
      else
        if (all (w(:, j) == 0.)) then
          call msg_bug ("[VEGAS] grid_resize: resize weights are zero.")
        end if
        pts_per_bin = sum(w(:, j)) / self%n_bins
      end if
      d_width = 0.
      k = 0
      do i = 2, self%n_bins
        do while (pts_per_bin > d_width)
          k = k + 1
          d_width = d_width + w(k, j)
        end do
        d_width = d_width - pts_per_bin
      end do
    end do
  end subroutine vegas_grid_resize

```

```

        associate (x_upper => self%xi(k + 1, j), x_lower => self%xi(k, j))
            xi_new(i) = x_upper - (x_upper - x_lower) * d_width / w(k, j)
        end associate
    end do
    self%xi(:, j) = 0. ! Reset grid explicitly
    self%xi(2:n_bins, j) = xi_new(2:n_bins)
    self%xi(n_bins + 1, j) = 1.
end do
end subroutine vegas_grid_resize

```

Find the probability for a given x in the unit hypercube.

For the case `n_bins < N_BINARY_SEARCH`, we utilize linear search which is faster for short arrays. Else we make use of a binary search. Furthermore, we calculate the inverse of the probability and invert the result only at the end (saving some time on division).

```

<vegas: vegas grid: TBP>+≡
    procedure, public :: get_probability => vegas_grid_get_probability

<vegas: procedures>+≡
    function vegas_grid_get_probability (self, x) result (g)
        class(vegas_grid_t), intent(in) :: self
        real(default), dimension(:), intent(in) :: x
        real(default) :: g
        integer :: j, i_lower, i_higher, i_mid
        real(default), dimension(size(x)) :: y
        g = 1
        y = (x - self%x_lower) / self%delta_x
        if (any (y < 0 .or. y > 1)) then
            g = 0; return
        end if
        ndim: do j = 1, self%n_dim
            i_lower = 1
            i_higher = self%n_bins + 1
            !! Left-most search
            search: do while (i_lower < i_higher - 1)
                i_mid = floor ((i_higher + i_lower) / 2.)
                if (y(j) > self%xi(i_mid, j)) then
                    i_lower = i_mid
                else
                    i_higher = i_mid
                end if
            end do search
            g = g * (self%delta_x(j) * &
                & self%n_bins * (self%xi(i_lower + 1, j) - self%xi(i_lower, j)))
        end do ndim
        ! Move division to the end, which is more efficient.
        if (g /= 0) g = 1 / g
    end function vegas_grid_get_probability

```

Broadcast the grid information. As safety measure, we get the actual grid object from VEGAS (correctly allocated, but for non-root unfilled) and broadcast the root object. On success, we set grid into VEGAS.

We use the non-blocking broadcast routine, because we have to send quite a bunch of integers and reals.

We have to be very careful with `n_bins`, the number of bins can actually change during different iterations. If we reuse a grid, we have to take that, every grid uses the same `n_bins`. We expect, that the number of dimension does not change, which is in principle possible, but will be checked onto in `vegas_set_grid`.

```

<MPI: vegas: vegas_grid: TBP>≡
  procedure, public :: broadcast => vegas_grid_broadcast

<MPI: vegas: procedures>≡
  subroutine vegas_grid_broadcast (self, comm)
    class(vegas_grid_t), intent(inout) :: self
    type(MPI_COMM), intent(in) :: comm
    integer :: j, ierror
    type(MPI_Request), dimension(self%n_dim + 4) :: status
    ! Blocking
    call MPI_Bcast (self%n_bins, 1, MPI_INTEGER, 0, comm)
    ! Non blocking
    call MPI_Ibcast (self%n_dim, 1, MPI_INTEGER, 0, comm, status(1))
    call MPI_Ibcast (self%x_lower, self%n_dim, &
      & MPI_DOUBLE_PRECISION, 0, comm, status(2))
    call MPI_Ibcast (self%x_upper, self%n_dim, &
      & MPI_DOUBLE_PRECISION, 0, comm, status(3))
    call MPI_Ibcast (self%delta_x, self%n_dim, &
      & MPI_DOUBLE_PRECISION, 0, comm, status(4))
    ndim: do j = 1, self%n_dim
      call MPI_Ibcast (self%xi(1:self%n_bins + 1, j), self%n_bins + 1, &
        & MPI_DOUBLE_PRECISION, 0, comm, status(4 + j))
    end do ndim
    call MPI_Waitall (self%n_dim + 4, status, MPI_STATUSES_IGNORE)
  end subroutine vegas_grid_broadcast

```

20.5 Type: vegas_result_t

We store the result of the latest iteration(s) in a transparent container. The `vegas_result_t` object inside VEGAS must not be directly accessible. We export the a copy of the result via a get-method of the `vegas_t` object.

We store latest event weight in `evt_weight` and a (possible) evebt weight excess in `evt_weight_excess`, if the event weight is larger than `max_abs_f`.

```

<vegas: public>+≡
  public :: vegas_result_t

<vegas: types>+≡
  type :: vegas_result_t
    integer :: it_start = 0
    integer :: it_num = 0
    integer :: samples = 0
    real(default) :: sum_int_wgtd = 0.
    real(default) :: sum_wgts
    real(default) :: sum_chi = 0.

```

```

real(default) :: chi2 = 0.
real(default) :: efficiency = 0.
real(default) :: efficiency_pos = 0.
real(default) :: efficiency_neg = 0.
real(default) :: max_abs_f = 0.
real(default) :: max_abs_f_pos = 0.
real(default) :: max_abs_f_neg = 0.
real(default) :: result = 0.
real(default) :: std = 0.
real(default) :: evt_weight = 0.
real(default) :: evt_weight_excess = 0.
contains
  <vegas: vegas result: TBP>
end type vegas_result_t

```

Write out the current status of the integration result.

```

<vegas: vegas result: TBP>≡
  procedure, public :: write => vegas_result_write
<vegas: procedures>+≡
  subroutine vegas_result_write (self, unit, indent)
    class(vegas_result_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(2x,A,I0)" &
      & "Start iteration" = ", self%it_start
    call write_indent (u, ind)
    write (u, "(2x,A,I0)" &
      & "Iteration number" = ", self%it_num
    call write_indent (u, ind)
    write (u, "(2x,A,I0)" &
      & "Sample number" = ", self%samples
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
      & "Sum of weighted integrals" = ", self%sum_int_wgtd
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
      & "Sum of weights" = ", self%sum_wgts
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
      & "Sum of chi" = ", self%sum_chi
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
      & "chi2" = ", self%chi2
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
      & "Overall efficiency" = ", self%efficiency
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
      & "f-positive efficiency" = ", self%efficiency_pos

```



```

call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
    & "f-negative efficiency" = ", self%efficiency_neg
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
    & "Maximum absolute overall value" = ", self%max_abs_f
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
    & "Maximum absolute positive value" = ", self%max_abs_f_pos
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
    & "Maximum absolute negative value" = ", self%max_abs_f_neg
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
    & "Integral (of latest iteration)" = ", self%result
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
    & "Standard deviation" = ", self%std
write (u, "(2x,A," // FMT_17 // ")") &
    & "Event weight" = ", self%evt_weight
write (u, "(2x,A," // FMT_17 // ")") &
    & "Event weight excess" = ", self%evt_weight_excess
end subroutine vegas_result_write

```

Update results and efficiency.

We define

$$\max_x w(x) = \frac{f(x)}{p(x)} \Delta_{\text{jac}}. \quad (20.1)$$

In the implementation we have to factor out `n_calls` in the jacobian. Also, during event generation.

```

<vegas: vegas result: TBP>+≡
    procedure, public :: update => vegas_result_update
    procedure, public :: update_efficiency => vegas_result_update_efficiency

<vegas: procedures>+≡
    subroutine vegas_result_update (result, integral, variance)
        class(vegas_result_t), intent(inout) :: result
        real(default), intent(in) :: integral
        real(default), intent(in) :: variance
        real(default) :: guarded_variance, sq_integral
        real(default) :: wgt, chi
        !! Guard against zero (or negative) variance.
        !! \Delta = I * \epsilon -> I = \Delta.
        if (variance < &
            max ((epsilon (integral) * integral)**2, tiny(integral))) then
            guarded_variance = &
                max ((epsilon (integral) * integral)**2, &
                    tiny (integral))
        else
            guarded_variance = variance
        end if
        wgt = 1._default / guarded_variance
        sq_integral = integral**2
    end subroutine

```

```

result%result = integral
result%std = sqrt (guarded_variance)
result%samples = result%samples + 1
if (result%samples == 1) then
    result%chi2 = 0._default
else
    chi = integral
    if (result%sum_wgts > 0) then
        chi = chi - result%sum_int_wgtd / result%sum_wgts
    end if
    result%chi2 = result%chi2 * (result%samples - 2.0_default)
    result%chi2 = (wgt / (1._default + (wgt / result%sum_wgts))) &
        & * chi**2
    result%chi2 = result%chi2 / (result%samples - 1._default)
end if
result%sum_wgts = result%sum_wgts + wgt
result%sum_int_wgtd = result%sum_int_wgtd + (integral * wgt)
result%sum_chi = result%sum_chi + (sq_integral * wgt)
end subroutine vegas_result_update

subroutine vegas_result_update_efficiency (result, &
    n_calls, max_pos, max_neg, sum_pos, sum_neg)
class(vegas_result_t), intent(inout) :: result
integer, intent(in) :: n_calls
real(default), intent(in) :: max_pos
real(default), intent(in) :: max_neg
real(default), intent(in) :: sum_pos
real(default), intent(in) :: sum_neg
result%max_abs_f_pos = n_calls * max_pos
result%max_abs_f_neg = n_calls * max_neg
result%max_abs_f = &
    & max (result%max_abs_f_pos, result%max_abs_f_neg)
result%efficiency_pos = 0
if (max_pos > 0) then
    result%efficiency_pos = &
        & sum_pos / max_pos
end if
result%efficiency_neg = 0
if (max_neg > 0) then
    result%efficiency_neg = &
        & sum_neg / max_neg
end if
result%efficiency = 0
if (result%max_abs_f > 0.) then
    result%efficiency = (sum_pos + sum_neg) &
        & / result%max_abs_f
end if
end subroutine vegas_result_update_efficiency

```

Reset results.

```

<vegas: vegas result: TBP>+≡
    procedure, public :: reset => vegas_result_reset
<vegas: procedures>+≡

```

```

subroutine vegas_result_reset (result)
  class(vegas_result_t), intent(inout) :: result
  result%sum_int_wgtd = 0
  result%sum_wgts = 0
  result%sum_chi = 0
  result%it_num = 0
  result%samples = 0
  result%chi2 = 0
  result%efficiency = 0
  result%efficiency_pos = 0
  result%efficiency_neg = 0
  result%max_abs_f = 0
  result%max_abs_f_pos = 0
  result%max_abs_f_neg = 0
end subroutine vegas_result_reset

```

Send the result object to specified rank, internally in a non-blocking way.

We do not need to handle the event results, because each event result is atomic.

(MPI: vegas: vegas result: TBP)≡

```

  procedure, public :: send => vegas_result_send

```

(MPI: vegas: procedures)+≡

```

subroutine vegas_result_send (self, receiver, tag, comm, request)
  class(vegas_result_t), intent(in) :: self
  integer, intent(in) :: receiver
  integer, intent(in) :: tag
  type(MPI_COMM), intent(in) :: comm
  type(MPI_Request), dimension(:), intent(inout) :: request
  if (size(request) /= self%get_n_requests ()) &
    call msg_bug ("VEGAS: number of requests does not match.")
  call MPI_Isend (self%it_start, 1, MPI_INTEGER, receiver, tag + 1,&
    & comm, request(1))
  call MPI_Isend (self%it_num, 1, MPI_INTEGER, receiver, tag + 2,&
    & comm, request(2))
  call MPI_Isend (self%samples, 1, MPI_INTEGER, receiver, tag + 3,&
    & comm, request(3))
  call MPI_Isend (self%sum_int_wgtd, 1, MPI_DOUBLE_PRECISION, receiver, tag + 4,&
    & comm, request(4))
  call MPI_Isend (self%sum_wgts, 1, MPI_DOUBLE_PRECISION, receiver, tag + 5,&
    & comm, request(5))
  call MPI_Isend (self%sum_chi, 1, MPI_DOUBLE_PRECISION, receiver, tag + 6,&
    & comm, request(6))
  call MPI_Isend (self%chi2, 1, MPI_DOUBLE_PRECISION, receiver, tag + 7,&
    & comm, request(7))
  call MPI_Isend (self%efficiency, 1, MPI_DOUBLE_PRECISION, receiver, tag + 8,&
    & comm, request(8))
  call MPI_Isend (self%efficiency_pos, 1, MPI_DOUBLE_PRECISION, receiver, tag + 9,&
    & comm, request(9))
  call MPI_Isend (self%efficiency_neg, 1, MPI_DOUBLE_PRECISION, receiver, tag + 10,&
    & comm, request(10))
  call MPI_Isend (self%max_abs_f, 1, MPI_DOUBLE_PRECISION, receiver, tag + 11,&
    & comm, request(11))
  call MPI_Isend (self%max_abs_f_pos, 1, MPI_DOUBLE_PRECISION, receiver, tag + 12,&

```

```

        & comm, request(12))
call MPI_Isend (self%max_abs_f_neg, 1, MPI_DOUBLE_PRECISION, receiver, tag + 13,&
    & comm, request(13))
call MPI_Isend (self%result, 1, MPI_DOUBLE_PRECISION, receiver, tag + 14,&
    & comm, request(14))
call MPI_Isend (self%std, 1, MPI_DOUBLE_PRECISION, receiver, tag + 15,&
    & comm, request(15))
end subroutine vegas_result_send

```

Receive the result object from a specified rank, internally in a non-blocking way.

(MPI: vegas: vegas result: TBP)+≡

```

    procedure, public :: receive => vegas_result_receive

```

(MPI: vegas: procedures)+≡

```

subroutine vegas_result_receive (self, sender, tag, comm, request)
    class(vegas_result_t), intent(inout) :: self
    integer, intent(in) :: sender
    integer, intent(in) :: tag
    type(MPI_COMM), intent(in) :: comm
    type(MPI_REQUEST), dimension(:), intent(inout) :: request
    if (size (request) /= self%get_n_requests ()) &
        call msg_bug ("VEGAS: number of requests does not match.")
    call MPI_Irecv (self%it_start, 1, MPI_INTEGER, sender, tag + 1,&
        & comm, request(1))
    call MPI_Irecv (self%it_num, 1, MPI_INTEGER, sender, tag + 2,&
        & comm, request(2))
    call MPI_Irecv (self%samples, 1, MPI_INTEGER, sender, tag + 3,&
        & comm, request(3))
    call MPI_Irecv (self%sum_int_wgtd, 1, MPI_DOUBLE_PRECISION, sender, tag + 4,&
        & comm, request(4))
    call MPI_Irecv (self%sum_wgts, 1, MPI_DOUBLE_PRECISION, sender, tag + 5,&
        & comm, request(5))
    call MPI_Irecv (self%sum_chi, 1, MPI_DOUBLE_PRECISION, sender, tag + 6,&
        & comm, request(6))
    call MPI_Irecv (self%chi2, 1, MPI_DOUBLE_PRECISION, sender, tag + 7,&
        & comm, request(7))
    call MPI_Irecv (self%efficiency, 1, MPI_DOUBLE_PRECISION, sender, tag + 8,&
        & comm, request(8))
    call MPI_Irecv (self%efficiency_pos, 1, MPI_DOUBLE_PRECISION, sender, tag + 9,&
        & comm, request(9))
    call MPI_Irecv (self%efficiency_neg, 1, MPI_DOUBLE_PRECISION, sender, tag + 10,&
        & comm, request(10))
    call MPI_Irecv (self%max_abs_f, 1, MPI_DOUBLE_PRECISION, sender, tag + 11,&
        & comm, request(11))
    call MPI_Irecv (self%max_abs_f_pos, 1, MPI_DOUBLE_PRECISION, sender, tag + 12,&
        & comm, request(12))
    call MPI_Irecv (self%max_abs_f_neg, 1, MPI_DOUBLE_PRECISION, sender, tag + 13,&
        & comm, request(13))
    call MPI_Irecv (self%result, 1, MPI_DOUBLE_PRECISION, sender, tag + 14,&
        & comm, request(14))
    call MPI_Irecv (self%std, 1, MPI_DOUBLE_PRECISION, sender, tag + 15,&
        & comm, request(15))
end subroutine vegas_result_receive

```

```

<MPI: vegas: vegas result: TBP>+≡
    procedure, private :: get_n_requests => vegas_result_get_n_requests

<MPI: vegas: procedures>+≡
    pure integer function vegas_result_get_n_requests (result) result (n_requests)
        class(vegas_result_t), intent(in) :: result
        n_requests = 15
    end function vegas_result_get_n_requests

```

20.6 Type: vegas_handler_t

Callback handler for VEGAS result and grid.

```

<MPI: vegas: public>≡
    public :: vegas_handler_t

<MPI: vegas: types>≡
    type, extends(request_handler_t) :: vegas_handler_t
        type(vegas_result_t), pointer :: result => null ()
        real(default), dimension(:, :), pointer :: d => null ()
    contains
        <vegas: vegas handler: TBP>
    end type vegas_handler_t

```

Provide the actual communication between master and client.

The communication for `vegas_result_t` is done in a separate procedure, where we only have to pass the MPI requests. Collecting of the distribution array is done directly.

```

<MPI: vegas: vegas handler: TBP>≡
    procedure :: init => vegas_handler_init
    procedure :: write => vegas_handler_write
    procedure :: handle => vegas_handler_handle
    procedure :: client_handle => vegas_handler_client_handle
    final :: vegas_handler_final

<MPI: vegas: procedures>+≡
    subroutine vegas_handler_init (handler, handler_id, result, d)
        class(vegas_handler_t), intent(inout) :: handler
        integer, intent(in) :: handler_id
        type(vegas_result_t), intent(in), target :: result
        real(default), dimension(:, :), intent(in), target :: d
        integer :: n_requests, tag_offset
        handler%result => result
        handler%d => d
        handler%finished = .false.
        !! Add one request for handling of the distribution d.
        n_requests = result%get_n_requests () + 1
        tag_offset = max(handler_id - 1, 0) * n_requests
        call handler%allocate (n_requests, tag_offset)
    end subroutine vegas_handler_init

    subroutine vegas_handler_write (handler, unit)
        class(vegas_handler_t), intent(in) :: handler
        integer, intent(in), optional :: unit
        integer :: u, j

```

```

u = given_output_unit (unit)
write (u, "(A)") "[VEGAS_HANDLER]"
call handler%base_write (unit)
call handler%result%write (u)
write (u, "(A)") "BEGIN D"
do j = 1, size (handler%d, dim=2)
    write (u, "(1X,I3,999(1X," // FMT_17 // "))" j, handler%d(:, j)
end do
write (u, "(A)") "END D"
end subroutine vegas_handler_write

subroutine vegas_handler_handle (handler, source_rank, comm)
class(vegas_handler_t), intent(inout) :: handler
integer, intent(in) :: source_rank
type(MPI_COMM), intent(in) :: comm
!! Take the complete contiguous array memory.
call MPI_Irecv (handler%d, size (handler%d), &
    & MPI_DOUBLE_PRECISION, source_rank, handler%tag_offset, comm, &
    & handler%request(1))
call handler%result%receive (source_rank, handler%tag_offset, comm, &
    handler%request(2:))
handler%activated = .true.
handler%finished = .false.
end subroutine vegas_handler_handle

subroutine vegas_handler_client_handle (handler, dest_rank, comm)
class(vegas_handler_t), intent(inout) :: handler
integer, intent(in) :: dest_rank
type(MPI_COMM), intent(in) :: comm
!! Take the complete contiguous array memory.
call MPI_Isend (handler%d, size (handler%d), &
    & MPI_DOUBLE_PRECISION, dest_rank, handler%tag_offset, comm, &
    & handler%request(1))
call handler%result%send (dest_rank, handler%tag_offset, comm, &
    handler%request(2:))
handler%activated = .true.
handler%finished = .false.
end subroutine vegas_handler_client_handle

!> Finalize vegas_handler_t.
!!
!! Nullify pointer to object.
subroutine vegas_handler_final (handler)
type(vegas_handler_t), intent(inout) :: handler
nullify (handler%result)
nullify (handler%d)
end subroutine vegas_handler_final

```

20.7 Type: vegas_t

The VEGAS object contains the methods for integration and grid resize- and refinement. We store the grid configuration and the (current) result in transparent

containers alongside with the actual grid and the distribution.

The values of the distribution depend on the chosen mode whether the function value or the variance is stored. The distribution is used after each iteration to refine the grid.

```

<vegas: public>+≡
    public :: vegas_t

<vegas: types>+≡
    type :: vegas_t
    private
    type(vegas_config_t) :: config
    real(default) :: hypercube_volume = 0.
    real(default) :: jacobian = 0.
    real(default), dimension(:, :), allocatable :: d
    type(vegas_grid_t) :: grid
    integer, dimension(:), allocatable :: bin
    integer, dimension(:), allocatable :: box
    type(vegas_result_t) :: result
    <vegas: vegas: type>
    contains
    <vegas: vegas: TBP>
end type vegas_t

```

Add members for MPI communication and parallel mode. Must be set before calling to `vegas_integrate`, likewise `vegas_set_calls`.

```

<MPI: vegas: vegas: type>≡
    type(MPI_COMM) :: comm
    logical :: parallel_mode = .false.

```

We overload the type constructor of `vegas_t` which initialises the mandatory argument `n_dim` and allocate memory for the grid.

```

<vegas: interfaces>+≡
    interface vegas_t
        module procedure vegas_init
    end interface vegas_t

<vegas: procedures>+≡
    type(vegas_t) function vegas_init (n_dim, alpha, n_bins_max, iterations, mode) result (self)
        integer, intent(in) :: n_dim
        integer, intent(in), optional :: n_bins_max
        real(default), intent(in), optional :: alpha
        integer, intent(in), optional :: iterations
        integer, intent(in), optional :: mode
        self%config%n_dim = n_dim
        if (present (alpha)) self%config%alpha = alpha
        if (present (n_bins_max)) self%config%n_bins_max = n_bins_max
        if (present (iterations)) self%config%iterations = iterations
        if (present (mode)) self%config%mode = mode
        self%grid = vegas_grid_t (n_dim, self%config%n_bins_max)
        allocate (self%d(self%config%n_bins_max, n_dim), source=0.0_default)
        allocate (self%box(n_dim), source=1)
        allocate (self%bin(n_dim), source=1)
        self%config%n_bins = 1
        self%config%n_boxes = 1
    end function vegas_init

```

```

        call self%set_limits (self%grid%x_lower, self%grid%x_upper)
        call self%reset_grid ()
        call self%reset_result ()
    <vegas: vegas init>
end function vegas_init

```

<vegas: vegas init>≡

Prepare VEGAS to be run in parallel modules (when compiled with MPI).

<MPI: vegas: vegas init>≡

```

        call self%prepare_parallel_integrate (MPI_COMM_WORLD, &
            duplicate_comm = .false., &
            parallel_mode = .true.)

```

Finalize the grid. Deallocate grid memory.

<vegas: vegas: TBP>≡

```

        procedure, public :: final => vegas_final

```

<vegas: procedures>+≡

```

        subroutine vegas_final (self)
            class(vegas_t), intent(inout) :: self
            deallocate (self%grid%x_upper)
            deallocate (self%grid%x_lower)
            deallocate (self%grid%delta_x)
            deallocate (self%d)
            deallocate (self%grid%xi)
            deallocate (self%box)
            deallocate (self%bin)
        end subroutine vegas_final

```

20.8 Get-/Set-methods

The VEGAS object prohibits direct access from outside. Communication is handled via get- or set-methods. Set the limits of integration. The default limits correspond to the n -dimensional unit hypercube.

Remark: After setting the limits, the grid is initialised, again. Previous results are lost due to recalculation of the overall jacobian.

<vegas: vegas: TBP>+≡

```

        procedure, public :: set_limits => vegas_set_limits

```

<vegas: procedures>+≡

```

        subroutine vegas_set_limits (self, x_lower, x_upper)
            class(vegas_t), intent(inout) :: self
            real(default), dimension(:), intent(in) :: x_lower
            real(default), dimension(:), intent(in) :: x_upper
            if (size (x_lower) /= self%config%n_dim &
                & .or. size (x_upper) /= self%config%n_dim) then
                write (msg_buffer, "(A, I5, A, I5, A, I5)") &
                    "VEGAS: [set_limits] n_dim of new lower/upper integration limit&
                    & does not match previously set n_dim. ", self%config%n_dim, " /=&
                    & ", size (x_lower), " /= ", size (x_upper)
                call msg_fatal ()
            end if

```



```

    if (any(x_upper < x_lower)) then
        call msg_fatal ("VEGAS: [set_limits] upper limits are smaller than lower limits.")
    end if
    if (any((x_upper - x_lower) > huge(0._default))) then
        call msg_fatal ("VEGAS: [set_limits] upper and lower limits exceed rendering.")
    end if
    self%grid%x_upper = x_upper
    self%grid%x_lower = x_lower
    self%grid%delta_x = self%grid%x_upper - self%grid%x_lower
    self%hypercube_volume = product (self%grid%delta_x)
    call self%reset_result ()
end subroutine vegas_set_limits

```

Set the number of calls. If the number of calls changed during different passes, we resize the grid preserving the probability density. We should reset the results after changing the number of calls which change the size of the grid and the running mode of VEGAS. But, this is a set method only for the number of calls.

```

<vegas: vegas: TBP>+≡
    procedure, public :: set_calls => vegas_set_n_calls

<vegas: procedures>+≡
    subroutine vegas_set_n_calls (self, n_calls)
        class(vegas_t), intent(inout) :: self
        integer, intent(in) :: n_calls
        if (.not. (n_calls > 0)) then
            write (msg_buffer, "(A, I5)") &
                "VEGAS: [set_calls] number of calls must be a positive number. Keep&
                & number of calls = ", self%config%n_calls
            call msg_warning ()
        else
            self%config%n_calls = max (n_calls, self%config%n_calls_min)
            if (self%config%n_calls /= n_calls) then
                write (msg_buffer, "(A,I5)") &
                    "VEGAS: [set calls] number of calls is too few, reset to ", self%config%n_calls
                call msg_warning ()
            end if
            call self%init_grid ()
        end if
    end subroutine vegas_set_n_calls

```

Get the grid object and set n_bins, n_dim inside grid container.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_grid => vegas_get_grid

<vegas: procedures>+≡
    type(vegas_grid_t) function vegas_get_grid (self) result (grid)
        class(vegas_t), intent(in) :: self
        grid = self%grid
        grid%n_dim = self%config%n_dim
        grid%n_bins = self%config%n_bins
    end function vegas_get_grid

```

Set grid. We need a set method for the parallelisation. We do some additional checks before copying the object. Be careful, we do not check on `n_bins`, because the number of bins can change after setting `n_calls`. We remind you, that you will loose all your current progress, if you use set the grid. Hence, it will only be used when compiled with MPI.

```

<MPI: vegas: vegas: TBP>≡
  procedure, public :: set_grid => vegas_set_grid

<MPI: vegas: procedures>+≡
  subroutine vegas_set_grid (self, grid)
    class(vegas_t), intent(inout) :: self
    type(vegas_grid_t), intent(in) :: grid
    integer :: j
    logical :: success
    success = .true.
    success = (success .and. (grid%n_dim .eq. self%config%n_dim))
    success = (success .and. all (grid%x_lower .eq. self%grid%x_lower))
    success = (success .and. all (grid%x_upper .eq. self%grid%x_upper))
    success = (success .and. all (grid%delta_x .eq. self%grid%delta_x))
    if (success) then
      self%config%n_bins = grid%n_bins
      do j = 1, self%config%n_dim
        self%grid%xi(1, j) = 0._default
        self%grid%xi(2:self%config%n_bins, j) = grid%xi(2:grid%n_bins, j)
        self%grid%xi(self%config%n_bins + 1, j) = 1._default
      end do
    else
      call msg_bug ("VEGAS: set grid: boundary conditions do not match.")
    end if
  end subroutine vegas_set_grid

```

Prepare a parallel integration.

A parallel integration requires a communicator, which may be duplicated in order to provide a safe communication context for the current VEGAS instance. Furthermore, given an optional parameter, the behavior with regards to the parallel evaluation can be changed (e.g. embbed integration).

```

<MPI: vegas: vegas: TBP>+≡
  procedure, public :: prepare_parallel_integrate => vegas_prepare_parallel_integrate

<MPI: vegas: procedures>+≡
  subroutine vegas_prepare_parallel_integrate (self, comm, duplicate_comm, parallel_mode)
    class(vegas_t), intent(inout) :: self
    type(MPI_COMM), intent(in) :: comm
    logical, intent(in), optional :: duplicate_comm
    logical, intent(in), optional :: parallel_mode
    logical :: flag
    flag = .true.; if (present (duplicate_comm)) flag = duplicate_comm
    if (duplicate_comm) then
      call MPI_COMM_DUP (comm, self%comm)
    else
      self%comm = comm
    end if
    self%parallel_mode = .true.; if (present (parallel_mode)) &
      self%parallel_mode = parallel_mode
  end subroutine vegas_prepare_parallel_integrate

```

```
end subroutine vegas_prepare_parallel_integrate
```

We check if it is sensible to parallelize the actual grid. In simple, this means that `n_boxes` has to be larger than 2. With the result that we could have an actual superimposed stratified grid. In advance, we can give the size of communicator `n_size` and check whether we have enough boxes to distribute.

```
<MPI: vegas: vegas: TBP>+≡
  procedure, public :: is_parallelizable => vegas_is_parallelizable

<MPI: vegas: procedures>+≡
  elemental logical function vegas_is_parallelizable (self, opt_n_size) result (flag)
    class(vegas_t), intent(in) :: self
    integer, intent(in), optional :: opt_n_size
    integer :: n_size
    n_size = 2; if (present (opt_n_size)) n_size = opt_n_size
    flag = (self%config%n_boxes**floor (self%config%n_dim / 2.) >= n_size)
  end function vegas_is_parallelizable
```

Get the config object.

```
<vegas: vegas: TBP>+≡
  procedure, public :: get_config => vegas_get_config

<vegas: procedures>+≡
  subroutine vegas_get_config (self, config)
    class(vegas_t), intent(in) :: self
    type(vegas_config_t), intent(out) :: config
    config = self%config
  end subroutine vegas_get_config
```

Set non-runtime dependent configuration. It will no be possible to change `n_bins_max`.

```
<vegas: vegas: TBP>+≡
  procedure, public :: set_config => vegas_set_config

<vegas: procedures>+≡
  subroutine vegas_set_config (self, config)
    class(vegas_t), intent(inout) :: self
    class(vegas_config_t), intent(in) :: config
    self%config%alpha = config%alpha
    self%config%iterations = config%iterations
    self%config%mode = config%mode
    self%config%n_calls_min = config%n_calls_min
  end subroutine vegas_set_config
```

Get the result object.

```
<vegas: vegas: TBP>+≡
  procedure, public :: get_result => vegas_get_result

<vegas: procedures>+≡
  type(vegas_result_t) function vegas_get_result (self) result (result)
    class(vegas_t), intent(in) :: self
    result = self%result
  end function vegas_get_result
```

Set the result object. Be reminded, that you will loose your current results, if you are not careful! Hence, it will only be available during usage with MPI.

```

<MPI: vegas: vegas: TBP>+≡
    procedure, public :: set_result => vegas_set_result

<MPI: vegas: procedures>+≡
    subroutine vegas_set_result (self, result)
        class(vegas_t), intent(inout) :: self
        type(vegas_result_t), intent(in) :: result
        self%result = result
    end subroutine vegas_set_result

```

Get (actual) number of calls.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_calls => vegas_get_n_calls

<vegas: procedures>+≡
    elemental real(default) function vegas_get_n_calls (self) result (n_calls)
        class(vegas_t), intent(in) :: self
        n_calls = self%config%n_calls
    end function vegas_get_n_calls

```

Get the cumulative result of the integration. Recalculate weighted average of the integration.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_integral => vegas_get_integral

<vegas: procedures>+≡
    elemental real(default) function vegas_get_integral (self) result (integral)
        class(vegas_t), intent(in) :: self
        integral = 0.
        if (self%result%sum_wgts > 0.) then
            integral = self%result%sum_int_wgtd / self%result%sum_wgts
        end if
    end function vegas_get_integral

```

Get the cumulative variance of the integration. Recalculate the variance.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_variance => vegas_get_variance

<vegas: procedures>+≡
    elemental real(default) function vegas_get_variance (self) result (variance)
        class(vegas_t), intent(in) :: self
        variance = 0.
        if (self%result%sum_wgts > 0.) then
            variance = 1.0 / self%result%sum_wgts
        end if
    end function vegas_get_variance

```

Get efficiency.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_efficiency => vegas_get_efficiency

```

```

<vegas: procedures>+≡
    elemental real(default) function vegas_get_efficiency (self) result (efficiency)
        class(vegas_t), intent(in) :: self
        efficiency = 0.
        if (self%result%efficiency > 0. ) then
            efficiency = self%result%efficiency
        end if
    end function vegas_get_efficiency

```

Get f_max.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_max_abs_f => vegas_get_max_abs_f

<vegas: procedures>+≡
    elemental real(default) function vegas_get_max_abs_f (self) result (max_abs_f)
        class(vegas_t), intent(in) :: self
        max_abs_f = 0.
        if (self%result%max_abs_f > 0.) then
            max_abs_f = self%result%max_abs_f
        end if
    end function vegas_get_max_abs_f

```

Get sum of absolute (positive and negative) values.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_sum_abs_f_pos => vegas_get_sum_abs_f_pos
    procedure, public :: get_sum_abs_f_neg => vegas_get_sum_abs_f_neg

<vegas: procedures>+≡
    elemental real(default) function vegas_get_sum_abs_f_pos (self) result (sum_abs_f)
        class(vegas_t), intent(in) :: self
        sum_abs_f = self%result%efficiency_pos * self%result%max_abs_f_pos
    end function vegas_get_sum_abs_f_pos

    elemental real(default) function vegas_get_sum_abs_f_neg (self) result (sum_abs_f)
        class(vegas_t), intent(in) :: self
        sum_abs_f = self%result%efficiency_neg * self%result%max_abs_f_neg
    end function vegas_get_sum_abs_f_neg

```

Get f_max_pos.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_max_abs_f_pos => vegas_get_max_abs_f_pos

<vegas: procedures>+≡
    elemental real(default) function vegas_get_max_abs_f_pos (self) result (max_abs_f)
        class(vegas_t), intent(in) :: self
        max_abs_f = 0.
        if (self%result%max_abs_f_pos > 0.) then
            max_abs_f = self%result%max_abs_f_pos
        end if
    end function vegas_get_max_abs_f_pos

```

Get f_max_neg.

```

<vegas: vegas: TBP>+≡
    procedure, public :: get_max_abs_f_neg => vegas_get_max_abs_f_neg

```

```

<vegas: procedures>+≡
  elemental real(default) function vegas_get_max_abs_f_neg (self) result (max_abs_f)
    class(vegas_t), intent(in) :: self
    max_abs_f = 0.
    if (self%result%max_abs_f_neg > 0.) then
      max_abs_f = self%result%max_abs_f_neg
    end if
  end function vegas_get_max_abs_f_neg

```

Get event weight and excess.

```

<vegas: vegas: TBP>+≡
  procedure, public :: get_evt_weight => vegas_get_evt_weight
  procedure, public :: get_evt_weight_excess => vegas_get_evt_weight_excess

<vegas: procedures>+≡
  real(default) function vegas_get_evt_weight (self) result (evt_weight)
    class(vegas_t), intent(in) :: self
    evt_weight = self%result%evt_weight
  end function vegas_get_evt_weight

  real(default) function vegas_get_evt_weight_excess (self) result (evt_weight_excess)
    class(vegas_t), intent(in) :: self
    evt_weight_excess = self%result%evt_weight_excess
  end function vegas_get_evt_weight_excess

```

Get and set distribution.

We allow the distribution to be manipulated by an external call. The integration result cannot be changed by this, however, the error behavior may worsen and the efficiency may fall pretty low. But, also, the opposite is possible, see `vamp2.equivalences`.

```

<vegas: vegas: TBP>+≡
  procedure, public :: get_distribution => vegas_get_distribution
  procedure, public :: set_distribution => vegas_set_distribution

<vegas: procedures>+≡
  function vegas_get_distribution (self) result (d)
    class(vegas_t), intent(in) :: self
    real(default), dimension(:, :), allocatable :: d
    d = self%d
  end function vegas_get_distribution

  subroutine vegas_set_distribution (self, d)
    class(vegas_t), intent(inout) :: self
    real(default), dimension(:, :), intent(in) :: d
    if (size (d, dim = 2) /= self%config%n_dim) then
      call msg_bug ("[VEGAS] set_distribution: new distribution has wrong size of dimension")
    end if
    if (size (d, dim = 1) /= self%config%n_bins_max) then
      call msg_bug ("[VEGAS] set_distribution: new distribution has wrong number of bins")
    end if
    self%d = d
  end subroutine vegas_set_distribution

```

Allocate result handler from VEGAS integrator object.

```

(MPI: vegas: vegas: TBP)+≡
  procedure, public :: allocate_handler => vegas_allocate_handler

(MPI: vegas: procedures)+≡
  subroutine vegas_allocate_handler (self, handler_id, handler)
    class(vegas_t), intent(in), target :: self
    integer, intent(in) :: handler_id
    class(request_handler_t), pointer, intent(out) :: handler
    allocate (vegas_handler_t :: handler)
    select type (handler)
      type is (vegas_handler_t)
        call handler%init (handler_id, result = self%result, d = self%d)
    end select
  end subroutine vegas_allocate_handler

```

20.9 Grid resize- and refinement

Before integration the grid itself must be initialised. Given the number of `n_calls` and `n_dim` we prepare the grid for the integration.

The grid is binned according to the VEGAS mode and `n_calls`. If the mode is not set to `vegas_importance_only`, the grid is divided in to equal boxes. We try for 2 calls per box

$$boxes = \sqrt[n_{dim}]{\frac{calls}{2}}. \quad (20.2)$$

If the numbers of boxes exceeds the number of bins, which is the case for low dimensions, the algorithm switches to stratified sampling. Otherwise, we are still using importance sampling, but keep the boxes for book keeping. If the number of bins changes from the previous invocation, bins are expanded or contracted accordingly, while preserving bin density.

```

(vegas: vegas: TBP)+≡
  procedure, private :: init_grid => vegas_init_grid

(vegas: procedures)+≡
  subroutine vegas_init_grid (self)
    class(vegas_t), intent(inout) :: self
    integer :: n_bins, n_boxes, box_per_bin, n_total_boxes
    real(default), dimension(:, :), allocatable :: w
    n_bins = self%config%n_bins_max
    n_boxes = 1
    if (self%config%mode /= VEGAS_MODE_IMPORTANCE_ONLY) then
      ! We try for 2 calls per box
      n_boxes = max (floor ((self%config%n_calls / 2.)*(1. / self%config%n_dim)), 1)
      self%config%mode = VEGAS_MODE_IMPORTANCE
      if (2 * n_boxes >= self%config%n_bins_max) then
        ! if n_bins/box < 2
        box_per_bin = max (n_boxes / self%config%n_bins_max, 1)
        n_bins = min (n_boxes / box_per_bin, self%config%n_bins_max)
        n_boxes = box_per_bin * n_bins
        self%config%mode = VEGAS_MODE_STRATIFIED
      end if
    end if
  end subroutine vegas_init_grid

```

```

end if
n_total_boxes = n_boxes**self%config%n_dim
self%config%calls_per_box = max (floor (real (self%config%n_calls) / n_total_boxes), 2)
self%config%n_calls = self%config%calls_per_box * n_total_boxes
! Total volume of x-space/(average n_calls per bin)
self%jacobian = self%hypercube_volume * real(n_bins, default)&
&***self%config%n_dim / real(self%config%n_calls, default)
self%config%n_boxes = n_boxes
if (n_bins /= self%config%n_bins) then
  allocate (w(self%config%n_bins, self%config%n_dim), source=1.0_default)
  call self%grid%resize (n_bins, w)
  self%config%n_bins = n_bins
end if
end subroutine vegas_init_grid

```

Reset the cumulative result, and efficiency and max. grid values.

```

<vegas: vegas: TBP>+≡
  procedure, public :: reset_result => vegas_reset_result

<vegas: procedures>+≡
  subroutine vegas_reset_result (self)
    class(vegas_t), intent(inout) :: self
    call self%result%reset ()
  end subroutine vegas_reset_result

```

Reset the grid. Purge the adapted grid and the distribution. Furthermore, reset the results. The maximal size of the grid remains.

Note: Handle `vegas_reset_grid` with great care! Instead of reusing an old object, create a new one.

```

<vegas: vegas: TBP>+≡
  procedure, public :: reset_grid => vegas_reset_grid

<vegas: procedures>+≡
  subroutine vegas_reset_grid (self)
    class(vegas_t), intent(inout) :: self
    self%config%n_bins = 1
    self%d = 0._default
    self%grid%xi = 0._default
    self%grid%xi(1, :) = 0._default
    self%grid%xi(2, :) = 1._default
    call self%reset_result ()
  end subroutine vegas_reset_grid

```

Refine the grid to match the distribution `d`.

Average the distribution over neighbouring bins, then contract or expand the bins. The averaging dampens high fluctuations among the integrand or the variance.

We make the type-bound procedure public accessible because the multi-channel integration refines each grid after integration over all grids.

```

<vegas: vegas: TBP>+≡
  procedure, public :: refine => vegas_refine_grid

```



```

<vegas: procedures>+≡
  subroutine vegas_refine_grid (self, average)
    class(vegas_t), intent(inout) :: self
    logical, intent(in), optional :: average
    logical :: opt_average
    opt_average = .true.; if (present (average)) opt_average = average
    if (opt_average) call self%average_distribution ()
    call self%grid%resize (self%config%n_bins, self%d(:self%config%n_bins, :))
  end subroutine vegas_refine_grid

```

We average the collected values d of the (sq.) weighted f over neighbouring bins. The averaged d are then again damped by a logarithm to enhance numerical stability. The results are then the refinement weights w .

We have to take care of the special case where we have a very low sampling rate. In those cases we can not be sure that the distribution is satisfying filled, although we have already averaged over neighbouring bins. This will lead to a squashing of the unfilled bins and such the boundaries of those will be pushed together. We circumvent this problem by setting those unfilled bins to the smallest representable value of a default real.

The problem becomes very annoying in the multi-channel formulae where have to look up via binary search the corresponding probability of x and if the width is zero, the point will be neglected.

Another issue arises when NaNs appear during sampling. A single NaN may spoil the complete adaption as the refinement depends on all weights for a single axis, c.f. `vegas_grid_resize` for the details of the mechanism. Therefore, if we find a single (or more) NaNs in the distribution of an axis, then we won't adapt that specific axis by setting the weights to one. Hence, we skip the adaption for parts of the grid, where NaN appeared during evaluation.

```

<vegas: vegas: TBP>+≡
  procedure, private :: average_distribution => vegas_average_distribution

<vegas: procedures>+≡
  subroutine vegas_average_distribution (self)
    !! use, intrinsic :: ieee_arithmetic, only: ieee_is_nan
    class(vegas_t), intent(inout) :: self
    integer :: j
    ndim: do j = 1, self%config%n_dim
      associate (d => self%d(:self%config%n_bins, j), &
        n_bins => self%config%n_bins)
        !! Non-portable and compiler-flag sensitive test, may replace with ieee_is_nan
        if (any (d /= d)) then
          d = 1.0_default
          cycle ndim
        end if
        if (n_bins > 2) then
          d(1) = (d(1) + d(2)) / 2.0_default
          d(2:n_bins - 1) = (d(1:n_bins - 2) + d(2:n_bins - 1) + d(3:n_bins)) / &
            & 3.0_default
          d(n_bins) = d(n_bins - 1) + d(n_bins) / 2.0_default
        end if
        if (all (d < tiny (d))) then
          d = 1.0_default; cycle ndim
        end if
      end associate
    end do
  end subroutine vegas_average_distribution

```

```

end if
d = d / sum (d)
where (d < tiny (1.0_default))
  d = tiny (1.0_default)
end where
where (d /= 1.0_default)
  d = ((d - 1.0_default) / log(d))**self%config%alpha
elsewhere
  ! Analytic limes for d -> 1
  d = 1.0_default
end where
end associate
end do ndim
end subroutine vegas_average_distribution

```

20.10 Integration

Integrate `func`, in the previous set bounds `x.lower` to `x.upper`, with `n.calls`. Use results from previous invocations of `integrate` with `opt.reset.result = .false.` and better with subsequent calls.

Before we walk through the hybercube, we initialise the grid (at a central position).

We step through the (equidistant) boxes which ensure we do not miss any place in the n -dim. hypercube. In each box we sample `calls_per_box` random points and transform them to bin coordinates. The total integral and the total (sample) variance over each box i is then calculated by

$$E(I)_i = \sum_j^{\text{calls per box}} I_{i,j},$$

$$V(I)_i = \text{calls per box} \frac{\sum_j^{\text{calls per box}^2} I_{i,j}^2}{I} - \left(\sum_j^{\text{calls per box}} I_{i,j} \right) * 2 \frac{\text{calls per box}}{\text{calls per box} - 1}.$$

The stratification of the n -dimensional hybercube allows a simple parallelisation of the algorithm (R. Kreckel, "Parallelization of adaptive MC integrators", Computer Physics Communications, vol. 106, no. 3, pp. 258–266, Nov. 1997.). We have to ensure that all boxes are sampled, but the number of boxes to distribute is too large. We allow each thread to sample a fraction r of all boxes k such that $r \ll k$. Furthermore, we constrain that the number of process p is much smaller than r .

The overall constraint is

$$p \ll r \ll k. \quad (20.3)$$

We divide the integration into a parallel and a perpendicular subspace. The number of parallel dimensions is $D_{\parallel} = \lfloor \frac{D}{2} \rfloor$.

`<vegas: vegas: TBP>+≡`

`procedure, public :: integrate => vegas_integrate`

```

<vegas: procedures>+≡
subroutine vegas_integrate (self, func, rng, iterations, reset_result,&
    & refine_grid, verbose, result, abserr)
    class(vegas_t), intent(inout) :: self
    class(vegas_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    integer, intent(in), optional :: iterations
    logical, intent(in), optional :: reset_result
    logical, intent(in), optional :: refine_grid
    logical, intent(in), optional :: verbose
    real(default), optional, intent(out) :: result, abserr
    integer :: it, k
    real(default), dimension(self%config%n_dim) :: x
    real(default) :: fval, fval_sq, bin_volume
    real(default) :: fval_box, fval_sq_box
    real(default) :: total_integral, total_sq_integral
    real(default) :: cumulative_int, cumulative_std
    real(default) :: sum_abs_f_pos, max_abs_f_pos
    real(default) :: sum_abs_f_neg, max_abs_f_neg
    logical :: opt_reset_result
    logical :: opt_refine_grid
    logical :: opt_verbose
    integer :: n_size
    integer :: n_dim_par
    logical :: box_success
<vegas: vegas integrate: variables>
    call set_options ()
    call self%init_grid ()
    if (opt_reset_result) call self%result%reset ()
    self%result%it_start = self%result%it_num
    cumulative_int = 0.
    cumulative_std = 0.
    n_dim_par = floor (self%config%n_dim / 2.)
    n_size = 1
<vegas: vegas integrate: init>
    if (opt_verbose) then
        call msg_message ("Results: [it, calls, integral, error, chi^2, eff.]")
    end if
    iteration: do it = 1, self%config%iterations
        self%result%it_num = self%result%it_start + it
        self%d = 0.
        self%box = 1
        self%bin = 1
        total_integral = 0.
        total_sq_integral = 0.
        sum_abs_f_pos = 0.
        max_abs_f_pos = 0.
        sum_abs_f_neg = 0.
        max_abs_f_neg = 0.
        box_success = .true.
        select type (rng)
            type is (rng_stream_t)
                call rng%next_substream ()
            end select

```

```

<vegas: vegas integrate: presampling>
  loop_over_par_boxes: do while (box_success)
    loop_over_perp_boxes: do while (box_success)
      fval_box = 0._default
      fval_sq_box = 0._default
      do k = 1, self%config%calls_per_box
        call self%random_point (rng, x, bin_volume)
        ! Call the function, yeah, call it...
        fval = self%jacobian * bin_volume * func%evaluate (x)
        fval_sq = fval**2
        fval_box = fval_box + fval
        fval_sq_box = fval_sq_box + fval_sq
        if (fval > 0.) then
          max_abs_f_pos = max(abs (fval), max_abs_f_pos)
          sum_abs_f_pos = sum_abs_f_pos + abs(fval)
        else
          max_abs_f_neg = max(abs (fval), max_abs_f_neg)
          sum_abs_f_neg = sum_abs_f_neg + abs(fval)
        end if
        if (self%config%mode /= VEGAS_MODE_STRATIFIED) then
          call self%accumulate_distribution (fval_sq)
        end if
      end do
      fval_sq_box = sqrt (fval_sq_box * self%config%calls_per_box)
      ! (a - b) * (a + b) = a**2 - b**2
      fval_sq_box = (fval_sq_box - fval_box) * (fval_sq_box + fval_box)
      if (fval_sq_box <= 0.0) fval_sq_box = fval_box**2 * epsilon (1.0_default)
      total_integral = total_integral + fval_box
      total_sq_integral = total_sq_integral + fval_sq_box
      if (self%config%mode == VEGAS_MODE_STRATIFIED) then
        call self%accumulate_distribution (fval_sq_box)
      end if
      call increment_box_coord (self%box(n_dim_par + 1:self%config%
        &n_dim), box_success)
    end do loop_over_perp_boxes
    shift: do k = 1, n_size
      call increment_box_coord (self%box(1:n_dim_par), box_success)
      if (.not. box_success) exit shift
    end do shift
  <vegas: vegas integrate: loop>
end do loop_over_par_boxes
<vegas: vegas integrate: postsampling>
associate (result => self%result)
! Compute final results for this iterations
call result%update (total_integral, variance = &
  total_sq_integral / (self%config%calls_per_box - 1._default))
call result%update_efficiency (n_calls = self%config%n_calls, &
  max_pos = max_abs_f_pos, max_neg = max_abs_f_neg, &
  sum_pos = sum_abs_f_pos, sum_neg = sum_abs_f_neg)
cumulative_int = result%sum_int_wgtd / result%sum_wgts
cumulative_std = sqrt (1 / result%sum_wgts)
end associate
if (opt_verbose) then
  write (msg_buffer, "(I0,1x,I0,1x, 4(E24.16E4,1x))") &

```

```

        & it, self%config%n_calls, cumulative_int, cumulative_std, &
        & self%result%chi2, self%result%efficiency
    call msg_message ()
end if
if (opt_refine_grid) then
    call self%refine (average = .true.)
else
    !! Skip grid refinement, but average the (grid) distribution.
    !! \note Now, we always average and dampen the distribution,
    !!         even when not adapting (e.g. final pass).
    call self%average_distribution ()
end if
end do iteration
if (present(result)) result = cumulative_int
if (present(abserr)) abserr = abs(cumulative_std)
contains
<vegas: vegas integrate: procedures>
end subroutine vegas_integrate

```

Set optional arguments of `vegas_integrate`.

```

<vegas: vegas integrate: procedures>≡
subroutine set_options ()
    if (present (iterations)) self%config%iterations = iterations
    opt_reset_result = .true.
    if (present (reset_result)) opt_reset_result = reset_result
    opt_refine_grid = .true.
    if (present (refine_grid)) opt_refine_grid = refine_grid
    opt_verbose = .false.
    if (present (verbose)) opt_verbose = verbose
end subroutine set_options

```

We define additional chunk, which will be used later on for inserting MPI/general MPI code. The code is then removed by additional `noweb` filter if not compiled with the corresponding compiler flag.

Overall variables, some additionally introduced due to the MPI parallelization and needed in sequential version.

```

<vegas: vegas integrate: variables>≡

```

Overall initialization.

```

<vegas: vegas integrate: init>≡

```

Reset all last-iteration results before sampling.

```

<vegas: vegas integrate: presampling>≡

```

Adjust rng between parallel and perpendicular loops.

```

<vegas: vegas integrate: loop>≡

```

```

<vegas: vegas integrate: postsampling>≡

```

Increment the box coordinates by 1. If we reach the largest value for the current axis (starting with the largest dimension number), we reset the counter to 1 and increment the next axis counter by 1. And so on, until we reach the maximum counter value of the axis with the lowest dimension, then we set `success` to false and the box coord is set to 1.

```

<vegas: vegas integrate: procedures>+=

```

```

subroutine increment_box_coord (box, success)
  integer, dimension(:), intent(inout) :: box
  logical, intent(out) :: success
  integer :: j
  success = .true.
  do j = size (box), 1, -1
    box(j) = box(j) + 1
    if (box(j) <= self%config%n_boxes) return
    box(j) = 1
  end do
  success = .false.
end subroutine increment_box_coord

```

We parallelize VEGAS in simple forward manner. The hyper-cube is dissambled in to equidistant boxes in which we sample the integrand `calls_per_box` times. The workload of calculating those boxes is distributed along the worker.

The number of dimensions which will be parallelised are $\lfloor \frac{D}{2} \rfloor$, such MPI Variables for `vegas_integrate`. We have to duplicate all buffers for `MPI_Ireduce`, because we cannot use the same send or receive buffer.

We temporarily store a (empty) grid, before communicating.

(MPI: vegas: vegas integrate: variables)≡

```

integer :: rank
logical :: parallel_mode
type(vegas_grid_t) :: grid

```

MPI procedure-specific initialization.

Allow for (external) veto on parallel mode.

(MPI: vegas: vegas integrate: init)≡

```

parallel_mode = self%parallel_mode .and. self%is_parallelizable ()
if (parallel_mode) then
  call MPI_Comm_size (self%comm, n_size)
  call MPI_Comm_rank (self%comm, rank)
else
  n_size = 1
  rank = 0
end if

```

Pre-sampling communication.

We make a copy of the (actual) grid, which is unfilled when non-root. The actual grid is then broadcasted among the workers and inserted into the VEGAS object.

(MPI: vegas: vegas integrate: presampling)≡

```

if (parallel_mode) then
  grid = self%get_grid ()
  call grid%broadcast (self%comm)
  call self%set_grid (grid)

```

Start index of the boxes for different ranks. If the random number generator is `RngStream`, we can advance the current stream in such a way, that we will getting matching numbers. Iff `n_boxes` is larger than 2, otherwise parallelization is useless.

(MPI: vegas: vegas integrate: presampling)+≡

```

do k = 1, rank
  call increment_box_coord (self%box(1:n_dim_par), box_success)

```

```

        if (.not. box_success) exit
    end do
    select type (rng)
    type is (rng_stream_t)
        call rng%advance_state (self%config%n_dim * self%config%calls_per_box&
            & * self%config%n_boxes**(self%config%n_dim - n_dim_par) * rank)
    end select
end if

```

Increment `n_size` times the box coordinates.

```

<MPI: vegas: vegas integrate: loop>≡
    if (parallel_mode) then
        select type (rng)
        type is (rng_stream_t)
            call rng%advance_state (self%config%n_dim * self%config%calls_per_box&
                & * self%config%n_boxes**(self%config%n_dim - n_dim_par) * (n_size - 1))
        end select
    end if

```

Call to `vegas_integrate_collect`.

```

<MPI: vegas: vegas integrate: postsampling>≡
    if (parallel_mode) then
        call vegas_integrate_collect ()
        if (rank /= 0) cycle iteration
    end if

```

Reduce (in an non-blocking fashion) all sampled information via `MPI_SUM` or `MPI_MAX`.

```

<MPI: vegas: vegas integrate: procedures>≡
    subroutine vegas_integrate_collect ()
        integer :: j
        real(default) :: root_total_integral, root_total_sq_integral
        real(default) :: root_sum_abs_f_pos, root_max_abs_f_pos
        real(default) :: root_sum_abs_f_neg, root_max_abs_f_neg
        real(default), dimension(self%config%n_bins_max, self%config%n_dim) :: root_d
        type(MPI_Request), dimension(self%config%n_dim + 6) :: status
        root_d = 0._default
        root_sum_abs_f_pos = 0._default
        root_sum_abs_f_neg = 0._default
        root_max_abs_f_pos = 0._default
        root_sum_abs_f_neg = 0._default
        root_total_integral = 0._default
        root_total_sq_integral = 0._default
        call MPI_Ireduce (sum_abs_f_pos, root_sum_abs_f_pos, 1, MPI_DOUBLE_PRECISION,&
            & MPI_SUM, 0, self%comm, status(1))
        call MPI_Ireduce (sum_abs_f_neg, root_sum_abs_f_neg, 1, MPI_DOUBLE_PRECISION,&
            & MPI_SUM, 0, self%comm, status(2))
        call MPI_Ireduce (max_abs_f_pos, root_max_abs_f_pos, 1, MPI_DOUBLE_PRECISION,&
            & MPI_MAX, 0, self%comm, status(3))
        call MPI_Ireduce (max_abs_f_neg, root_max_abs_f_neg, 1, MPI_DOUBLE_PRECISION,&
            & MPI_MAX, 0, self%comm, status(4))
        call MPI_Ireduce (total_integral, root_total_integral, 1, MPI_DOUBLE_PRECISION,&
            & MPI_SUM, 0, self%comm, status(5))
        call MPI_Ireduce (total_sq_integral, root_total_sq_integral, 1,&
            & MPI_DOUBLE_PRECISION, MPI_SUM, 0, self%comm, status(6))
    end subroutine

```

```

do j = 1, self%config%n_dim
  call MPI_Ireduce (self%d(1:self%config%n_bins, j), root_d(1:self%config%
    &n_bins, j), self%config%n_bins, MPI_DOUBLE_PRECISION, MPI_SUM, 0,&
    & self%comm, status(6 + j))
end do
call MPI_Waitall (self%config%n_dim + 6, status, MPI_STATUSES_IGNORE)
if (rank == 0) sum_abs_f_pos = root_sum_abs_f_pos
if (rank == 0) sum_abs_f_neg = root_sum_abs_f_neg
if (rank == 0) max_abs_f_pos = root_max_abs_f_pos
if (rank == 0) max_abs_f_neg = root_max_abs_f_neg
if (rank == 0) total_integral = root_total_integral
if (rank == 0) total_sq_integral = root_total_sq_integral
if (rank == 0) self%d = root_d
end subroutine vegas_integrate_collect

```

Obtain a random point inside the n -dimensional hypercube, transform onto the correct interval and calculate the bin volume. The additional factor `n_bins` is already applied to the jacobian (per dimension).

(vegas: vegas: TBP)+≡

```

  procedure, private :: random_point => vegas_random_point

```

(vegas: procedures)+≡

```

subroutine vegas_random_point (self, rng, x, bin_volume)
  class(vegas_t), intent(inout) :: self
  class(rng_t), intent(inout) :: rng
  real(default), dimension(self%config%n_dim), intent(out) :: x
  real(default), intent(out) :: bin_volume
  integer :: j
  real(default) :: r, y, z, bin_width
  bin_volume = 1.
  ndim: do j = 1, self%config%n_dim
    call rng%generate (r)
    z = ((self%box(j) - 1 + r) / self%config%n_boxes) * self%config%n_bins + 1
    self%bin(j) = max (min (int (z), self%config%n_bins), 1)
    if (self%bin(j) == 1) then
      bin_width = self%grid%xi(2, j)
      y = (z - self%bin(j)) * bin_width
    else
      bin_width = self%grid%xi(self%bin(j) + 1, j) - self%grid%xi(self%bin(j), j)
      y = self%grid%xi(self%bin(j), j) + (z - self%bin(j)) * bin_width
    end if
    x(j) = self%grid%x_lower(j) + y * self%grid%delta_x(j)
    bin_volume = bin_volume * bin_width
  end do ndim
end subroutine vegas_random_point

```

Obtain a random point inside the n -dimensional hyper-cube. We neglect stratification and generate the random point in the most simple way. Hence, we do not need to know in which box we are actually sampling. This is useful for only for event generation.

(vegas: vegas: TBP)+≡

```

  procedure, private :: simple_random_point => vegas_simple_random_point

```


<vegas: procedures>+≡

```

subroutine vegas_simple_random_point (self, rng, x, bin_volume)
  class(vegas_t), intent(inout) :: self
  class(rng_t), intent(inout) :: rng
  real(default), dimension(self%config%n_dim), intent(out) :: x
  real(default), intent(out) :: bin_volume
  integer :: j, k
  real(default) :: r, y, z, bin_width
  bin_volume = 1.
  ndim: do j = 1, self%config%n_dim
    call rng%generate (r)
    z = r * self%config%n_bins + 1
    k = max (min (int (z), self%config%n_bins), 1)
    if (k == 1) then
      bin_width = self%grid%xi(2, j)
      y = (z - 1) * bin_width
    else
      bin_width = self%grid%xi(k + 1, j) - self%grid%xi(k, j)
      y = self%grid%xi(k, j) + (z - k) * bin_width
    end if
    x(j) = self%grid%x_lower(j) + y * self%grid%delta_x(j)
    bin_volume = bin_volume * bin_width
  end do ndim
end subroutine vegas_simple_random_point

```

<vegas: vegas: TBP>+≡

```

procedure, private :: accumulate_distribution => vegas_accumulate_distribution

```

<vegas: procedures>+≡

```

subroutine vegas_accumulate_distribution (self, y)
  class(vegas_t), intent(inout) :: self
  real(default), intent(in) :: y
  integer :: j
  do j = 1, self%config%n_dim
    self%d(self%bin(j), j) = self%d(self%bin(j), j) + y
  end do
end subroutine vegas_accumulate_distribution

```

Generate weighted random event.

The weight given by the overall jacobian

$$\Delta_{\text{jac}} = \prod_{j=1}^d (x_j^+ - x_j^-) \frac{N_{\text{bins}}^d}{N_{\text{calls}}} \quad (20.4)$$

includes the overall non-changing factors $\frac{1}{N_{\text{calls}}}$ -factor (divisions are expensive) and N_{bins}^d , the latter combined with `bin_volume` gives rise to the probability, see `vegas_init_grid` for details. We have to factor out N_{calls} to retrieve the correct weight.

<vegas: vegas: TBP>+≡

```

procedure :: generate_weighted => vegas_generate_weighted_event

```

```

<vegas: procedures>+≡
  subroutine vegas_generate_weighted_event (self, func, rng, x)
    class(vegas_t), intent(inout) :: self
    class(vegas_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(inout) :: x
    real(default) :: bin_volume
    call self%simple_random_point (rng, x, bin_volume)
    ! Cancel n_calls from jacobian with n_calls
    self%result%evt_weight = self%config%n_calls * self%jacobian * bin_volume &
      & * func%evaluate (x)
  end subroutine vegas_generate_weighted_event

```

Generate random event. We accept on the rate

$$\frac{|f(x)|}{\max_x |f(x)|}. \quad (20.5)$$

We keep separate maximum weights for positive and negative weights, and use them, accordingly. In the case of unweighted event generation, if the current weight exceeds the the maximum weight, we update the maximum, accordingly.

```

<vegas: vegas: TBP>+≡
  procedure, public :: generate_unweighted=> vegas_generate_unweighted_event

<vegas: procedures>+≡
  subroutine vegas_generate_unweighted_event (self, func, rng, x)
    class(vegas_t), intent(inout) :: self
    class(vegas_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(out) :: x
    real(default) :: bin_volume
    real(default) :: max_abs_f
    real(default) :: r
    associate (result => self%result)
      generate: do
        call self%generate_weighted (func, rng, x)
        max_abs_f = merge (result%max_abs_f_pos, result%max_abs_f_neg, &
          & result%evt_weight > 0.)
        if (result%evt_weight > max_abs_f) then
          result%evt_weight_excess = &
            & result%evt_weight / max_abs_f - 1._default
          exit generate
        end if
        call rng%generate (r)
        ! Do not use division, because max_abs_f could be zero.
        if (max_abs_f * r <= abs(result%evt_weight)) then
          exit generate
        end if
      end do generate
    end associate
  end subroutine vegas_generate_unweighted_event

```

20.11 I/O operation

Write grid to file. We use the original VAMP formatter.

```

<vegas: parameters>+≡
  character(len=*), parameter, private :: &
    descr_fmt =      "(1X,A)", &
    integer_fmt =     "(1X,A18,1X,I15)", &
    integer_array_fmt = "(1X,I18,1X,I15)", &
    logical_fmt =     "(1X,A18,1X,L1)", &
    double_fmt =      "(1X,A18,1X,E24.16E4)", &
    double_array_fmt = "(1X,I18,1X,E24.16E4)", &
    double_array_pac_fmt = "(1X,I18,1X,E16.8E4)", &
    double_array2_fmt = "(1X,2(1X,I8),1X,E24.16E4)", &
    double_array2_pac_fmt = "(1X,2(1X,I8),1X,E16.8E4)"

<vegas: vegas: TBP>+≡
  procedure, public :: write_grid => vegas_write_grid

<vegas: procedures>+≡
  subroutine vegas_write_grid (self, unit)
    class(vegas_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer :: u
    integer :: i, j
    u = given_output_unit (unit)
    write (u, descr_fmt) "begin type(vegas_t)"
    write (u, integer_fmt) "n_dim =", self%config%n_dim
    write (u, integer_fmt) "n_bins_max =", self%config%n_bins_max
    write (u, double_fmt) "alpha =", self%config%alpha
    write (u, integer_fmt) "iterations =", self%config%iterations
    write (u, integer_fmt) "mode =", self%config%mode
    write (u, integer_fmt) "calls_per_box =", self%config%calls_per_box
    write (u, integer_fmt) "n_calls =", self%config%n_calls
    write (u, integer_fmt) "n_calls_min =", self%config%n_calls_min
    write (u, integer_fmt) "n_boxes =", self%config%n_boxes
    write (u, integer_fmt) "n_bins =", self%config%n_bins
    write (u, integer_fmt) "it_start =", self%result%it_start
    write (u, integer_fmt) "it_num =", self%result%it_num
    write (u, integer_fmt) "samples =", self%result%samples
    write (u, double_fmt) "sum_int_wgtd =", self%result%sum_int_wgtd
    write (u, double_fmt) "sum_wgts =", self%result%sum_wgts
    write (u, double_fmt) "sum_chi =", self%result%sum_chi
    write (u, double_fmt) "chi2 =", self%result%chi2
    write (u, double_fmt) "efficiency =", self%result%efficiency
    write (u, double_fmt) "efficiency =", self%result%efficiency_pos
    write (u, double_fmt) "efficiency =", self%result%efficiency_neg
    write (u, double_fmt) "max_abs_f =", self%result%max_abs_f
    write (u, double_fmt) "max_abs_f_pos =", self%result%max_abs_f_pos
    write (u, double_fmt) "max_abs_f_neg =", self%result%max_abs_f_neg
    write (u, double_fmt) "result =", self%result%result
    write (u, double_fmt) "std =", self%result%std
    write (u, double_fmt) "hypercube_volume =", self%hypercube_volume
    write (u, double_fmt) "jacobian =", self%jacobian
    write (u, descr_fmt) "begin x_lower"

```

```

do j = 1, self%config%n_dim
  write (u, double_array_fmt) j, self%grid%x_lower(j)
end do
write (u, descr_fmt) "end x_lower"
write (u, descr_fmt) "begin x_upper"
do j = 1, self%config%n_dim
  write (u, double_array_fmt) j, self%grid%x_upper(j)
end do
write (u, descr_fmt) "end x_upper"
write (u, descr_fmt) "begin delta_x"
do j = 1, self%config%n_dim
  write (u, double_array_fmt) j, self%grid%delta_x(j)
end do
write (u, descr_fmt) "end delta_x"
write (u, integer_fmt) "n_bins =", self%config%n_bins
write (u, descr_fmt) "begin bin"
do j = 1, self%config%n_dim
  write (u, integer_array_fmt) j, self%bin(j)
end do
write (u, descr_fmt) "end n_bin"
write (u, integer_fmt) "n_boxes =", self%config%n_boxes
write (u, descr_fmt) "begin box"
do j = 1, self%config%n_dim
  write (u, integer_array_fmt) j, self%box(j)
end do
write (u, descr_fmt) "end box"
write (u, descr_fmt) "begin d"
do j = 1, self%config%n_dim
  do i = 1, self%config%n_bins_max
    write (u, double_array2_fmt) i, j, self%d(i, j)
  end do
end do
write (u, descr_fmt) "end d"
write (u, descr_fmt) "begin xi"
do j = 1, self%config%n_dim
  do i = 1, self%config%n_bins_max + 1
    write (u, double_array2_fmt) i, j, self%grid%xi(i, j)
  end do
end do
write (u, descr_fmt) "end xi"
write (u, descr_fmt) "end type(vegas_t)"
end subroutine vegas_write_grid

```

Read grid configuration from file.

```

<vegas: vegas: TBP>+≡
  procedure, public :: read_grid => vegas_read_grid

<vegas: procedures>+≡
  subroutine vegas_read_grid (self, unit)
    class(vegas_t), intent(out) :: self
    integer, intent(in) :: unit
    integer :: i, j
    character(len=80) :: buffer
    integer :: ibuffer, jbuffer

```

```

read (unit, descr_fmt) buffer
read (unit, integer_fmt) buffer, ibuffer
read (unit, integer_fmt) buffer, jbuffer
select type(self)
type is (vegas_t)
    self = vegas_t (n_dim = ibuffer, n_bins_max = jbuffer)
end select
read (unit, double_fmt) buffer, self%config%alpha
read (unit, integer_fmt) buffer, self%config%iterations
read (unit, integer_fmt) buffer, self%config%mode
read (unit, integer_fmt) buffer, self%config%calls_per_box
read (unit, integer_fmt) buffer, self%config%n_calls
read (unit, integer_fmt) buffer, self%config%n_calls_min
read (unit, integer_fmt) buffer, self%config%n_boxes
read (unit, integer_fmt) buffer, self%config%n_bins
self%grid%n_bins = self%config%n_bins
read (unit, integer_fmt) buffer, self%result%it_start
read (unit, integer_fmt) buffer, self%result%it_num
read (unit, integer_fmt) buffer, self%result%samples
read (unit, double_fmt) buffer, self%result%sum_int_wgtd
read (unit, double_fmt) buffer, self%result%sum_wgts
read (unit, double_fmt) buffer, self%result%sum_chi
read (unit, double_fmt) buffer, self%result%chi2
read (unit, double_fmt) buffer, self%result%efficiency
read (unit, double_fmt) buffer, self%result%efficiency_pos
read (unit, double_fmt) buffer, self%result%efficiency_neg
read (unit, double_fmt) buffer, self%result%max_abs_f
read (unit, double_fmt) buffer, self%result%max_abs_f_pos
read (unit, double_fmt) buffer, self%result%max_abs_f_neg
read (unit, double_fmt) buffer, self%result%result
read (unit, double_fmt) buffer, self%result%std
read (unit, double_fmt) buffer, self%hypercube_volume
read (unit, double_fmt) buffer, self%jacobian
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, double_array_fmt) jbuffer, self%grid%x_lower(j)
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, double_array_fmt) jbuffer, self%grid%x_upper(j)
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, double_array_fmt) jbuffer, self%grid%delta_x(j)
end do
read (unit, descr_fmt) buffer
read (unit, integer_fmt) buffer, self%config%n_bins
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, integer_array_fmt) jbuffer, self%bin(j)
end do
read (unit, descr_fmt) buffer

```

```

read (unit, integer_fmt) buffer, self%config%n_boxes
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    read (unit, integer_array_fmt) jbuffer, self%box(j)
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    do i = 1, self%config%n_bins_max
        read (unit, double_array2_fmt) ibuffer, jbuffer, self%d(i, j)
    end do
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
do j = 1, self%config%n_dim
    do i = 1, self%config%n_bins_max + 1
        read (unit, double_array2_fmt) ibuffer, jbuffer, self%grid%xi(i, j)
    end do
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
end subroutine vegas_read_grid

```

Read and write a grid from an unformatted file.

<vegas: vegas: TBP>+≡

```

procedure :: write_binary_grid => vegas_write_binary_grid
procedure :: read_binary_grid => vegas_read_binary_grid

```

<vegas: procedures>+≡

```

subroutine vegas_write_binary_grid (self, unit)
    class(vegas_t), intent(in) :: self
    integer, intent(in) :: unit
    integer :: i, j
    write (unit) self%config%n_dim
    write (unit) self%config%n_bins_max
    write (unit) self%config%alpha
    write (unit) self%config%iterations
    write (unit) self%config%mode
    write (unit) self%config%calls_per_box
    write (unit) self%config%n_calls
    write (unit) self%config%n_calls_min
    write (unit) self%config%n_boxes
    write (unit) self%config%n_bins
    write (unit) self%result%it_start
    write (unit) self%result%it_num
    write (unit) self%result%samples
    write (unit) self%result%sum_int_wgtd
    write (unit) self%result%sum_wgts
    write (unit) self%result%sum_chi
    write (unit) self%result%chi2
    write (unit) self%result%efficiency
    write (unit) self%result%efficiency_pos
    write (unit) self%result%efficiency_neg
    write (unit) self%result%max_abs_f

```

```

write (unit) self%result%max_abs_f_pos
write (unit) self%result%max_abs_f_neg
write (unit) self%result%result
write (unit) self%result%std
write (unit) self%hypercube_volume
write (unit) self%jacobian
do j = 1, self%config%n_dim
  write (unit) j, self%grid%x_lower(j)
end do
do j = 1, self%config%n_dim
  write (unit) j, self%grid%x_upper(j)
end do
do j = 1, self%config%n_dim
  write (unit) j, self%grid%delta_x(j)
end do
write (unit) self%config%n_bins
do j = 1, self%config%n_dim
  write (unit) j, self%bin(j)
end do
write (unit) self%config%n_boxes
do j = 1, self%config%n_dim
  write (unit) j, self%box(j)
end do
do j = 1, self%config%n_dim
  do i = 1, self%config%n_bins_max
    write (unit) i, j, self%d(i, j)
  end do
end do
do j = 1, self%config%n_dim
  do i = 1, self%config%n_bins_max + 1
    write (unit) i, j, self%grid%xi(i, j)
  end do
end do
end subroutine vegas_write_binary_grid

subroutine vegas_read_binary_grid (self, unit)
  class(vegas_t), intent(out) :: self
  integer, intent(in) :: unit
  integer :: i, j
  integer :: ibuffer, jbuffer
  read (unit) ibuffer
  read (unit) jbuffer
  select type(self)
  type is (vegas_t)
    self = vegas_t (n_dim = ibuffer, n_bins_max = jbuffer)
  end select
  read (unit) self%config%alpha
  read (unit) self%config%iterations
  read (unit) self%config%mode
  read (unit) self%config%calls_per_box
  read (unit) self%config%n_calls
  read (unit) self%config%n_calls_min
  read (unit) self%config%n_boxes
  read (unit) self%config%n_bins

```

```

self%grid%n_bins = self%config%n_bins
read (unit) self%result%it_start
read (unit) self%result%it_num
read (unit) self%result%samples
read (unit) self%result%sum_int_wgtd
read (unit) self%result%sum_wgts
read (unit) self%result%sum_chi
read (unit) self%result%chi2
read (unit) self%result%efficiency
read (unit) self%result%efficiency_pos
read (unit) self%result%efficiency_neg
read (unit) self%result%max_abs_f
read (unit) self%result%max_abs_f_pos
read (unit) self%result%max_abs_f_neg
read (unit) self%result%result
read (unit) self%result%std
read (unit) self%hypercube_volume
read (unit) self%jacobian
do j = 1, self%config%n_dim
    read (unit) jbuffer, self%grid%x_lower(j)
end do
do j = 1, self%config%n_dim
    read (unit) jbuffer, self%grid%x_upper(j)
end do
do j = 1, self%config%n_dim
    read (unit) jbuffer, self%grid%delta_x(j)
end do
read (unit) self%config%n_bins
do j = 1, self%config%n_dim
    read (unit) jbuffer, self%bin(j)
end do
read (unit) self%config%n_boxes
do j = 1, self%config%n_dim
    read (unit) jbuffer, self%box(j)
end do
do j = 1, self%config%n_dim
    do i = 1, self%config%n_bins_max
        read (unit) ibuffer, jbuffer, self%d(i, j)
    end do
end do
do j = 1, self%config%n_dim
    do i = 1, self%config%n_bins_max + 1
        read (unit) ibuffer, jbuffer, self%grid%xi(i, j)
    end do
end do
end subroutine vegas_read_binary_grid

```

20.12 Unit tests

Test module, followed by the corresponding implementation module.

(vegas.ut.f90)≡


```

<File header>

module vegas_ut
  use unit_tests
  use vegas_util

<Standard module head>

<vegas: public test>

contains
  <vegas: test driver>
end module vegas_ut

<vegas_util.f90>≡
<File header>

module vegas_util
  <Use kinds>
  use io_units
  use constants, only: pi
  use format_defs, only: FMT_10, FMT_12
  use rng_base
  use rng_stream
  use vegas

<Standard module head>

<vegas: test declaration>

<vegas: test types>

contains
  <vegas: tests>
end module vegas_util
API: driver for the unit tests below.
<vegas: public test>≡
  public :: vegas_test
<vegas: test driver>≡
  subroutine vegas_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <vegas: execute tests>
  end subroutine vegas_test

```

Test function

We use the example from the Monte Carlo Examples of the GSL library

$$I = \int_{-pi}^{+pi} dk_x / (2pi) \int_{-pi}^{+pi} dk_y / (2pi) \int_{-pi}^{+pi} dk_z / (2pi) 1 / (1 - \cos(k_x) \cos(k_y) \cos(k_z)). \quad (20.6)$$

The integral is reduced to region $(0,0,0) \rightarrow (\pi, \pi, \pi)$ and multiplied by 8.

```

<vegas: test types>≡
  type, extends (vegas_func_t) :: vegas_test_func_t
  !
  contains
    <vegas: vegas test func: TBP>
  end type vegas_test_func_t

```

Evaluate the integrand.

```

<vegas: vegas test func: TBP>≡
  procedure, public :: evaluate => vegas_test_func_evaluate

<vegas: tests>≡
  real(default) function vegas_test_func_evaluate (self, x) result (f)
    class(vegas_test_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    f = 1.0 / (pi**3)
    f = f / ( 1.0 - cos (x(1)) * cos (x(2)) * cos (x(3)))
  end function vegas_test_func_evaluate

```

The second test function is the normalised n-dim. gaussian distribution.

```

<vegas: test types>+≡
  type, extends (vegas_func_t) :: vegas_gaussian_test_func_t
  !
  contains
    <vegas: vegas gaussian test func: TBP>
  end type vegas_gaussian_test_func_t

```

Evaluate the integrand.

```

<vegas: vegas gaussian test func: TBP>≡
  procedure, public :: evaluate => vegas_gaussian_evaluate

<vegas: tests>+≡
  real(default) function vegas_gaussian_evaluate (self, x) result (f)
    class(vegas_gaussian_test_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    real(default), parameter :: inv_sqrt_pi = 1._default / sqrt(pi)
    f = inv_sqrt_pi**size (x)
    f = f * exp (- dot_product(x, x))
  end function vegas_gaussian_evaluate

```

The third test function is a three-dimensional polynomial function which factorises. The function is defined in such a way that the integral in the unit range is normalised to zero.

$$f(x) = -\frac{8}{3}(x+1) * (y-1) * z \quad (20.7)$$

```

<vegas: test types>+≡
  type, extends (vegas_func_t) :: vegas_polynomial_func_t
  !
  contains
    <vegas: vegas polynomial func: TBP>
  end type vegas_polynomial_func_t

```

```

<vegas: vegas polynomial func: TBP>≡
    procedure, public :: evaluate => vegas_polynomial_evaluate

<vegas: tests>+≡
    real(default) function vegas_polynomial_evaluate (self, x) result (f)
        class(vegas_polynomial_func_t), intent(inout) :: self
        real(default), dimension(:), intent(in) :: x
        f = - 8. / 3. * (x(1) + 1.) * (x(2) - 1.) * x(3)
    end function vegas_polynomial_evaluate

```

MC Integrator check

Initialise the VEGAS MC integrator and call to `vegas_init_grid` for the initialisation of the grid.

```

<vegas: execute tests>≡
    call test (vegas_1, "vegas_1", "VEGAS initialisation and&
        & grid preparation", u, results)

<vegas: test declaration>≡
    public :: vegas_1

<vegas: tests>+≡
    subroutine vegas_1 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vegas_func_t), allocatable :: func
        real(default), dimension(3), parameter :: x_lower = 0., &
            x_upper = pi
        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vegas_1"
        write (u, "(A)") "* Purpose: initialise the VEGAS MC integrator and the grid"
        write (u, "(A)")

        write (u, "(A)") "* Initialise random number generator (default seed)"
        write (u, "(A)")

        allocate (rng_stream_t :: rng)
        call rng%init ()

        call rng%write (u)

        write (u, "(A)")
        write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
        write (u, "(A)")

        allocate (vegas_test_func_t :: func)
        mc_integrator = vegas_t (3)

        write (u, "(A)")
        write (u, "(A)") "* Initialise grid with n_calls = 10000"
        write (u, "(A)")

```

```

call mc_integrator%set_limits (x_lower, x_upper)
call mc_integrator%set_calls (10000)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vegas_1

```

Configuration and result check

Initialise the MC integrator. Get and write the config object, also the (empty) result object.

```

<vegas: execute tests>+≡
    call test (vegas_2, "vegas_2", "VEGAS configuration and result object", u, results)

<vegas: test declaration>+≡
    public :: vegas_2

<vegas: tests>+≡
    subroutine vegas_2 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        type(vegas_config_t) :: mc_integrator_config
        type(vegas_result_t) :: mc_integrator_result

        write (u, "(A)") "* Test output: vegas_2"
        write (u, "(A)") "* Purpose: use transparent containers for&
            & configuration and result."
        write (u, "(A)")

        write (u, "(A)")
        write (u, "(A)") "* Initialise MC integrator with n_dim = 10"
        write (u, "(A)")

        mc_integrator = vegas_t (10)

```

```

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 10000 (Importance Sampling)"
write (u, "(A)")

call mc_integrator%set_calls (10000)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS config object and write out"
write (u, "(A)")

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS empty result object and write out"
write (u, "(A)")

mc_integrator_result = mc_integrator%get_result ()
call mc_integrator_result%write (u)

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_2

```

Grid check

Initialise the MC integrator. Get and write the config object. Integrate the gaussian distribution. Get and write the result object. Before and after integration get the grid object and output both. Repeat with different number of dimensions.

```

<vegas: execute tests>+≡
    call test (vegas_3, "vegas_3", "VEGAS integration of multi-dimensional gaussian", u, results)
<vegas: test declaration>+≡
    public :: vegas_3
<vegas: tests>+≡
    subroutine vegas_3 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vegas_func_t), allocatable :: func
        real(default), dimension(3), parameter :: x_lower_3 = -10._default, &
            x_upper_3 = 10._default
        type(vegas_config_t) :: mc_integrator_config
        type(vegas_grid_t) :: mc_integrator_grid
        type(vegas_result_t) :: mc_integrator_result

        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vegas_3"
        write (u, "(A)") "* Purpose: Integrate gaussian distribution."

```

```

write (u, "(A)")

allocate (rng_stream_t :: rng)
call rng%init ()

call rng%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
write (u, "(A)")

allocate (vegas_gaussian_test_func_t :: func)
mc_integrator = vegas_t (3)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 10000"
write (u, "(A)")

call mc_integrator%set_limits (x_lower_3, x_upper_3)
call mc_integrator%set_calls (10000)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS config object and write out"
write (u, "(A)")

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS grid object and write out"
write (u, "(A)")

mc_integrator_grid = mc_integrator%get_grid ()
call mc_integrator_grid%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 20000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

```

```

write (u, "(A)")
write (u, "(A)") "* Get VEGAS result object and write out"
write (u, "(A)")

mc_integrator_result = mc_integrator%get_result ()
call mc_integrator_result%write (u)

write (u, "(A)")
write (u, "(A)") "* Get VEGAS grid object and write out"
write (u, "(A)")

mc_integrator_grid = mc_integrator%get_grid ()
call mc_integrator_grid%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_3

```

Three-dimensional integration with polynomial function

Initialise the MC integrator. Get and write the config object. Integrate the factorisable polynomial function. Get and write the result object. Repeat with different number of dimensions.

```

<vegas: execute tests>+≡
  call test (vegas_4, "vegas_4", "VEGAS integration of three&
    &-dimensional factorisable polynomial function", u, results)

<vegas: test declaration>+≡
  public :: vegas_4

<vegas: tests>+≡
  subroutine vegas_4 (u)
    integer, intent(in) :: u
    type(vegas_t) :: mc_integrator
    class(rng_t), allocatable :: rng
    class(vegas_func_t), allocatable :: func
    real(default), dimension(3), parameter :: x_lower_3 = 0._default, &
      x_upper_3 = 1._default
    type(vegas_config_t) :: mc_integrator_config
    type(vegas_result_t) :: mc_integrator_result

    real(default) :: result, abserr

    write (u, "(A)") "* Test output: vegas_4"
    write (u, "(A)") "* Purpose: Integrate gaussian distribution."
    write (u, "(A)")

    allocate (rng_stream_t :: rng)
    call rng%init ()

```

```

call rng%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
write (u, "(A)")

allocate (vegas_polynomial_func_t :: func)
mc_integrator = vegas_t (3)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 2000"
write (u, "(A)")

call mc_integrator%set_limits (x_lower_3, x_upper_3)
call mc_integrator%set_calls (2000)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")

write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 20000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (20000)

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_4

```

Event generation

Initialise the MC integrator. Integrate the gaussian distribution. Get and write the result object. Finally, generate events in accordance to the adapted grid

and print them out.

```

<vegas: execute tests>+≡
    call test (vegas_5, "vegas_5", "VEGAS integration and event&
        & generation of multi-dimensional gaussian", u, results)

<vegas: test declaration>+≡
    public :: vegas_5

<vegas: tests>+≡
    subroutine vegas_5 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vegas_func_t), allocatable :: func
        real(default), dimension(1), parameter :: x_lower_1 = -10._default, &
            x_upper_1 = 10._default
        type(vegas_config_t) :: mc_integrator_config
        type(vegas_result_t) :: mc_integrator_result

        integer :: i, u_event
        real(default), dimension(1) :: event, mean, delta, M2
        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vegas_5"
        write (u, "(A)") "* Purpose: Integrate gaussian distribution."
        write (u, "(A)")

        allocate (rng_stream_t :: rng)
        call rng%init ()

        call rng%write (u)

        write (u, "(A)")
        write (u, "(A)") "* Initialise MC integrator with n_dim = 1"
        write (u, "(A)")

        allocate (vegas_gaussian_test_func_t :: func)
        mc_integrator = vegas_t (1)

        write (u, "(A)")
        write (u, "(A)") "* Initialise grid with n_calls = 20000"
        write (u, "(A)")

        call mc_integrator%set_limits (x_lower_1, x_upper_1)
        call mc_integrator%set_calls (20000)

        write (u, "(A)")
        write (u, "(A)") "* Integrate with n_it = 3 (Adaptation)"
        write (u, "(A)")

        call mc_integrator%integrate (func, rng, 3, verbose=.true., result=result, abserr=abserr)
        call mc_integrator%get_config (mc_integrator_config)
        call mc_integrator_config%write (u)
        write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") &
            & "Result: ", result, " +/- ", abserr

```

```

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%integrate (func, rng, 3, verbose=.true., result=result, abserr=abserr)
call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") &
    & "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Generate 10000 events based on the adaptation and&
    & calculate mean and variance"
write (u, "(A)")

mean = 0._default
M2 = 0._default
do i = 1, 10000
    call mc_integrator%generate_unweighted (func, rng, event)
    delta = event - mean
    mean = mean + delta / i
    M2 = M2 + delta * (event - mean)
end do

write (u, "(2X,A)") "Result:"
write (u, "(4X,A," // FMT_12 // ")") &
    & "mean          = ", mean
write (u, "(4X,A," // FMT_12 // ")") &
    & "(sample) std. dev. = ", sqrt (M2 / (9999))

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_5

```

Grid I/O

Initialise the MC integrator. Get and write the config object. Integrate the factorisable polynomial function. Get and write the result object. Write grid to file and start with fresh grid.

```

<vegas: execute tests>+≡
    call test (vegas_6, "vegas_6", "VEGAS integrate and write grid, &
        & read grid and continue", u, results)

<vegas: test declaration>+≡
    public :: vegas_6

<vegas: tests>+≡
    subroutine vegas_6 (u)
        integer, intent(in) :: u

```

```

type(vegas_t) :: mc_integrator
class(rng_t), allocatable :: rng
class(vegas_func_t), allocatable :: func
real(default), dimension(3), parameter :: x_lower_3 = 0._default, &
      x_upper_3 = 1._default
type(vegas_config_t) :: mc_integrator_config
type(vegas_result_t) :: mc_integrator_result

real(default) :: result, abserr
integer :: unit

write (u, "(A)") "* Test output: vegas_6"
write (u, "(A)") "* Purpose: Write and read grid, and continue."
write (u, "(A)")

allocate (rng_stream_t :: rng)
call rng%init ()

call rng%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
write (u, "(A)")

allocate (vegas_polynomial_func_t :: func)
mc_integrator = vegas_t (3)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 2000"
write (u, "(A)")

call mc_integrator%set_limits (x_lower_3, x_upper_3)
call mc_integrator%set_calls (2000)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")

write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Write grid to file vegas_io.grid"
write (u, "(A)")

unit = free_unit ()
open (unit, file = "vegas_io.grid", &
      action = "write", status = "replace")

```

```

call mc_integrator%write_grid (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Read grid from file vegas_io.grid"
write (u, "(A)")

call mc_integrator%final ()
open (unit, file = "vegas_io.grid", &
      action = "read", status = "old")
call mc_integrator%read_grid (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 20000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (20000)

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)

call mc_integrator%get_config (mc_integrator_config)
call mc_integrator_config%write (u)

write (u, "(A)")
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
end subroutine vegas_6

```

Numeric stability

We wrap a previous testing function to produce a single NaN.

```

<vegas: test types>+≡
  type, extends (vegas_test_func_t) :: vegas_nan_test_func_t
  private
  logical :: evaluate_to_nan = .true.
  contains
  <vegas: vegas nan test func: TBP>
end type vegas_nan_test_func_t

```

Evaluate the integrand.

```

<vegas: vegas nan test func: TBP>≡
  procedure, public :: evaluate => vegas_nan_test_func_evaluate

<vegas: tests>+≡
  real(default) function vegas_nan_test_func_evaluate (self, x) result (f)
  use, intrinsic :: ieee_arithmetic, only: ieee_value, ieee_quiet_nan
  class(vegas_nan_test_func_t), intent(inout) :: self

```

```

real(default), dimension(:), intent(in) :: x
if (self%evaluate_to_nan) then
    f = ieee_value(1.0_default, ieee_quiet_nan)
    self%evaluate_to_nan = .false.
else
    f = self%vegas_test_func_t%evaluate (x)
end if
end function vegas_nan_test_func_evaluate

```

Initialise the VEGAS MC integrator. Run a integration pass and insert a single NaN that leads to a NaN result. However, the integration grid will be fine.

Proceed with a second pass, and get the correct result.

```

<vegas: execute tests>+≡
    !!! Disabled for the moment as NAGFOR stops execution on NaNs as intended
    ! call test (vegas_7, "vegas_7", "VEGAS NaN stability test", u, results)

<vegas: test declaration>+≡
    public :: vegas_7

<vegas: tests>+≡
    subroutine vegas_7 (u)
        integer, intent(in) :: u
        type(vegas_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vegas_func_t), allocatable :: func
        real(default), dimension(3), parameter :: x_lower = 0., &
            x_upper = pi
        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vegas_7"
        write (u, "(A)") "* Purpose: initialise the VEGAS MC integrator and the grid"
        write (u, "(A)")

        write (u, "(A)") "* Initialise random number generator (default seed)"
        write (u, "(A)")

        allocate (rng_stream_t :: rng)
        call rng%init ()

        call rng%write (u)

        write (u, "(A)")
        write (u, "(A)") "* Initialise MC integrator with n_dim = 3"
        write (u, "(A)")

        allocate (vegas_nan_test_func_t :: func)
        mc_integrator = vegas_t (3)

        write (u, "(A)")
        write (u, "(A)") "* Initialise grid with n_calls = 10000"
        write (u, "(A)")

        call mc_integrator%set_limits (x_lower, x_upper)
        call mc_integrator%set_calls (10000)

```

```

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (2000)
call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vegas_7

```

20.13 VAMP2

We concentrate all configuration and run-time data in a derived-type, such that, `mci_t` can spawn each time a distinctive MCI VEGAS integrator object.

```
<vamp2.f90>≡  
  <File header>  
  
  module vamp2  
  
    <Use kinds>  
    use io_units  
    use format_utils, only: pac_fmt  
    use format_utils, only: write_separator, write_indent  
    use format_defs, only: FMT_17  
    use diagnostics  
    use iterator  
    use rng_base  
    use rng_stream, only: rng_stream_t  
  
    use vegas  
  
    <vamp2: modules>  
  
    <Standard module head>  
  
    <vamp2: public>  
  
    <vamp2: parameters>  
  
    <vamp2: types>  
  
    <vamp2: interfaces>  
  
    contains  
  
    <vamp2: procedures>  
  
  end module vamp2  
<vamp2: modules>≡  
<MPI: vamp2: modules>≡  
  use request_base  
  use request_simple  
  use request_caller  
  use balancer_base  
  use request_callback  
  use mpi_f08 !NODEP!
```

20.13.1 Type: `vamp2_func_t`

We extend `vegas_func_t` with the multi-channel weights and the `vegas_grid_t`, such that, the overall multi-channel weight can be calculated by the function itself.

We add an additional logical `valid_x`, if it is set to `.false.`, we do not compute weighted function and just set the weighted integrand to zero. This behavior is in particular very useful, if a mapping is prohibited or fails. Or in the case of WHIZARD, a phase cut is applied.

```

<vamp2: public>≡
  public :: vamp2_func_t

<vamp2: types>≡
  type, abstract, extends(vegas_func_t) :: vamp2_func_t
    integer :: current_channel = 0
    integer :: n_dim = 0
    integer :: n_channel = 0
    integer :: n_calls = 0
    logical :: valid_x = .false.
    real(default), dimension(:, :), allocatable :: xi
    real(default), dimension(:), allocatable :: det
    real(default), dimension(:), allocatable :: wi
    real(default), dimension(:), allocatable :: gi
    type(vegas_grid_t), dimension(:), allocatable :: grids
    real(default) :: g = 0.
  contains
    <vamp2: vamp2_func: TBP>
  end type vamp2_func_t

```

Init.

```

<vamp2: vamp2_func: TBP>≡
  procedure, public :: init => vamp2_func_init

<vamp2: procedures>≡
  subroutine vamp2_func_init (self, n_dim, n_channel)
    class(vamp2_func_t), intent(out) :: self
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
    self%n_dim = n_dim
    self%n_channel = n_channel
    allocate (self%xi(n_dim, n_channel), source=0._default)
    allocate (self%det(n_channel), source=1._default)
    allocate (self%wi(n_channel), source=0._default)
    allocate (self%gi(n_channel), source=0._default)
    allocate (self%grids(n_channel))
  end subroutine vamp2_func_init

```

Set current channel.

```

<vamp2: vamp2_func: TBP>+≡
  procedure, public :: set_channel => vamp2_func_set_channel

<vamp2: procedures>+≡
  subroutine vamp2_func_set_channel (self, channel)
    class(vamp2_func_t), intent(inout) :: self
    integer, intent(in) :: channel
    self%current_channel = channel
  end subroutine vamp2_func_set_channel

```


Get number of function calls for which $f \neq 0$.

```

<vamp2: vamp2 func: TBP>+≡
  procedure, public :: get_n_calls => vamp2_func_get_n_calls

<vamp2: procedures>+≡
  integer function vamp2_func_get_n_calls (self) result (n_calls)
    class(vamp2_func_t), intent(in) :: self
    n_calls = self%n_calls
  end function vamp2_func_get_n_calls

```

Reset number of calls.

```

<vamp2: vamp2 func: TBP>+≡
  procedure, public :: reset_n_calls => vamp2_func_reset_n_calls

<vamp2: procedures>+≡
  subroutine vamp2_func_reset_n_calls (self)
    class(vamp2_func_t), intent(inout) :: self
    self%n_calls = 0
  end subroutine vamp2_func_reset_n_calls

```

Evaluate mappings. We defer this method to be implemented by the user. The result must be written to `xi` and `det`.

The mapping is defined by $\phi : U \rightarrow M$. We map $x \in M$ to the different mappings of the hypercube U_i , such that $x_i \in U_i$.

The mapping should determine, whether `x` is a valid point, e.g. can be mapped, or is restricted otherwise.

```

<vamp2: vamp2 func: TBP>+≡
  procedure(vamp2_func_evaluate_maps), deferred :: evaluate_maps

<vamp2: interfaces>≡
  abstract interface
    subroutine vamp2_func_evaluate_maps (self, x)
      import :: vamp2_func_t, default
      class(vamp2_func_t), intent(inout) :: self
      real(default), dimension(:), intent(in) :: x
    end subroutine vamp2_func_evaluate_maps
  end interface

```

Evaluate channel weights.

The calling procedure must handle the case of a vanishing overall probability density where either a channel weight or a channel probability vanishes.

```

<vamp2: vamp2 func: TBP>+≡
  procedure, private :: evaluate_weight => vamp2_func_evaluate_weight

<vamp2: procedures>+≡
  subroutine vamp2_func_evaluate_weight (self)
    class(vamp2_func_t), intent(inout) :: self
    integer :: ch
    self%g = 0.
    self%gi = 0.
    !$OMP PARALLEL DO PRIVATE(ch) SHARED(self)
    do ch = 1, self%n_channel
      if (self%wi(ch) /= 0) then

```

```

        self%gi(ch) = self%grids(ch)%get_probability (self%xi(:, ch))
    end if
end do
!$OMP END PARALLEL DO
if (self%gi(self%current_channel) /= 0) then
    do ch = 1, self%n_channel
        if (self%wi(ch) /= 0 .and. self%det(ch) /= 0) then
            self%g = self%g + self%wi(ch) * self%gi(ch) / self%det(ch)
        end if
    end do
    self%g = self%g / self%gi(self%current_channel)
end if
end subroutine vamp2_func_evaluate_weight

```

Evaluate function at x. We call this procedure in `vamp2_func_evaluate`.

```

<vamp2: vamp2 func: TBP>+≡
    procedure(vamp2_func_evaluate_func), deferred :: evaluate_func

<vamp2: interfaces>+≡
    abstract interface
        real(default) function vamp2_func_evaluate_func (self, x) result (f)
            import :: vamp2_func_t, default
            class(vamp2_func_t), intent(in) :: self
            real(default), dimension(:), intent(in) :: x
        end function vamp2_func_evaluate_func
    end interface

<vamp2: vamp2 func: TBP>+≡
    procedure, public :: evaluate => vamp2_func_evaluate

<vamp2: procedures>+≡
    real(default) function vamp2_func_evaluate (self, x) result (f)
        class(vamp2_func_t), intent(inout) :: self
        real(default), dimension(:), intent(in) :: x
        call self%evaluate_maps (x)
        f = 0.
        self%gi = 0.
        self%g = 1
        if (self%valid_x) then
            call self%evaluate_weight ()
            if (self%g /= 0) then
                f = self%evaluate_func (x) / self%g
                self%n_calls = self%n_calls + 1
            end if
        end if
    end function vamp2_func_evaluate

```

20.13.2 Type: `vamp2_config_t`

This is a transparent container which incorporates and extends the definitions in `vegas_config`. The parent object can then be used to parametrise the VEGAS grids directly, where the new parameters are exclusively used in

the multi-channel implementation of VAMP2. `n_calls_min` is calculated by `n_calls_min_per_channel` and `n_channel`. The channels weights (and the result `n_calls` for each channel) are calculated regarding `n_calls_threshold`.

```

<vamp2: public>+≡
    public :: vamp2_config_t

<vamp2: types>+≡
    type, extends(vegas_config_t) :: vamp2_config_t
        integer :: n_channel = 0
        integer :: n_calls_min_per_channel = 20
        integer :: n_calls_threshold = 10
        integer :: n_chains = 0
        logical :: stratified = .true.
        logical :: equivalences = .false.
        real(default) :: beta = 0.5_default
        real(default) :: accuracy_goal = 0._default
        real(default) :: error_goal = 0._default
        real(default) :: rel_error_goal = 0._default
    contains
        <vamp2: vamp2 config: TBP>
    end type vamp2_config_t

```

Write.

```

<vamp2: vamp2 config: TBP>≡
    procedure, public :: write => vamp2_config_write

<vamp2: procedures>+≡
    subroutine vamp2_config_write (self, unit, indent)
        class(vamp2_config_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        integer :: u, ind
        u = given_output_unit (unit)
        ind = 0; if (present (indent)) ind = indent
        call self%vegas_config_t%write (unit, indent)
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Number of channels" = ", self%n_channel
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Min. number of calls per channel (setting calls) = ", &
            & self%n_calls_min_per_channel
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Threshold number of calls (adapting weights) = ", &
            & self%n_calls_threshold
        call write_indent (u, ind)
        write (u, "(2x,A,I0)") &
            & "Number of chains" = ", self%n_chains
        call write_indent (u, ind)
        write (u, "(2x,A,L1)") &
            & "Stratified" = ", self%stratified
        call write_indent (u, ind)
        write (u, "(2x,A,L1)") &

```

```

        & "Equivalences
call write_indent (u, ind)
write (u, "(2x,A," // FMT_17 // ")") &
        & "Adaption power (beta)
if (self%accuracy_goal > 0) then
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
        & "accuracy_goal
end if
if (self%error_goal > 0) then
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
        & "error_goal
end if
if (self%rel_error_goal > 0) then
    call write_indent (u, ind)
    write (u, "(2x,A," // FMT_17 // ")") &
        & "rel_error_goal
end if
end subroutine vamp2_config_write
= ", self%equivalences
= ", self%beta
= ", self%accuracy_goal
= ", self%error_goal
= ", self%rel_error_goal

```

20.13.3 Type: vamp2_result_t

This is a transparent container which incorporates and extends the definitions of `vegas_result_t`.

```

<vamp2: public>+≡
    public :: vamp2_result_t

<vamp2: types>+≡
    type, extends(vegas_result_t) :: vamp2_result_t
    contains
    <vamp2: vamp2 result: TBP>
end type vamp2_result_t

```

Output.

```

<vamp2: vamp2 result: TBP>≡
    procedure, public :: write => vamp2_result_write

<vamp2: procedures>+≡
    subroutine vamp2_result_write (self, unit, indent)
        class(vamp2_result_t), intent(in) :: self
        integer, intent(in), optional :: unit
        integer, intent(in), optional :: indent
        integer :: u, ind
        u = given_output_unit (unit)
        ind = 0; if (present (indent)) ind = indent
        call self%vegas_result_t%write (unit, indent)
    end subroutine vamp2_result_write

```

20.13.4 Type: vamp2_equivalences_t

```
<vamp2: parameters>≡  
  integer, parameter, public :: &  
    VEQ_IDENTITY = 0, VEQ_INVERT = 1, VEQ_SYMMETRIC = 2, VEQ_INVARIANT = 3
```

Channel equivalences. Store retrieving and sourcing channel.

```
<vamp2: types>+≡  
  type :: vamp2_equi_t  
    integer :: ch  
    integer :: ch_src  
    integer, dimension(:), allocatable :: perm  
    integer, dimension(:), allocatable :: mode  
    contains  
    <vamp2: vamp2 equi: TBP>  
  end type vamp2_equi_t
```

Write equivalence.

```
<vamp2: vamp2 equi: TBP>≡  
  procedure :: write => vamp2_equi_write  
  
<vamp2: procedures>+≡  
  subroutine vamp2_equi_write (self, unit, indent)  
    class(vamp2_equi_t), intent(in) :: self  
    integer, intent(in), optional :: unit  
    integer, intent(in), optional :: indent  
    integer :: u, ind  
    u = given_output_unit (unit)  
    ind = 0; if (present (indent)) ind = indent  
    call write_indent (u, ind)  
    write (u, "(2(A,1X,I0))") "src:", self%ch_src, "-> dest:", self%ch  
    call write_indent (u, ind)  
    write (u, "(A,99(1X,I0))") "Perm: ", self%perm  
    call write_indent (u, ind)  
    write (u, "(A,99(1X,I0))") "Mode: ", self%mode  
  end subroutine vamp2_equi_write
```

```
<vamp2: public>+≡  
  public :: vamp2_equivalences_t
```

```
<vamp2: types>+≡  
  type :: vamp2_equivalences_t  
    private  
    integer :: n_eqv = 0  
    integer :: n_channel = 0  
    integer :: n_dim = 0  
    type(vamp2_equi_t), dimension(:), allocatable :: eqv  
    integer, dimension(:), allocatable :: map  
    integer, dimension(:), allocatable :: multiplicity  
    integer, dimension(:), allocatable :: symmetry  
    logical, dimension(:), allocatable :: independent  
    integer, dimension(:), allocatable :: equivalent_to_ch  
    logical, dimension(:, :), allocatable :: dim_is_invariant  
    contains  
    <vamp2: vamp2 equivalences: TBP>
```

```
end type vamp2_equivalences_t
```

Constructor.

```
{vamp2: interfaces}+≡
```

```
interface vamp2_equivalences_t
  module procedure vamp2_equivalences_init
end interface vamp2_equivalences_t
```

```
{vamp2: procedures}+≡
```

```
type(vamp2_equivalences_t) function vamp2_equivalences_init (&
  n_eqv, n_channel, n_dim) result (eqv)
  integer, intent(in) :: n_eqv, n_channel, n_dim
  eqv%n_eqv = n_eqv
  eqv%n_channel = n_channel
  eqv%n_dim = n_dim
  allocate (eqv%eqv(n_eqv))
  allocate (eqv%map(n_channel), source = 0)
  allocate (eqv%multiplicity(n_channel), source = 0)
  allocate (eqv%symmetry(n_channel), source = 0)
  allocate (eqv%independent(n_channel), source = .true.)
  allocate (eqv%equivalent_to_ch(n_channel), source = 0)
  allocate (eqv%dim_is_invariant(n_dim, n_channel), source = .false.)
end function vamp2_equivalences_init
```

Write equivalences.

```
{vamp2: vamp2 equivalences: TBP}≡
```

```
procedure :: write => vamp2_equivalences_write
```

```
{vamp2: procedures}+≡
```

```
subroutine vamp2_equivalences_write (self, unit, indent)
  class(vamp2_equivalences_t), intent(in) :: self
  integer, intent(in), optional :: unit
  integer, intent(in), optional :: indent
  integer :: u, ind, i_eqv, ch
  u = given_output_unit (unit)
  ind = 0; if (present (indent)) ind = indent
  write (u, "(A)") "Inequivalent channels:"
  if (allocated (self%independent)) then
    do ch = 1, self%n_channel
      if (self%independent(ch)) then
        write (u, "(2X,A,1x,I0,A,4x,A,I0,4x,A,I0,4x,A,999(L1))") &
          "Channel", ch, ":", &
          "Mult. = ", self%multiplicity(ch), &
          "Symm. = ", self%symmetry(ch), &
          "Invar.: ", self%dim_is_invariant(:, ch)
      end if
    end do
  else
    write (u, "(A)") "[not allocated]"
  end if
  write (u, "(A)") "Equivalence list:"
  if (allocated (self%eqv)) then
    do i_eqv = 1, self%n_eqv
```

```

        write (u, "(2X,A,1X,I0)") "i_eqv:", i_eqv
        call self%eqv(i_eqv)%write (unit, indent = ind + 4)
    end do
else
    write (u, "(A)") "[not allocated]"
end if
end subroutine vamp2_equivalences_write

```

Is allocated.

```

<vamp2: vamp2 equivalences: TBP>+≡
    procedure, public :: is_allocated => vamp2_equivalences_is_allocated

<vamp2: procedures>+≡
    logical function vamp2_equivalences_is_allocated (self) result (yorn)
        class(vamp2_equivalences_t), intent(in) :: self
        yorn = allocated (self%eqv)
    end function vamp2_equivalences_is_allocated

```

Get source channel and destination channel for given equivalence.

```

<vamp2: vamp2 equivalences: TBP>+≡
    procedure, public :: get_channels => vamp2_equivalences_get_channels

<vamp2: procedures>+≡
    subroutine vamp2_equivalences_get_channels (eqv, i_eqv, dest, src)
        class(vamp2_equivalences_t), intent(in) :: eqv
        integer, intent(in) :: i_eqv
        integer, intent(out) :: dest, src
        dest = eqv%eqv(i_eqv)%ch
        src = eqv%eqv(i_eqv)%ch_src
    end subroutine vamp2_equivalences_get_channels

```

```

<vamp2: vamp2 equivalences: TBP>+≡
    procedure, public :: get_mode => vamp2_equivalences_get_mode
    procedure, public :: get_perm => vamp2_equivalences_get_perm

<vamp2: procedures>+≡
    function vamp2_equivalences_get_mode (eqv, i_eqv) result (mode)
        class(vamp2_equivalences_t), intent(in) :: eqv
        integer, intent(in) :: i_eqv
        integer, dimension(:), allocatable :: mode
        mode = eqv%eqv(i_eqv)%mode
    end function vamp2_equivalences_get_mode

    function vamp2_equivalences_get_perm (eqv, i_eqv) result (perm)
        class(vamp2_equivalences_t), intent(in) :: eqv
        integer, intent(in) :: i_eqv
        integer, dimension(:), allocatable :: perm
        perm = eqv%eqv(i_eqv)%perm
    end function vamp2_equivalences_get_perm

```

```

<vamp2: vamp2 equivalences: TBP>+≡
    procedure, public :: set_equivalence => vamp2_equivalences_set_equivalence

```

```

<vamp2: procedures>+≡
  subroutine vamp2_equivalences_set_equivalence &
    (eqv, i_eqv, dest, src, perm, mode)
    class(vamp2_equivalences_t), intent(inout) :: eqv
    integer, intent(in) :: i_eqv
    integer, intent(in) :: dest, src
    integer, dimension(:), intent(in) :: perm, mode
    integer :: i
    if (dest < 1 .or. dest > eqv%n_channel) call msg_bug &
      ("VAMP2: set_equivalences: destination channel out of range.")
    if (src < 1 .or. src > eqv%n_channel) call msg_bug &
      ("VAMP2: set_equivalences: source channel out of range.")
    if (size(perm) /= eqv%n_dim) call msg_bug &
      ("VAMP2: set_equivalences: size(perm) does not match n_dim.")
    if (size(mode) /= eqv%n_dim) call msg_bug &
      ("VAMP2: set_equivalences: size(mode) does not match n_dim.")
    eqv%eqv(i_eqv)%ch = dest
    eqv%eqv(i_eqv)%ch_src = src
    allocate (eqv%eqv(i_eqv)%perm (size (perm)))
    do i = 1, size (perm)
      eqv%eqv(i_eqv)%perm(i) = perm(i)
    end do
    allocate (eqv%eqv(i_eqv)%mode (size (mode)))
    do i = 1, size (mode)
      eqv%eqv(i_eqv)%mode(i) = mode(i)
    end do
  end subroutine vamp2_equivalences_set_equivalence

```

Freeze equivalences.

```

<vamp2: vamp2 equivalences: TBP>+≡
  procedure, public :: freeze => vamp2_equivalences_freeze

<vamp2: procedures>+≡
  subroutine vamp2_equivalences_freeze (self)
    class(vamp2_equivalences_t), intent(inout) :: self
    integer :: i_eqv, ch, upper, lower
    ch = 0
    do i_eqv = 1, self%n_eqv
      if (ch /= self%eqv(i_eqv)%ch) then
        ch = self%eqv(i_eqv)%ch
        self%map(ch) = i_eqv
      end if
    end do
    do ch = 1, self%n_channel
      lower = self%map(ch)
      if (ch == self%n_channel) then
        upper = self%n_eqv
      else
        upper = self%map(ch + 1) - 1
      end if
      associate (eqv => self%eqv, n_eqv => size (self%eqv(lower:upper)))
        if (.not. all(eqv(lower:upper)%ch == ch) .or. &
          eqv(lower)%ch_src > ch) then
          do i_eqv = lower, upper

```



```

        call self%eqv(i_eqv)%write ()
    end do
    call msg_bug ("VAMP2: vamp2_equivalences_freeze: &
        &equivalence order is not correct.")
end if
self%symmetry(ch) = count (eqv(lower:upper)%ch_src == ch)
if (mod (n_eqv, self%symmetry(ch)) /= 0) then
    do i_eqv = lower, upper
        call self%eqv(i_eqv)%write ()
    end do
    call msg_bug ("VAMP2: vamp2_equivalences_freeze: &
        &permutation count is not correct.")
end if
self%multiplicity(ch) = n_eqv / self%symmetry(ch)
self%independent(ch) = all (eqv(lower:upper)%ch_src >= ch)
self%equivalent_to_ch(ch) = eqv(lower)%ch_src
self%dim_is_invariant(:, ch) = eqv(lower)%mode == VEQ_INVARIANT
end associate
end do
end subroutine vamp2_equivalences_freeze

```

20.13.5 Type: vamp2_t

```

<vamp2: public>+≡
    public :: vamp2_t

<vamp2: types>+≡
    type :: vamp2_t
    private
    type(vamp2_config_t) :: config
    type(vegas_t), dimension(:), allocatable :: integrator
    integer, dimension(:), allocatable :: chain
    real(default), dimension(:), allocatable :: weight
    real(default), dimension(:), allocatable :: integral
    real(default), dimension(:), allocatable :: variance
    real(default), dimension(:), allocatable :: efficiency
    type(vamp2_result_t) :: result
    type(vamp2_equivalences_t) :: equivalences
    logical :: event_prepared
    real(default), dimension(:), allocatable :: event_weight
    <vamp2: vamp2: type>
    contains
    <vamp2: vamp2: TBP>
    end type vamp2_t

<MPI: vamp2: vamp2: type>≡
    class(request_base_t), allocatable :: request

<vamp2: interfaces>+≡
    interface vamp2_t
        module procedure vamp2_init
    end interface vamp2_t

```

Constructor.

```

<vamp2: procedures>+=
  type(vamp2_t) function vamp2_init (n_channel, n_dim, alpha, beta, n_bins_max,&
    & n_calls_min_per_channel, iterations, mode) result (self)
    integer, intent(in) :: n_channel
    integer, intent(in) :: n_dim
    integer, intent(in), optional :: n_bins_max
    integer, intent(in), optional :: n_calls_min_per_channel
    real(default), intent(in), optional :: alpha
    real(default), intent(in), optional :: beta
    integer, intent(in), optional :: iterations
    integer, intent(in), optional :: mode
    integer :: ch
    self%config%n_dim = n_dim
    self%config%n_channel = n_channel
    call set_options ()
    allocate (self%chain(n_channel), source=0)
    allocate (self%integrator(n_channel))
    allocate (self%weight(n_channel), source=0._default)
    do ch = 1, n_channel
      self%integrator(ch) = vegas_t (n_dim, alpha, n_bins_max, 1, mode)
    end do
    self%weight = 1._default / self%config%n_channel
    call self%reset_result ()
    allocate (self%event_weight(self%config%n_channel), source = 0._default)
    self%event_prepared = .false.
  contains
    subroutine set_options ()
      if (present (n_bins_max)) self%config%n_bins_max = n_bins_max
      if (present (n_calls_min_per_channel)) self%config%n_calls_min_per_channel = n_calls_min_per_channel
      if (present (alpha)) self%config%alpha = alpha
      if (present (beta)) self%config%beta = beta
      if (present (iterations)) self%config%iterations = iterations
      if (present (mode)) self%config%mode = mode
    end subroutine set_options
  end function vamp2_init

```

<vamp2: vamp2: TBP>=

```

  procedure, public :: final => vamp2_final

```

<vamp2: procedures>+=

```

  subroutine vamp2_final (self)
    class(vamp2_t), intent(inout) :: self
    integer :: ch
    do ch = 1, self%config%n_channel
      call self%integrator(ch)%final ()
    end do
  end subroutine vamp2_final

```

Output.

<vamp2: vamp2: TBP>+=

```

  procedure, public :: write => vamp2_write

```

```

<vamp2: procedures>+=
  subroutine vamp2_write (self, unit, indent)
    class(vamp2_t), intent(in) :: self
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
    integer :: u, ind, ch
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(A)") "VAMP2: VEGAS AMPlified 2"
    call write_indent (u, ind)
    call self%config%write (unit, indent)
    call self%result%write (unit, indent)
  end subroutine vamp2_write

```

Get the config object.

```

<vamp2: vamp2: TBP>+=
  procedure, public :: get_config => vamp2_get_config

<vamp2: procedures>+=
  subroutine vamp2_get_config (self, config)
    class(vamp2_t), intent(in) :: self
    type(vamp2_config_t), intent(out) :: config
    config = self%config
  end subroutine vamp2_get_config

```

Set non-runtime dependent configuration. It will no be possible to change `n.bins_max`.

```

<vamp2: vamp2: TBP>+=
  procedure, public :: set_config => vamp2_set_config

<vamp2: procedures>+=
  subroutine vamp2_set_config (self, config)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_config_t), intent(in) :: config
    integer :: ch
    self%config%equivalences = config%equivalences
    self%config%n_calls_min_per_channel = config%n_calls_min_per_channel
    self%config%n_calls_threshold = config%n_calls_threshold
    self%config%n_calls_min = config%n_calls_min
    self%config%beta = config%beta
    self%config%accuracy_goal = config%accuracy_goal
    self%config%error_goal = config%error_goal
    self%config%rel_error_goal = config%rel_error_goal
    do ch = 1, self%config%n_channel
      call self%integrator(ch)%set_config (config)
    end do
  end subroutine vamp2_set_config

```

Set the overall number of calls. The number of calls each channel is scaled by the channel weights

$$N_i = \alpha_i N. \quad (20.8)$$

```

<vamp2: vamp2: TBP>+=

```

```

    procedure, public :: set_calls => vamp2_set_n_calls
<vamp2: procedures>+≡
    subroutine vamp2_set_n_calls (self, n_calls)
        class(vamp2_t), intent(inout) :: self
        integer, intent(in) :: n_calls
        integer :: ch
        self%config%n_calls_min = self%config%n_calls_min_per_channel &
            & * self%config%n_channel
        self%config%n_calls = max(n_calls, self%config%n_calls_min)
        if (self%config%n_calls > n_calls) then
            write (msg_buffer, "(A,I0)") "VAMP2: [set_calls] number of calls too few,&
                & reset to = ", self%config%n_calls
            call msg_message ()
        end if
        do ch = 1, self%config%n_channel
            call self%integrator(ch)%set_calls (max (nint (self%config%n_calls *&
                & self%weight(ch)), self%config%n_calls_min_per_channel))
        end do
    end subroutine vamp2_set_n_calls

```

Set limits. We only support same limits for all channels.

```

<vamp2: vamp2: TBP>+≡
    procedure, public :: set_limits => vamp2_set_limits
<vamp2: procedures>+≡
    subroutine vamp2_set_limits (self, x_upper, x_lower)
        class(vamp2_t), intent(inout) :: self
        real(default), dimension(:), intent(in) :: x_upper
        real(default), dimension(:), intent(in) :: x_lower
        integer :: ch
        do ch = 1, self%config%n_channel
            call self%integrator(ch)%set_limits (x_upper, x_lower)
        end do
    end subroutine vamp2_set_limits

```

Set `n_chains` and the (actual) chains. `chain` must have size `n_channels` and each elements must store an index to a corresponding chain. This means, that channels with equal index correspond to the same chain, and we refer to those as chained weights, where we average the contributions of the chained weights in `vamp2_adapt_weights`.

```

<vamp2: vamp2: TBP>+≡
    procedure, public :: set_chain => vamp2_set_chain
<vamp2: procedures>+≡
    subroutine vamp2_set_chain (self, n_chains, chain)
        class(vamp2_t), intent(inout) :: self
        integer, intent(in) :: n_chains
        integer, dimension(:), intent(in) :: chain
        if (size (chain) /= self%config%n_channel) then
            call msg_bug ("VAMP2: set chain: size of chain array does not match n_channel.")
        else
            call msg_message ("VAMP2: set chain: use chained weights.")
        end if
    end subroutine

```

```

        self%config%n_chains = n_chains
        self%chain = chain
    end subroutine vamp2_set_chain

```

Set channel equivalences.

```

<vamp2: vamp2: TBP>+≡
    procedure, public :: set_equivalences => vamp2_set_equivalences

<vamp2: procedures>+≡
    subroutine vamp2_set_equivalences (self, equivalences)
        class(vamp2_t), intent(inout) :: self
        type(vamp2_equivalences_t), intent(in) :: equivalences
        self%equivalences = equivalences
    end subroutine vamp2_set_equivalences

```

Move allocated (and prepared!) request object into VAMP2.

```

<MPI: vamp2: vamp2: TBP>≡
    generic, public :: allocate_request => allocate_request_by_method, &
        allocate_request_by_object
    procedure, private :: allocate_request_by_method => vamp2_allocate_request_by_method
    procedure, private :: allocate_request_by_object => vamp2_allocate_request_by_object

<MPI: vamp2: procedures>≡
    subroutine vamp2_allocate_request_by_method (self, method)
        class(vamp2_t), intent(inout) :: self
        character(len=*), intent(in) :: method
        class(request_base_t), allocatable :: request
        select case (trim(method))
            case("simple", "Simple", "SIMPLE")
                allocate (request_simple_t :: request)
            case("load", "Load", "LOAD")
                allocate (request_caller_t :: request)
            case default
                call msg_bug ("VAMP2: Unknown method for MPI request module.")
        end select
        select type (request)
            type is (request_simple_t)
                call request%init (MPI_COMM_WORLD, n_channels = self%config%n_channel)
            type is (request_caller_t)
                call request%init (MPI_COMM_WORLD, n_channels = self%config%n_channel)
        end select
        call self%allocate_request_by_object (request)
    end subroutine vamp2_allocate_request_by_method

    subroutine vamp2_allocate_request_by_object (self, request)
        class(vamp2_t), intent(inout) :: self
        class(request_base_t), allocatable, intent(inout) :: request
        !! Only output in case of "parallel" integration.
        if (request%has_workers ()) then
            select type (request)
                type is (request_simple_t)
                    call msg_message ("VAMP2: Simple Request Balancing.")
                type is (request_caller_t)
                    call msg_message ("VAMP2: Request with load balancing.")
            end select
        end if
    end subroutine vamp2_allocate_request_by_object

```

```

class default
  call msg_bug ("VAMP2: Unknown extension of request_base.")
end select
end if
call move_alloc (request, self%request)
end subroutine vamp2_allocate_request_by_object

```

Get `n_calls` calculated by VEGAS.

```

<vamp2: vamp2: TBP>+≡
  procedure, public :: get_n_calls => vamp2_get_n_calls

<vamp2: procedures>+≡
  elemental real(default) function vamp2_get_n_calls (self) result (n_calls)
    class(vamp2_t), intent(in) :: self
    n_calls = sum (self%integrator%get_calls ())
  end function vamp2_get_n_calls

```

Get the cumulative result of the integration. Recalculate weighted average of the integration.

```

<vamp2: vamp2: TBP>+≡
  procedure, public :: get_integral => vamp2_get_integral

<vamp2: procedures>+≡
  elemental real(default) function vamp2_get_integral (self) result (integral)
    class(vamp2_t), intent(in) :: self
    integral = 0.
    if (self%result%sum_wgts > 0.) then
      integral = self%result%sum_int_wgtd / self%result%sum_wgts
    end if
  end function vamp2_get_integral

```

Get the cumulative variance of the integration. Recalculate the variance.

```

<vamp2: vamp2: TBP>+≡
  procedure, public :: get_variance => vamp2_get_variance

<vamp2: procedures>+≡
  elemental real(default) function vamp2_get_variance (self) result (variance)
    class(vamp2_t), intent(in) :: self
    variance = 0.
    if (self%result%sum_wgts > 0.) then
      variance = 1.0 / self%result%sum_wgts
    end if
  end function vamp2_get_variance

```

Get efficiency.

```

<vamp2: vamp2: TBP>+≡
  procedure, public :: get_efficiency => vamp2_get_efficiency

<vamp2: procedures>+≡
  elemental real(default) function vamp2_get_efficiency (self) result (efficiency)
    class(vamp2_t), intent(in) :: self
    efficiency = 0.
    if (self%result%efficiency > 0.) then

```

```

        efficiency = self%result%efficiency
    end if
end function vamp2_get_efficiency

```

Get event weight and event weight excess.

```

<vamp2: vamp2: TBP>+≡
    procedure :: get_evt_weight => vamp2_get_evt_weight
    procedure :: get_evt_weight_excess => vamp2_get_evt_weight_excess

<vamp2: procedures>+≡
    real(default) function vamp2_get_evt_weight (self) result (evt_weight)
        class(vamp2_t), intent(in) :: self
        evt_weight = self%result%evt_weight
    end function vamp2_get_evt_weight

    real(default) function vamp2_get_evt_weight_excess (self) result (evt_weight_excess)
        class(vamp2_t), intent(in) :: self
        evt_weight_excess = self%result%evt_weight_excess
    end function vamp2_get_evt_weight_excess

```

Get procedure to retrieve channel-th grid.

```

<vamp2: vamp2: TBP>+≡
    procedure :: get_grid => vamp2_get_grid

<vamp2: procedures>+≡
    type(vegas_grid_t) function vamp2_get_grid (self, channel) result (grid)
        class(vamp2_t), intent(in) :: self
        integer, intent(in) :: channel
        if (channel < 1 .or. channel > self%config%n_channel) &
            call msg_bug ("VAMP2: vamp2_get_grid: channel index < 1 or > n_channel.")
        grid = self%integrator(channel)%get_grid ()
    end function vamp2_get_grid

```

Adapt. We adapt the weights due the contribution of variances with $\beta > 0$.

$$\alpha_i = \frac{\alpha_i V_i^\beta}{\sum_i \alpha_i V_i^\beta} \quad (20.9)$$

If `n.calls.threshold` is set, we rescale the weights in such a way, that the `n.calls` for each channel are greater than `n.calls.threshold`. We calculate the distance of the weights to the `weight_min` and reset those weights which are less than `weight_mins` to this value. The other values are accordingly resized to fit the boundary condition of the partition of unity.

```

<vamp2: vamp2: TBP>+≡
    procedure, private :: adapt_weights => vamp2_adapt_weights

<vamp2: procedures>+≡
    subroutine vamp2_adapt_weights (self)
        class(vamp2_t), intent(inout) :: self
        integer :: n_weights_underflow
        real(default) :: weight_min, sum_weights_underflow
        self%weight = self%weight * self%integrator%get_variance ()**self%config%beta
        if (sum (self%weight) == 0) self%weight = real(self%config%n_calls, default)
    end subroutine vamp2_adapt_weights

```

```

if (self%config%n_chains > 0) then
  call chain_weights ()
end if
self%weight = self%weight / sum(self%weight)
if (self%config%n_calls_threshold /= 0) then
  weight_min = real(self%config%n_calls_threshold, default) &
    & / self%config%n_calls
  sum_weights_underflow = sum (self%weight, self%weight < weight_min)
  n_weights_underflow = count (self%weight < weight_min)
  where (self%weight < weight_min)
    self%weight = weight_min
  elsewhere
    self%weight = self%weight * (1. - n_weights_underflow * weight_min) &
      & / (1. - sum_weights_underflow)
  end where
end if
call self%set_calls (self%config%n_calls)
contains
<vamp2: vamp2 adapt weights: procedures>
end subroutine vamp2_adapt_weights

```

We average the weights over their respective chain members.

```

<vamp2: vamp2 adapt weights: procedures>≡
  subroutine chain_weights ()
    integer :: ch
    real(default) :: average
    do ch = 1, self%config%n_chains
      average = max (sum (self%weight, self%chain == ch), 0._default)
      if (average /= 0) then
        average = average / count (self%chain == ch)
        where (self%chain == ch)
          self%weight = average
        end where
      end if
    end do
  end subroutine chain_weights

<vamp2: vamp2: TBP>+≡
  procedure, private :: apply_equivalences => vamp2_apply_equivalences

<vamp2: procedures>+≡
  subroutine vamp2_apply_equivalences (self)
    class(vamp2_t), intent(inout) :: self
    integer :: ch, ch_src, j, j_src, i_eqv
    real(default), dimension(:, :, :), allocatable :: d
    real(default), dimension(:, :), allocatable :: d_src
    integer, dimension(:), allocatable :: mode, perm
    if (.not. self%equivalences%is_allocated ()) then
      call msg_bug ("VAMP2: vamp2_apply_equivalences: &
        &cannot apply not-allocated equivalences.")
    end if
    allocate (d(self%config%n_bins_max, self%config%n_dim, &
      self%config%n_channel), source=0._default)
    associate (eqv => self%equivalences, nb => self%config%n_bins_max)

```



```

do i_eqv = 1, self%equivalences%n_eqv
  call eqv%get_channels (i_eqv, ch, ch_src)
  d_src = self%integrator(ch_src)%get_distribution ()
  mode = eqv%get_mode (i_eqv)
  perm = eqv%get_perm (i_eqv)
  do j = 1, self%config%n_dim
    select case (mode (j))
    case (VEQ_IDENTITY)
      d(:, j, ch) = d(:, j, ch) + &
        d_src(:, perm(j))
    case (VEQ_INVERT)
      d(:, j, ch) = d(:, j, ch) + &
        d_src(nb:1:-1, perm(j))
    case (VEQ_SYMMETRIC)
      d(:, j, ch) = d(:, j, ch) + &
        d_src(:, perm(j)) / 2. + &
        d_src(nb:1:-1, perm(j)) / 2.
    case (VEQ_INVARIANT)
      d(:, j, ch) = 1._default
    end select
  end do
end do
end associate
do ch = 1, self%config%n_channel
  call self%integrator(ch)%set_distribution (d(:, :, ch))
end do
end subroutine vamp2_apply_equivalences

```

Reset the cumulative result.

```

<vamp2: vamp2: TBP>+≡
  procedure, public :: reset_result => vamp2_reset_result

<vamp2: procedures>+≡
  subroutine vamp2_reset_result (self)
    class(vamp2_t), intent(inout) :: self
    call self%result%reset ()
  end subroutine vamp2_reset_result

```

Integrate. We integrate each channel separately and combine the results

$$I = \sum_i \alpha_i I_i, \quad (20.10)$$

$$\sigma^2 = \sum_i \alpha_i^2 \sigma_i^2. \quad (20.11)$$

Although, the (population) variance is given by

$$\begin{aligned}
\sigma^2 &= \frac{1}{N} \left(\sum_i \alpha_i I_i^2 - I^2 \right) \\
&= \frac{1}{N-1} \left(\sum_i (N_i \sigma_i^2 + I_i^2) - I^2 \right) \\
&= \frac{1}{N-1} \left(\sum_i \alpha_i \sigma_i^2 + \alpha_i I_i^2 - I^2 \right),
\end{aligned} \tag{20.12}$$

where we used $\sigma_i^2 = \frac{1}{N} (\langle I_i^2 \rangle - \langle I_i \rangle^2)$, we use the approximation for numeric stability. The population variance relates to sample variance

$$s^2 = \frac{n}{n-1} \sigma^2, \tag{20.13}$$

which gives an unbiased error estimate.

Beside those adaption to multichannel, the overall processing of `total_integral`, `total_sq_integral` and `total_variance` is the same as in `vegas_integrate`.

```

<vamp2: vamp2: TBP>+≡
  procedure, public :: integrate => vamp2_integrate

<vamp2: procedures>+≡
  subroutine vamp2_integrate (self, func, rng, iterations, reset_result,&
    & refine_grids, adapt_weights, verbose, result, abserr)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    integer, intent(in), optional :: iterations
    logical, intent(in), optional :: reset_result
    logical, intent(in), optional :: refine_grids
    logical, intent(in), optional :: adapt_weights
    logical, intent(in), optional :: verbose
    real(default), optional, intent(out) :: result, abserr
    integer :: it, ch
    type(iterator_t) :: channel_iterator
    real(default) :: cumulative_int, cumulative_std
    logical :: opt_reset_result
    logical :: opt_adapt_weights
    logical :: opt_refine_grids
    logical :: opt_verbose
  <vamp2: vamp2 integrate: variables>
    call set_options ()
    if (opt_verbose) then
      call msg_message ("Results: [it, calls, integral, error, chi^2, eff.]")
    end if
    if (opt_reset_result) call self%reset_result ()
  <vamp2: vamp2 integrate: init>
    iteration: do it = 1, self%config%iterations
      call channel_iterator%init (1, self%config%n_channel)
      call self%prepare_integrate_iteration (func)
    <vamp2: vamp2 integrate: presampling>
    channel: do

```

```

    <vamp2: vamp2 integrate: sampling>
    call func%set_channel (ch)
    call self%integrator(ch)%integrate ( &
        & func, rng, iterations, refine_grid = .false., verbose = .false.)
    <vamp2: vamp2 integrate: callback>
    call channel_iterator%next_step ()
end do channel
<vamp2: vamp2 integrate: postsampling>
call self%compute_result_and_efficiency ()
associate (result => self%result)
    cumulative_int = result%sum_int_wgtd / result%sum_wgts
    cumulative_std = sqrt (1 / result%sum_wgts)
    if (opt_verbose) then
        write (msg_buffer, "(I0,1x,I0,1x, 4(E24.16E4,1x))") &
            & it, self%config%n_calls, cumulative_int, cumulative_std, &
            & result%chi2, result%efficiency
        call msg_message ()
    end if
end associate
if (opt_adapt_weights) then
    call self%adapt_weights ()
end if
if (opt_refine_grids) then
    if (self%config%equivalences .and. self%equivalences%is_allocated ()) then
        call self%apply_equivalences ()
    end if
    do ch = 1, self%config%n_channel
        !! When we apply the grid refinement outside of VEGAS, then we do not average over di
        !! as VEGAS averaged the distribution internally.
        call self%integrator(ch)%refine (average = .false.)
    end do
end if
end do iteration
if (present (result)) result = cumulative_int
if (present (abserr)) abserr = abs (cumulative_std)
contains
<vamp2: vamp2 integrate: procedures>
end subroutine vamp2_integrate

```

Set optional parameters.

```

<vamp2: vamp2 integrate: procedures>≡
subroutine set_options ()
    if (present (iterations)) self%config%iterations = iterations
    opt_reset_result = .true.
    if (present (reset_result)) opt_reset_result = reset_result
    opt_adapt_weights = .true.
    if (present (adapt_weights)) opt_adapt_weights = adapt_weights
    opt_refine_grids = .true.
    if (present (refine_grids)) opt_refine_grids = refine_grids
    opt_verbose = .false.
    if (present (verbose)) opt_verbose = verbose
end subroutine set_options

```

We define additional chunks, which we use to insert parallel/MPI code.

```
<vamp2: vamp2 integrate: variables>≡
```

```
<vamp2: vamp2 integrate: init>≡
```

```
<vamp2: vamp2 integrate: presampling>≡
```

Conditional handling. We introduce a different behavior for the MPI-/non-MPI variant.

```
<NOMPI: vamp2: vamp2 integrate: sampling>≡
```

```
  if (.not. channel_iterator%is_iterable ()) exit channel
  ch = channel_iterator%get_current ()
```

```
<vamp2: vamp2 integrate: callback>≡
```

```
<vamp2: vamp2 integrate: postsampling>≡
```

```
<MPI: vamp2: vamp2 integrate: variables>≡
```

```
  type(request_t) :: request
```

Verify that we have an allocated request object, else fallback to simple method. Be aware that we keep the fallback silent (!) in order to keep any possible testing output uninterrupted.

```
<MPI: vamp2: vamp2 integrate: init>≡
```

```
  if (.not. allocated (self%request)) then
    call self%allocate_request_by_method ("simple")
  end if
```

```
<MPI: vamp2: vamp2 integrate: presampling>≡
```

```
  if (self%request%is_master ()) then
    select type (req => self%request)
    type is (request_caller_t)
      request%terminate = .true.
      call update_iter_and_rng (request, channel_iterator, rng)
      !! channel_iter is already drained for master.
      !! Do not descent into channel integration (later on).
      call req%handle_workload ()
    end select
  end if
```

Conditional handling for the MPI-version of sampling.

We have a request object and an advanced `channel_iterator` and have to consider three cases:

1. `channel_iterator` drained,
2. `request` terminated,
3. `request` received.

When the `channel_iterator` is drained by `update_iter_and_rng`, we send a terminate request to the master and await in the next cycle of channel loop the terminated request. When the request is terminated, we can gracefully exit the channel loop as `channel_iterator` and `rng` are already advanced by `update_iter_and_rng`. When we received a genuine request, then, we proceed as prophesied.

```
<MPI: vamp2: vamp2 integrate: sampling>≡
```

```
  select type (req => self%request)
```

```

type is (request_caller_t)
  if (self%request%is_master ()) exit channel
end select
call self%request%request_workload (request)
call update_iter_and_rng (request, channel_iterator, rng)
if (request%terminate) then
  exit channel
else if (.not. channel_iterator%is_iterable ()) then
  select type (req => self%request)
  type is (request_caller_t)
    call req%request_terminate ()
    cycle channel
  class is (request_base_t)
    exit channel
  end select
end if
if (request%group) call MPI_BARRIER (request%comm)
ch = request%handler_id
call self%integrator(ch)%prepare_parallel_integrate(request%comm, &
  duplicate_comm = .false., &
  parallel_mode = request%group)
<MPI: vamp2: vamp2 integrate: callback>≡
  if (request%group_master) then
    if (.not. self%request%is_master ()) &
      call allocate_handler (self%request, ch)
    call self%request%handle_and_release_workload (request)
  else
    call self%request%release_workload (request)
  end if
<MPI: vamp2: vamp2 integrate: postsampling>≡
  call reduce_func_calls (func)
  call self%request%await_handler ()
  call self%request%barrier ()
  if (.not. self%request%is_master ()) cycle
<MPI: vamp2: vamp2 integrate: procedures>≡
  subroutine allocate_handler (req, ch)
    class(request_base_t), intent(inout) :: req
    integer, intent(in) :: ch
    class(request_handler_t), pointer :: vegas_result_handler
    call self%integrator(ch)%allocate_handler (&
      handler_id = ch,&
      handler = vegas_result_handler)
    call req%add_handler (ch, vegas_result_handler)
  end subroutine allocate_handler

!! Advance the random number generator for the skipped channels.
!!
!! We set current_channel = request%handler_id, hence, we need to advance
!! the random number generator until th iterator returns the same channel.
subroutine update_iter_and_rng (request, iter, rng)
  type(request_t), intent(in) :: request
  type(iterator_t), intent(inout) :: iter
  class(rng_t), intent(inout) :: rng

```

```

advance: do while (iter%is_iterable ())
  !! Advance up to iterator%end when in terminate mode,
  !! else advance until we hit the previous channel (i.e. request%handler_id - 1):
  !! Proof: current_channel <= request%handler_id - 1
  if (.not. request%terminate) then
    if (iter%get_current () >= request%handler_id) &
      exit advance
    end if
    select type (rng)
    type is (rng_stream_t)
      call rng%next_substream ()
    end select
    call iter%next_step ()
  end do advance
end subroutine update_iter_and_rng

```

```

subroutine reduce_func_calls (func)
  class(vamp2_func_t), intent(inout) :: func
  type(MPI_COMM) :: comm
  integer :: root_n_calls
  call self%request%get_external_comm (comm)
  call MPI_reduce (func%n_calls, root_n_calls, 1, MPI_INTEGER, &
    MPI_SUM, 0, comm)
  if (self%request%is_master ()) then
    func%n_calls = root_n_calls
  else
    call func%reset_n_calls ()
  end if
end subroutine reduce_func_calls

```

Prepeare current integration's iteration.

Prepare iteration, i.e. provide weights and grids to function object.

<vamp2: vamp2: TBP>+≡

```

  procedure, private :: prepare_integrate_iteration => &
    vamp2_prepare_integrate_iteration

```

<vamp2: procedures>+≡

```

  subroutine vamp2_prepare_integrate_iteration (self, func)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_func_t), intent(inout) :: func
    <vamp2: vamp2 prepare integrate iteration: body>
    call fill_func_with_weights_and_grids (func)
  contains
    subroutine fill_func_with_weights_and_grids (func)
      class(vamp2_func_t), intent(inout) :: func
      integer :: ch
      do ch = 1, self%config%n_channel
        func%wi(ch) = self%weight(ch)
        !! \todo Use pointers instead of a deep copy.
        func%grids(ch) = self%integrator(ch)%get_grid ()
      end do
    end subroutine fill_func_with_weights_and_grids
    <vamp2: vamp2 prepare integrate iteration: procedures>
  end subroutine vamp2_prepare_integrate_iteration

```

```

<vamp2: vamp2 prepare integrate iteration: body>≡

<vamp2: vamp2 prepare integrate iteration: procedures>≡

<MPI: vamp2: vamp2 prepare integrate iteration: body>≡
  if (.not. allocated (self%request)) then
    call msg_bug ("VAMP2: prepare integration iteration failed: unallocated request.")
  end if
  call broadcast_weights_and_grids ()
  select type (req => self%request)
  type is (request_simple_t)
    call req%update (self%integrator%is_parallelizable ())
    call init_all_handler (req)
    call call_all_handler (req)
    !! Add all handlers, call all handlers.
  type is (request_caller_t)
    if (req%is_master ()) then
      call req%update_balancer (self%weight, self%integrator%is_parallelizable ())
      call init_all_handler (req)
    else
      call self%request%reset ()
    end if
  class default
    call msg_bug ("VAMP2: prepare integration iteration failed: unknown request type.")
  end select

<MPI: vamp2: vamp2 prepare integrate iteration: procedures>≡
  subroutine broadcast_weights_and_grids ()
    type(vegas_grid_t) :: grid
    type(MPI_COMM) :: comm
    integer :: ch
    call self%request%get_external_comm (comm)
    call MPI_BCAST (self%weight, self%config%n_channel, &
      MPI_DOUBLE_PRECISION, 0, comm)
    do ch = 1, self%config%n_channel
      grid = self%integrator(ch)%get_grid ()
      call grid%broadcast (comm)
      call self%integrator(ch)%set_grid (grid)
    end do
    call self%set_calls (self%config%n_calls)
  end subroutine broadcast_weights_and_grids

  subroutine init_all_handler (req)
    class(request_base_t), intent(inout) :: req
    class(request_handler_t), pointer :: vegas_result_handler
    integer :: ch
    !! The master worker needs always all handler (callback objects)
    !! in order to perform the communication to the client handler (callbacks).
    if (.not. req%is_master ()) return
    do ch = 1, self%config%n_channel
      call self%integrator(ch)%allocate_handler (&
        handler_id = ch,&
        handler = vegas_result_handler)
      call req%add_handler (ch, vegas_result_handler)
    end do

```

```

end subroutine init_all_handler

subroutine call_all_handler (req)
  class(request_base_t), intent(inout) :: req
  integer :: ch
  if (.not. req%is_master ()) return
  do ch = 1, self%config%n_channel
    select type (req)
    type is (request_simple_t)
      call req%call_handler (handler_id = ch, &
        source_rank = req%get_request_master (ch))
    end select
  end do
end subroutine call_all_handler

Compute the result and efficiency of the current status of the integrator.
<vamp2: vamp2: TBP>+=
  procedure, private :: compute_result_and_efficiency => &
    vamp2_compute_result_and_efficiency

<vamp2: procedures>+=
  subroutine vamp2_compute_result_and_efficiency (self)
    class(vamp2_t), intent(inout) :: self
    real(default) :: total_integral, total_variance
    real(default) :: max_abs_f_pos, max_abs_f_neg, &
      sum_abs_f_pos, sum_abs_f_neg
    call compute_integral_and_variance (total_integral, total_variance)
    call self%result%update (total_integral, total_variance)
    call compute_efficiency (max_pos = max_abs_f_pos, max_neg = max_abs_f_neg, &
      sum_pos = sum_abs_f_pos, sum_neg = sum_abs_f_neg)
    !! Do not average of number of calls, we have already averaged the efficiencies of all channel
    call self%result%update_efficiency (n_calls = 1, &
      max_pos = max_abs_f_pos, max_neg = max_abs_f_neg, &
      sum_pos = sum_abs_f_pos, sum_neg = sum_abs_f_neg)
contains
  subroutine compute_integral_and_variance (integral, variance)
    real(default), intent(out) :: integral, variance
    real(default) :: sq_integral
    integral = dot_product (self%weight, self%integrator%get_integral ())
    sq_integral = dot_product (self%weight, self%integrator%get_integral ()**2)
    variance = self%config%n_calls * dot_product (self%weight**2, self%integrator%get_variance ())
    variance = sqrt (variance + sq_integral)
    variance = 1._default / self%config%n_calls * &
      & (variance + integral) * (variance - integral)
  end subroutine compute_integral_and_variance

  !> We compute the weight-averaged sum and maximum of the channel (integration) weights \f$w_{i,j}$
  !!
  !! The averaged integration weight and maximum are
  !! \f[
  !! \langle w \rangle = \sum_i \alpha_i \frac{\sum_j w_{i,j}}{N_i},
  !! \f]
  !! \f[
  !! \langle \max w \rangle = \sum_i \alpha_i |\max_j w_{i,j}|.
  !! \f]

```



```

subroutine compute_efficiency (max_pos, max_neg, &
    sum_pos, sum_neg)
    real(default), intent(out) :: max_pos, max_neg
    real(default), intent(out) :: sum_pos, sum_neg
    max_abs_f_pos = dot_product (self%weight, self%integrator%get_max_abs_f_pos ())
    max_abs_f_neg = dot_product (self%weight, self%integrator%get_max_abs_f_neg ())
    sum_abs_f_pos = dot_product (self%weight, &
        self%integrator%get_sum_abs_f_pos () / self%integrator%get_calls ())
    sum_abs_f_neg = dot_product (self%weight, &
        self%integrator%get_sum_abs_f_neg () / self%integrator%get_calls ())
end subroutine compute_efficiency
end subroutine vamp2_compute_result_and_efficiency

```

Generate event from multi-channel weight $w(x) = f(x)/g(x)$.

We select a channel using the a-priori weights and f_i^{\max} , to flatten possible unbalanced channel weight(s).

An additional rescale factor `opt_event_rescale` is applied to `f_max`, iff set.

```

<vamp2: vamp2: TBP>+=
    procedure, public :: generate_weighted => vamp2_generate_weighted_event
<vamp2: procedures>+=
    subroutine vamp2_generate_weighted_event (&
        self, func, rng, x)
        class(vamp2_t), intent(inout) :: self
        class(vamp2_func_t), intent(inout) :: func
        class(rng_t), intent(inout) :: rng
        real(default), dimension(self%config%n_dim), intent(out) :: x
        integer :: ch, i
        real(default) :: r
        if (.not. self%event_prepared) then
            call prepare_event ()
        end if
        call rng%generate (r)
        nchannel: do ch = 1, self%config%n_channel
            r = r - self%event_weight(ch)
            if (r <= 0._default) exit nchannel
        end do nchannel
        ch = min (ch, self%config%n_channel)
        call func%set_channel (ch)
        call self%integrator(ch)%generate_weighted (func, rng, x)
        ! Norm weight by f_max, hidden in event_weight(ch), else by 1
        self%result%evt_weight = self%integrator(ch)%get_evt_weight () &
            * self%weight(ch) / self%event_weight(ch)
contains
    <vamp2: vamp2 generate event: procedures>
end subroutine vamp2_generate_weighted_event

```

Generate unweighted events.

After selecting a channel ch by the inversion method using a random number $r \in [0, 1]$

$$F^{-1}(r) := \inf\{c \in \{1, \dots, N_c\} | F(c) \geq r\}, F(c) = \sum_{c' \leq c} \alpha'_{c'}, \quad (20.14)$$

we try for an event from the previously selected channel. If the event is rejected, we also reject the selected channel.

The inversion method is implemented as a loop over the channel weights α_i until $\sum_c^{c^{prime}} \alpha_c - r \leq 0$, the last value of the loop index `ch` is then c' .

```

<vamp2: vamp2: TBP>+=
  procedure, public :: generate_unweighted => vamp2_generate_unweighted_event
<vamp2: procedures>+=
  subroutine vamp2_generate_unweighted_event ( &
    & self, func, rng, x, opt_event_rescale)
    class(vamp2_t), intent(inout) :: self
    class(vamp2_func_t), intent(inout) :: func
    class(rng_t), intent(inout) :: rng
    real(default), dimension(self%config%n_dim), intent(out) :: x
    real(default), intent(in), optional :: opt_event_rescale
    integer :: ch, i
    real(default) :: r, max_abs_f, event_rescale
    event_rescale = 1._default
    if (present (opt_event_rescale)) then
      event_rescale = opt_event_rescale
    end if
    if (.not. self%event_prepared) then
      call prepare_event ()
    end if
    generate: do
      call rng%generate (r)
      nchannel: do ch = 1, self%config%n_channel
        r = r - self%event_weight(ch)
        if (r <= 0._default) exit nchannel
      end do nchannel
      ch = min (ch, self%config%n_channel)
      call func%set_channel (ch)
      call self%integrator(ch)%generate_weighted (func, rng, x)
      self%result%evt_weight = self%integrator(ch)%get_evt_weight ()
      max_abs_f = merge ( &
        self%integrator(ch)%get_max_abs_f_pos (), &
        self%integrator(ch)%get_max_abs_f_neg (), &
        self%result%evt_weight > 0.)
      self%result%evt_weight_excess = 0._default
      if (self%result%evt_weight > max_abs_f) then
        self%result%evt_weight_excess = self%result%evt_weight / max_abs_f - 1._default
        exit generate
      end if
      call rng%generate (r)
      ! Do not use division, because max_abs_f could be zero.
      if (event_rescale * max_abs_f * r <= abs(self%result%evt_weight)) then
        exit generate
      end if
    end do generate
  contains
    <vamp2: vamp2 generate event: procedures>
  end subroutine vamp2_generate_unweighted_event

```

Prepare event generation. We have to set the channel weights and the grids for

the integrand's object.

We use an ansatz proposed by T. Ohl in the original VAMP code where we do not have to accept on

$$\frac{w_i(x)}{\sum_i \alpha_i \max_x w_i(x)},$$

after we have selected a channel by the weights α_i . But rather, we use a more efficient way where we rescale the channel weights α_i

$$\alpha_i \rightarrow \alpha_i \frac{\max_x w_i(x)}{\sum_i \alpha_i \max_x w_i(x)}.$$

The overall magic is to insert a "1" and to move the uneasy part into the channel selection, such that we can generate events likewise in the single channel mode. We generate an unweighted event by

$$\frac{w_i(x)}{\max_x w_i x},$$

after we have selected a channel by the rescaled event channel weights. The overall normalization $\max_{i,x}$ is not needed because we normalize the event channel weights to one and therefore the overall normalization cancels.

```
<vamp2: vamp2 generate event: procedures>≡
subroutine prepare_event ()
  integer :: i
  self%event_prepared = .false.
  do i = 1, self%config%n_channel
    func%wi(i) = self%weight(i)
    func%grids(i) = self%integrator(i)%get_grid ()
  end do
  if (any (self%integrator%get_max_abs_f () > 0)) then
    self%event_weight = self%weight * self%integrator%get_max_abs_f ()
  else
    self%event_weight = self%weight
  end if
  self%event_weight = self%event_weight / sum (self%event_weight)
  self%event_prepared = .true.
end subroutine prepare_event
```

Write grids to unit.

```
<vamp2: parameters>+≡
character(len=*), parameter, private :: &
  descr_fmt = "(1X,A)", &
  integer_fmt = "(1X,A18,1X,I15)", &
  integer_array_fmt = "(1X,I18,1X,I15)", &
  logical_fmt = "(1X,A18,1X,L1)", &
  double_fmt = "(1X,A18,1X,E24.16E4)", &
  double_array_fmt = "(1X,I18,1X,E24.16E4)", &
  double_array_pac_fmt = "(1X,I18,1X,E16.8E4)", &
  double_array2_fmt = "(1X,2(1X,I8),1X,E24.16E4)", &
  double_array2_pac_fmt = "(1X,2(1X,I8),1X,E16.8E4)"

<vamp2: vamp2: TBP>+≡
procedure, public :: write_grids => vamp2_write_grids
```

<vamp2: procedures>+≡

```

subroutine vamp2_write_grids (self, unit)
  class(vamp2_t), intent(in) :: self
  integer, intent(in), optional :: unit
  integer :: u
  integer :: ch
  u = given_output_unit (unit)
  write (u, descr_fmt) "begin type(vamp2_t)"
  write (u, integer_fmt) "n_channel =", self%config%n_channel
  write (u, integer_fmt) "n_dim =", self%config%n_dim
  write (u, integer_fmt) "n_calls_min_ch =", self%config%n_calls_min_per_channel
  write (u, integer_fmt) "n_calls_thres =", self%config%n_calls_threshold
  write (u, integer_fmt) "n_chains =", self%config%n_chains
  write (u, logical_fmt) "stratified =", self%config%stratified
  write (u, double_fmt) "alpha =", self%config%alpha
  write (u, double_fmt) "beta =", self%config%beta
  write (u, integer_fmt) "n_bins_max =", self%config%n_bins_max
  write (u, integer_fmt) "iterations =", self%config%iterations
  write (u, integer_fmt) "n_calls =", self%config%n_calls
  write (u, integer_fmt) "it_start =", self%result%it_start
  write (u, integer_fmt) "it_num =", self%result%it_num
  write (u, integer_fmt) "samples =", self%result%samples
  write (u, double_fmt) "sum_int_wgtd =", self%result%sum_int_wgtd
  write (u, double_fmt) "sum_wgts =", self%result%sum_wgts
  write (u, double_fmt) "sum_chi =", self%result%sum_chi
  write (u, double_fmt) "chi2 =", self%result%chi2
  write (u, double_fmt) "efficiency =", self%result%efficiency
  write (u, double_fmt) "efficiency_pos =", self%result%efficiency_pos
  write (u, double_fmt) "efficiency_neg =", self%result%efficiency_neg
  write (u, double_fmt) "max_abs_f =", self%result%max_abs_f
  write (u, double_fmt) "max_abs_f_pos =", self%result%max_abs_f_pos
  write (u, double_fmt) "max_abs_f_neg =", self%result%max_abs_f_neg
  write (u, double_fmt) "result =", self%result%result
  write (u, double_fmt) "std =", self%result%std
  write (u, descr_fmt) "begin weight"
  do ch = 1, self%config%n_channel
    write (u, double_array_fmt) ch, self%weight(ch)
  end do
  write (u, descr_fmt) "end weight"
  if (self%config%n_chains > 0) then
    write (u, descr_fmt) "begin chain"
    do ch = 1, self%config%n_channel
      write (u, integer_array_fmt) ch, self%chain(ch)
    end do
    write (u, descr_fmt) "end chain"
  end if
  write (u, descr_fmt) "begin integrator"
  do ch = 1, self%config%n_channel
    call self%integrator(ch)%write_grid (unit)
  end do
  write (u, descr_fmt) "end integrator"
  write (u, descr_fmt) "end type(vamp2_t)"
end subroutine vamp2_write_grids

```

Read grids from unit.

<vamp2: vamp2: TBP>+≡

procedure, public :: read_grids => vamp2_read_grids

<vamp2: procedures>+≡

```
subroutine vamp2_read_grids (self, unit)
  class(vamp2_t), intent(out) :: self
  integer, intent(in), optional :: unit
  integer :: u
  integer :: ibuffer, jbuffer, ch
  character(len=80) :: buffer
  read (unit, descr_fmt) buffer
  read (unit, integer_fmt) buffer, ibuffer
  read (unit, integer_fmt) buffer, jbuffer
  select type (self)
  type is (vamp2_t)
    self = vamp2_t (n_channel = ibuffer, n_dim = jbuffer)
  end select
  read (unit, integer_fmt) buffer, self%config%n_calls_min_per_channel
  read (unit, integer_fmt) buffer, self%config%n_calls_threshold
  read (unit, integer_fmt) buffer, self%config%n_chains
  read (unit, logical_fmt) buffer, self%config%stratified
  read (unit, double_fmt) buffer, self%config%alpha
  read (unit, double_fmt) buffer, self%config%beta
  read (unit, integer_fmt) buffer, self%config%n_bins_max
  read (unit, integer_fmt) buffer, self%config%iterations
  read (unit, integer_fmt) buffer, self%config%n_calls
  read (unit, integer_fmt) buffer, self%result%it_start
  read (unit, integer_fmt) buffer, self%result%it_num
  read (unit, integer_fmt) buffer, self%result%samples
  read (unit, double_fmt) buffer, self%result%sum_int_wgtd
  read (unit, double_fmt) buffer, self%result%sum_wgts
  read (unit, double_fmt) buffer, self%result%sum_chi
  read (unit, double_fmt) buffer, self%result%chi2
  read (unit, double_fmt) buffer, self%result%efficiency
  read (unit, double_fmt) buffer, self%result%efficiency_pos
  read (unit, double_fmt) buffer, self%result%efficiency_neg
  read (unit, double_fmt) buffer, self%result%max_abs_f
  read (unit, double_fmt) buffer, self%result%max_abs_f_pos
  read (unit, double_fmt) buffer, self%result%max_abs_f_neg
  read (unit, double_fmt) buffer, self%result%result
  read (unit, double_fmt) buffer, self%result%std
  read (unit, descr_fmt) buffer
  do ch = 1, self%config%n_channel
    read (unit, double_array_fmt) ibuffer, self%weight(ch)
  end do
  read (unit, descr_fmt) buffer
  if (self%config%n_chains > 0) then
    read (unit, descr_fmt) buffer
    do ch = 1, self%config%n_channel
      read (unit, integer_array_fmt) ibuffer, self%chain(ch)
    end do
    read (unit, descr_fmt) buffer
  end if
  read (unit, descr_fmt) buffer
```

```

do ch = 1, self%config%n_channel
  call self%integrator(ch)%read_grid (unit)
end do
read (unit, descr_fmt) buffer
read (unit, descr_fmt) buffer
end subroutine vamp2_read_grids

```

Read and write grids from an unformatted file.

```

<vamp2: vamp2: TBP>+=
  procedure :: write_binary_grids => vamp2_write_binary_grids
  procedure :: read_binary_grids => vamp2_read_binary_grids
<vamp2: procedures>+=
  subroutine vamp2_write_binary_grids (self, unit)
    class(vamp2_t), intent(in) :: self
    integer, intent(in) :: unit
    integer :: ch
    write (unit)
    write (unit) self%config%n_channel
    write (unit) self%config%n_dim
    write (unit) self%config%n_calls_min_per_channel
    write (unit) self%config%n_calls_threshold
    write (unit) self%config%n_chains
    write (unit) self%config%stratified
    write (unit) self%config%alpha
    write (unit) self%config%beta
    write (unit) self%config%n_bins_max
    write (unit) self%config%iterations
    write (unit) self%config%n_calls
    write (unit) self%result%it_start
    write (unit) self%result%it_num
    write (unit) self%result%samples
    write (unit) self%result%sum_int_wgtd
    write (unit) self%result%sum_wgts
    write (unit) self%result%sum_chi
    write (unit) self%result%chi2
    write (unit) self%result%efficiency
    write (unit) self%result%efficiency_pos
    write (unit) self%result%efficiency_neg
    write (unit) self%result%max_abs_f
    write (unit) self%result%max_abs_f_pos
    write (unit) self%result%max_abs_f_neg
    write (unit) self%result%result
    write (unit) self%result%std
    do ch = 1, self%config%n_channel
      write (unit) ch, self%weight(ch)
    end do
    if (self%config%n_chains > 0) then
      do ch = 1, self%config%n_channel
        write (unit) ch, self%chain(ch)
      end do
    end if
    do ch = 1, self%config%n_channel
      call self%integrator(ch)%write_binary_grid (unit)

```

```

        end do
    end subroutine vamp2_write_binary_grids

    subroutine vamp2_read_binary_grids (self, unit)
        class(vamp2_t), intent(out) :: self
        integer, intent(in) :: unit
        integer :: ch, ibuffer, jbuffer
        read (unit)
        read (unit) ibuffer
        read (unit) jbuffer
        select type (self)
        type is (vamp2_t)
            self = vamp2_t (n_channel = ibuffer, n_dim = jbuffer)
        end select
        read (unit) self%config%n_calls_min_per_channel
        read (unit) self%config%n_calls_threshold
        read (unit) self%config%n_chains
        read (unit) self%config%stratified
        read (unit) self%config%alpha
        read (unit) self%config%beta
        read (unit) self%config%n_bins_max
        read (unit) self%config%iterations
        read (unit) self%config%n_calls
        read (unit) self%result%it_start
        read (unit) self%result%it_num
        read (unit) self%result%samples
        read (unit) self%result%sum_int_wgtd
        read (unit) self%result%sum_wgts
        read (unit) self%result%sum_chi
        read (unit) self%result%chi2
        read (unit) self%result%efficiency
        read (unit) self%result%efficiency_pos
        read (unit) self%result%efficiency_neg
        read (unit) self%result%max_abs_f
        read (unit) self%result%max_abs_f_pos
        read (unit) self%result%max_abs_f_neg
        read (unit) self%result%result
        read (unit) self%result%std
        do ch = 1, self%config%n_channel
            read (unit) ibuffer, self%weight(ch)
        end do
        if (self%config%n_chains > 0) then
            do ch = 1, self%config%n_channel
                read (unit) ibuffer, self%chain(ch)
            end do
        end if
        do ch = 1, self%config%n_channel
            call self%integrator(ch)%read_binary_grid (unit)
        end do
    end subroutine vamp2_read_binary_grids

```

20.14 Unit tests

Test module, followed by the corresponding implementation module.

```
<vamp2.ut.f90>≡  
  <File header>
```

```
module vamp2_ut  
  use unit_tests  
  use vamp2_uti
```

```
  <Standard module head>
```

```
  <vamp2: public test>
```

```
contains  
  <vamp2: test driver>  
end module vamp2_ut
```

```
<vamp2.uti.f90>≡  
  <File header>
```

```
module vamp2_uti  
  <Use kinds>  
  use io_units  
  use constants, only: pi  
  use numeric_utils, only: nearly_equal  
  use format_defs, only: FMT_12  
  use rng_base  
  use rng_stream  
  use vegas, only: vegas_func_t, vegas_grid_t, operator(==)  
  use vamp2
```

```
  <Standard module head>
```

```
  <vamp2: test declaration>
```

```
  <vamp2: test types>
```

```
contains  
  <vamp2: tests>  
end module vamp2_uti
```

API: driver for the unit tests below.

```
<vamp2: public test>≡
```

```
  public :: vamp2_test
```

```
<vamp2: test driver>≡
```

```
  subroutine vamp2_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <vamp2: execute tests>  
  end subroutine vamp2_test
```


Test function

We use the example from the Monte Carlo Examples of the GSL library

$$I = \int_{-pi}^{+pi} dk_x / (2pi) \int_{-pi}^{+pi} dk_y / (2pi) \int_{-pi}^{+pi} dk_z / (2pi) 1 / (1 - \cos(k_x) \cos(k_y) \cos(k_z)). \quad (20.15)$$

The integral is reduced to region $(0,0,0) \rightarrow (\pi, \pi, \pi)$ and multiplied by 8.

```

<vamp2: test types>≡
    type, extends (vamp2_func_t) :: vamp2_test_func_t
    !
    contains
    <vamp2: vamp2 test func: TBP>
end type vamp2_test_func_t

<vamp2: vamp2 test func: TBP>≡
    procedure, public :: evaluate_maps => vamp2_test_func_evaluate_maps

<vamp2: tests>≡
    subroutine vamp2_test_func_evaluate_maps (self, x)
        class(vamp2_test_func_t), intent(inout) :: self
        real(default), dimension(:), intent(in) :: x
        self%xi(:, 1) = x
        self%det(1) = 1
        self%valid_x = .true.
    end subroutine vamp2_test_func_evaluate_maps

```

Evaluate the integrand.

```

<vamp2: vamp2 test func: TBP>+≡
    procedure, public :: evaluate_func => vamp2_test_func_evaluate

<vamp2: tests>+≡
    real(default) function vamp2_test_func_evaluate (self, x) result (f)
        class(vamp2_test_func_t), intent(in) :: self
        real(default), dimension(:), intent(in) :: x
        f = 1.0 / (pi**3)
        f = f / ( 1.0 - cos (x(1)) * cos (x(2)) * cos (x(3)))
    end function vamp2_test_func_evaluate

```

The second test function implements

$$f(\vec{x}) = 4 \sin^2(\pi x_1) \sin^2(\pi x_2) + 2 \sin^2(\pi v), \quad (20.16)$$

where

$$x = u^v y = u^{1-v} \quad (20.17)$$

$$u = xyv = \frac{1}{2} \left(1 + \frac{\log(x/y)}{\log(xy)} \right). \quad (20.18)$$

The jacobian is $\frac{\partial(x,y)}{\partial(u,v)}$.

```

<vamp2: test types>+≡
    type, extends(vamp2_func_t) :: vamp2_test_func_2_t

```

```

!
contains
  <vamp2: vamp2 test func 2: TBP>
end type vamp2_test_func_2_t

```

Evaluate maps.

```

<vamp2: vamp2 test func 2: TBP>≡
  procedure :: evaluate_maps => vamp2_test_func_2_evaluate_maps
<vamp2: tests>+≡
  subroutine vamp2_test_func_2_evaluate_maps (self, x)
    class(vamp2_test_func_2_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    select case (self%current_channel)
    case (1)
      self%xi(:, 1) = x
      self%xi(1, 2) = x(1) * x(2)
      self%xi(2, 2) = 0.5 * ( 1. + log(x(1) / x(2)) / log(x(1) * x(2)))
    case (2)
      self%xi(1, 1) = x(1)**x(2)
      self%xi(2, 1) = x(1)**(1. - x(2))
      self%xi(:, 2) = x
    end select
    self%det(1) = 1.
    self%det(2) = abs (log(self%xi(1, 2)))
    self%valid_x = .true.
  end subroutine vamp2_test_func_2_evaluate_maps

```

Evaluate func.

```

<vamp2: vamp2 test func 2: TBP>+≡
  procedure :: evaluate_func => vamp2_test_func_2_evaluate_func
<vamp2: tests>+≡
  real(default) function vamp2_test_func_2_evaluate_func (self, x) result (f)
    class(vamp2_test_func_2_t), intent(in) :: self
    real(default), dimension(:), intent(in) :: x
    f = 4. * sin(pi * self%xi(1, 1))**2 * sin(pi * self%xi(2, 1))**2 &
      + 2. * sin(pi * self%xi(2, 2))**2
  end function vamp2_test_func_2_evaluate_func

```

The third test function implements

$$f(\vec{x}) = 5x_1^4 + 5(1 - x_1)^4, \quad (20.19)$$

where

$$x_1 = u^{1/5} \quad \vee \quad x_1 = 1 - v^{1/5} \quad (20.20)$$

The jacobians are $\frac{\partial x_1}{\partial u} = \frac{1}{5}u^{-4/5}$ and $\frac{\partial x_1}{\partial v} = \frac{1}{5}v^{-4/5}$.

```

<vamp2: test types>+≡
  type, extends(vamp2_func_t) :: vamp2_test_func_3_t
  !
  contains
    <vamp2: vamp2 test func 3: TBP>
  end type vamp2_test_func_3_t

```

Evaluate maps.

```

<vamp2: vamp2 test func 3: TBP>≡
  procedure :: evaluate_maps => vamp2_test_func_3_evaluate_maps

<vamp2: tests>+≡
  subroutine vamp2_test_func_3_evaluate_maps (self, x)
    class(vamp2_test_func_3_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    real(default) :: u, v, xx
    select case (self%current_channel)
    case (1)
      u = x(1)
      xx = u**0.2_default
      v = (1 - xx)**5._default
    case (2)
      v = x(1)
      xx = 1 - v**0.2_default
      u = xx**5._default
    end select
    self%det(1) = 0.2_default * u**(-0.8_default)
    self%det(2) = 0.2_default * v**(-0.8_default)
    self%xi(:, 1) = [u]
    self%xi(:, 2) = [v]
    self%valid_x = .true.
  end subroutine vamp2_test_func_3_evaluate_maps

```

Evaluate func.

```

<vamp2: vamp2 test func 3: TBP>+≡
  procedure :: evaluate_func => vamp2_test_func_3_evaluate_func

<vamp2: tests>+≡
  real(default) function vamp2_test_func_3_evaluate_func (self, x) result (f)
    class(vamp2_test_func_3_t), intent(in) :: self
    real(default), dimension(:), intent(in) :: x
    real(default) :: xx
    select case (self%current_channel)
    case (1)
      xx = x(1)**0.2_default
    case (2)
      xx = 1 - x(1)**0.2_default
    end select
    f = 5 * xx**4 + 5 * (1 - xx)**4
  end function vamp2_test_func_3_evaluate_func

```

MC Integrator check

We reproduce the first test case of VEGAS. Initialise the VAMP2 MC integrator and call to `vamp2_init.grid` for the initialisation of the grid.

```

<vamp2: execute tests>≡
  call test (vamp2_1, "vamp2_1", "VAMP2 initialisation and&
    & grid preparation", u, results)

```

```

<vamp2: test declaration>≡
    public :: vamp2_1
<vamp2: tests>+≡
    subroutine vamp2_1 (u)
        integer, intent(in) :: u
        type(vamp2_t) :: mc_integrator
        class(rng_t), allocatable :: rng
        class(vamp2_func_t), allocatable :: func
        real(default), dimension(3), parameter :: x_lower = 0., &
            x_upper = pi
        real(default) :: result, abserr

        write (u, "(A)") "* Test output: vamp2_1"
        write (u, "(A)") "* Purpose: initialise the VAMP2 MC integrator and the grid"
        write (u, "(A)")

        write (u, "(A)") "* Initialise random number generator (default seed)"
        write (u, "(A)")

        allocate (rng_stream_t :: rng)
        call rng%init ()

        call rng%write (u)

        write (u, "(A)")
        write (u, "(A)") "* Initialise MC integrator with n_channel = 1 and n_dim = 3"
        write (u, "(A)")

        allocate (vamp2_test_func_t :: func)
        call func%init (n_dim = 3, n_channel = 1)
        mc_integrator = vamp2_t (1, 3)
        call mc_integrator%write (u)

        write (u, "(A)")
        write (u, "(A)") "* Initialise grid with n_calls = 10000"
        write (u, "(A)")

        call mc_integrator%set_limits (x_lower, x_upper)
        call mc_integrator%set_calls (10000)

        write (u, "(A)")
        write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
        write (u, "(A)")

        call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
        write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

        write (u, "(A)")
        write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
        write (u, "(A)")

        call mc_integrator%set_calls (2000)
        call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
        write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

```

```

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vamp2_1

```

Integrate a function with two-dimensional argument and two channels.

```

<vamp2: execute tests>+≡
  call test (vamp2_2, "vamp2_2", "VAMP2 intgeration of two-dimensional &
    & function with two channels", u, results)

<vamp2: test declaration>+≡
  public :: vamp2_2

<vamp2: tests>+≡
  subroutine vamp2_2 (u)
    integer, intent(in) :: u
    type(vamp2_t) :: mc_integrator
    class(rng_t), allocatable :: rng
    class(vamp2_func_t), allocatable :: func
    real(default), dimension(2), parameter :: x_lower = 0., &
      x_upper = 1.
    real(default) :: result, abserr

    write (u, "(A)") "* Test output: vamp2_2"
    write (u, "(A)") "* Purpose: intgeration of two-dimensional &
      & function with two channels"
    write (u, "(A)")

    write (u, "(A)") "* Initialise random number generator (default seed)"
    write (u, "(A)")

    allocate (rng_stream_t :: rng)
    call rng%init ()

    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Initialise MC integrator with n_channel = 1 and n_dim = 3"
    write (u, "(A)")

    allocate (vamp2_test_func_2_t :: func)
    call func%init (n_dim = 2, n_channel = 2)
    mc_integrator = vamp2_t (2, 2)
    call mc_integrator%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Initialise grid with n_calls = 10000"
    write (u, "(A)")

    call mc_integrator%set_limits (x_lower, x_upper)
    call mc_integrator%set_calls (1000)

```

```

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, verbose = .true., result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 2000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (200)
call mc_integrator%integrate (func, rng, 3, verbose = .true., result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vamp2_2

```

Integrate a function with two-dimensional argument and two channels.

```

<vamp2: execute tests>+≡
  call test (vamp2_3, "vamp2_3", "VAMP2 intgeration of two-dimensional &
    & function with two channels", u, results)

<vamp2: test declaration>+≡
  public :: vamp2_3

<vamp2: tests>+≡
  subroutine vamp2_3 (u)
    integer, intent(in) :: u
    type(vamp2_t) :: mc_integrator
    class(rng_t), allocatable :: rng
    class(vamp2_func_t), allocatable :: func
    real(default), dimension(2), parameter :: x_lower = 0., &
      x_upper = 1.
    real(default) :: result, abserr
    integer :: unit

    write (u, "(A)") "* Test output: vamp2_3"
    write (u, "(A)") "* Purpose: intgeration of two-dimensional &
      & function with two channels"
    write (u, "(A)")

    write (u, "(A)") "* Initialise random number generator (default seed)"
    write (u, "(A)")

    allocate (rng_stream_t :: rng)
    call rng%init ()

    call rng%write (u)

```

```

write (u, "(A)")
write (u, "(A)") "* Initialise MC integrator with n_channel = 1 and n_dim = 3"
write (u, "(A)")

allocate (vamp2_test_func_2_t :: func)
call func%init (n_dim = 2, n_channel = 2)
mc_integrator = vamp2_t (2, 2)
call mc_integrator%write (u)

write (u, "(A)")
write (u, "(A)") "* Initialise grid with n_calls = 20000"
write (u, "(A)")

call mc_integrator%set_limits (x_lower, x_upper)
call mc_integrator%set_calls (20000)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 20000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Write grid to file vamp2_3.grids"
write (u, "(A)")

unit = free_unit ()
open (unit, file = "vamp2_3.grids", &
      action = "write", status = "replace")
call mc_integrator%write_grids (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Read grid from file vamp2_3.grids"
write (u, "(A)")

call mc_integrator%final ()

unit = free_unit ()
open (unit, file = "vamp2_3.grids", &
      action = "read", status = "old")
call mc_integrator%read_grids (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 5000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (5000)
call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

```

```

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vamp2_3

```

Integrate a function with two-dimensional argument and two channels. Use chained weights, although we average over each weight itself.

```

<vamp2: execute tests>+≡
  call test (vamp2_4, "vamp2_4", "VAMP2 intgeration of two-dimensional &
    & function with two channels with chains", u, results)

<vamp2: test declaration>+≡
  public :: vamp2_4

<vamp2: tests>+≡
  subroutine vamp2_4 (u)
    integer, intent(in) :: u
    type(vamp2_t) :: mc_integrator
    class(rng_t), allocatable :: rng
    class(vamp2_func_t), allocatable :: func
    real(default), dimension(2), parameter :: x_lower = 0., &
      x_upper = 1.
    real(default) :: result, abserr
    integer :: unit

    write (u, "(A)") "* Test output: vamp2_4"
    write (u, "(A)") "* Purpose: intgeration of two-dimensional &
      & function with two channels with chains"
    write (u, "(A)")

    write (u, "(A)") "* Initialise random number generator (default seed)"
    write (u, "(A)")

    allocate (rng_stream_t :: rng)
    call rng%init ()

    call rng%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Initialise MC integrator with n_channel = 2 and n_dim = 2"
    write (u, "(A)")

    allocate (vamp2_test_func_2_t :: func)
    call func%init (n_dim = 2, n_channel = 2)
    mc_integrator = vamp2_t (2, 2)
    call mc_integrator%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Initialise grid with n_calls = 20000 and set chains"
    write (u, "(A)")

    call mc_integrator%set_limits (x_lower, x_upper)

```



```

call mc_integrator%set_calls (20000)
call mc_integrator%set_chain (2, [1, 2])

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 10000 (Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Write grid to file vamp2_4.grids"
write (u, "(A)")

unit = free_unit ()
open (unit, file = "vamp2_4.grids", &
      action = "write", status = "replace")
call mc_integrator%write_grids (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Read grid from file vamp2_4.grids"
write (u, "(A)")

call mc_integrator%final ()

unit = free_unit ()
open (unit, file = "vamp2_4.grids", &
      action = "read", status = "old")
call mc_integrator%read_grids (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 5000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (5000)
call mc_integrator%integrate (func, rng, 3, result=result, abserr=abserr)
write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ")") "Result: ", result, " +/- ", abserr

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vamp2_4

```

<vamp2: execute tests>+≡

```

call test (vamp2_5, "vamp2_5", "VAMP2 intgeration of two-dimensional &
& function with two channels with equivalences", u, results)

```

<vamp2: test declaration>+≡

```

public :: vamp2_5

```

```

<vamp2: tests>+≡
subroutine vamp2_5 (u)
  integer, intent(in) :: u
  type(vamp2_t) :: mc_integrator
  class(rng_t), allocatable :: rng
  class(vamp2_func_t), allocatable :: func
  real(default), dimension(1), parameter :: x_lower = 0., &
    x_upper = 1.
  real(default) :: result, abserr
  integer :: unit
  type(vamp2_config_t) :: config
  type(vamp2_equivalences_t) :: eqv
  type(vegas_grid_t), dimension(2) :: grid

  write (u, "(A)") "* Test output: vamp2_5"
  write (u, "(A)") "* Purpose: intgeration of two-dimensional &
    & function with two channels with equivalences"
  write (u, "(A)")

  write (u, "(A)") "* Initialise random number generator (default seed)"
  write (u, "(A)")

  allocate (rng_stream_t :: rng)
  call rng%init ()

  call rng%write (u)

  write (u, "(A)")
  write (u, "(A)") "* Initialise MC integrator with n_channel = 2 and n_dim = 1"
  write (u, "(A)")

  allocate (vamp2_test_func_3_t :: func)
  call func%init (n_dim = 1, n_channel = 2)
  config%equivalences = .true.
  mc_integrator = vamp2_t (n_channel = 2, n_dim = 1)
  call mc_integrator%set_config (config)
  call mc_integrator%write (u)

  write (u, "(A)")
  write (u, "(A)") "* Initialise grid with n_calls = 20000 and set chains"
  write (u, "(A)")

  call mc_integrator%set_limits (x_lower, x_upper)
  call mc_integrator%set_calls (20000)

  write (u, "(A)")
  write (u, "(A)") "* Initialise equivalences"
  write (u, "(A)")

  eqv = vamp2_equivalences_t (n_eqv = 4, n_channel = 2, n_dim = 1)
  call eqv%set_equivalence &
    (i_eqv = 1, dest = 2, src = 1, perm = [1], mode = [VEQ_IDENTITY])
  call eqv%set_equivalence &
    (i_eqv = 2, dest = 1, src = 2, perm = [1], mode = [VEQ_IDENTITY])

```

```

call eqv%set_equivalence &
    (i_eqv = 3, dest = 1, src = 1, perm = [1], mode = [VEQ_IDENTITY])
call eqv%set_equivalence &
    (i_eqv = 4, dest = 2, src = 2, perm = [1], mode = [VEQ_IDENTITY])
call eqv%write (u)
call mc_integrator%set_equivalences (eqv)

write (u, "(A)")
write (u, "(A)") &
    "* Integrate with n_it = 3 and n_calls = 10000 (Grid-only Adaptation)"
write (u, "(A)")

call mc_integrator%integrate (func, rng, 3, &
    adapt_weights = .false., result=result, abserr=abserr)
if (nearly_equal &
    (result, 2.000_default, rel_smallness = 0.003_default)) then
    write (u, "(2x,A)") "Result: 2.000 [ok]"
else
    write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ",A)") &
        "Result: ", result, " +/- ", abserr, " [not ok]"
end if

write (u, "(A)")
write (u, "(A)") "* Compare the grids of both channels"
write (u, "(A)")

grid(1) = mc_integrator%get_grid(channel = 1)
grid(2) = mc_integrator%get_grid(channel = 2)

write (u, "(2X,A,1X,L1)") "Equal grids =", (grid(1) == grid(2))

write (u, "(A)")
write (u, "(A)") "* Write grid to file vamp2_5.grids"
write (u, "(A)")

unit = free_unit ()
open (unit, file = "vamp2_5.grids", &
    action = "write", status = "replace")
call mc_integrator%write_grids (unit)
close (unit)

write (u, "(A)")
write (u, "(A)") "* Integrate with n_it = 3 and n_calls = 5000 (Precision)"
write (u, "(A)")

call mc_integrator%set_calls (5000)
call mc_integrator%integrate (func, rng, 3, adapt_weights = .false., &
    refine_grids = .false., result=result, abserr=abserr)
if (nearly_equal &
    (result, 2.000_default, rel_smallness = 0.003_default)) then
    write (u, "(2x,A)") "Result: 2.000 [ok]"
else
    write (u, "(2x,A," // FMT_12 // ",A," // FMT_12 // ",A)") &
        "Result: ", result, " +/- ", abserr, " [not ok]"

```

```

end if

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mc_integrator%final ()
call rng%final ()
deallocate (rng)
end subroutine vamp2_5

```

20.15 MPI Request

Request Direct interface for requests.

Balancer Sublibrary interfaces and types for implementation into **request**.

Callback Direct interface for non-blocking communication in callback fashion used in subsidiary in **request**.

20.15.1 Request Base

request Container type for current request, contains handler index and status of request.

request group cache Caching for communicator groups, tries to reduce the costly calls to `MPI_CREATE_COMM_GROUP`.

request base Base type for request handling, defines procedures and basic request scheme for direct implementation into **VAMP2**.

When a data type has an associated communicator field, it always must duplicate the communicator in order to ensure communication encapsulation. Only in special case (e.g. outside of object communication is required) the parent communicator should be directly used. For example, that is the case for the group cache, as it exports its newly created communicator to the outside of the request library.

```

(request_base.f90)≡
<File header>
module request_base
  use io_units

  use diagnostics

  use balancer_base
  use request_callback
  use mpi_f08 !NODEP!

  implicit none

  private

```

```

type :: request_t
  integer :: handler_id = 0
  logical :: terminate = .false.
  logical :: group = .false.
  logical :: group_master = .false.
  logical :: callback = .false.
  type(MPI_COMM) :: comm
end type request_t

type :: request_group_cache_t
  private
  type(MPI_COMM) :: parent_comm
  type(MPI_GROUP) :: parent_group
  type(MPI_COMM) :: comm
  type(MPI_GROUP) :: group
  integer, dimension(:), allocatable :: rank
contains
  procedure :: init => request_group_cache_init
  procedure :: reset => request_group_cache_reset
  procedure :: update => request_group_cache_update
  procedure :: get_comm => request_group_cache_get_comm
  procedure :: is_master => request_group_cache_is_master
end type request_group_cache_t

!> Base type for requesting and back calling.
!!
!! A short remark on the semantics of point-to-point communication (as its intended use in this
!! MPI is strict regarding the order of the messages (for blocking communication), as those can
!! For non-blocking communication, the standard extends it such that the order depends on "the e
!! The non-overtaking requirement is then extended to this definition of order.
!!
!! Color method for tracking communication?
!! We restrict each slave to a single callback (at once), which can communicate during the next
!! Before handling the next (current) callback, the former one has to finish (with a wait call o
!! On the server-side, we only test on the finishing, reporting a communication failure.
!!
!! Furthermore, the implementation has to take care that the order of the communication calls on
!!
!! Therefore, we need to secure the order of communication calls.
!! First, we let the master initiate all callback communication *before* polling.
!! This fixiates the order.
!! Second, we require that the implementation of the polling honors this order.
type, abstract :: request_base_t
  type(MPI_COMM) :: comm
  type(MPI_COMM) :: external_comm !! communicator for use outside of request, however, just a d
  class(balancer_base_t), allocatable :: balancer
  type(request_group_cache_t) :: cache
  type(request_handler_manager_t) :: handler
contains
  procedure :: base_init => request_base_init
  procedure :: base_write => request_base_write
  procedure(request_base_deferred_write), deferred :: write
  procedure :: is_master => request_base_is_master
  procedure(request_base_has_workers), deferred :: has_workers

```

```

    procedure :: get_external_comm => request_base_get_external_comm
    procedure :: add_balancer => request_base_add_balancer
    procedure :: add_handler => request_base_add_handler
    procedure :: reset => request_base_reset
    procedure :: call_handler => request_base_call_handler
    procedure :: call_client_handler => request_base_call_client_handler
    procedure :: await_handler => request_base_await_handler
    procedure :: barrier => request_base_barrier
    procedure(request_base_request_workload), deferred :: request_workload
    procedure(request_base_release_workload), deferred :: release_workload
    procedure(request_base_handle_and_release_workload), deferred :: handle_and_release_workload
end type request_base_t

!> The basic idea behind the request mechanism is that each associated worker can request a work
!!
!! We note that it is not necessary to differentiate between master and worker on this level of
!! Hence, the request interface ignores any notion regarding a possible parallelization concept.
abstract interface
    subroutine request_base_deferred_write (req, unit)
        import :: request_base_t
        class(request_base_t), intent(in) :: req
        integer, intent(in), optional :: unit
    end subroutine request_base_deferred_write

!> Verify if request object has workers.
!!
!! An implementation shall return if there at least two workers, or otherwise stated,
!! one master and one slave at least, when both are used as computing ranks.
logical function request_base_has_workers (req) result (flag)
    import :: request_base_t
    class(request_base_t), intent(in) :: req
end function request_base_has_workers

!> Request workload and returns an request_t object.
!!
!! The request_t object has an associated handler_id and provide several ways
!! to indicate whether the execution is to be terminated, or the request has an associated co
!! Finally, whether we expect that the handler id will be connected to an callback.
!!
!! \param[out] request Request container.
subroutine request_base_request_workload (req, request)
    import :: request_base_t, request_t
    class(request_base_t), intent(inout) :: req
    type(request_t), intent(out) :: request
end subroutine request_base_request_workload

!> Release workload with the information from the request container.
!!
!! The release procedure may notify the master about the finishing of the workload associated
!! Or, it may just bookkeep whether the workload has finished.
!! Additionally, if request%callback was true, it could handle the callback (from client side
subroutine request_base_release_workload (req, request)
    import :: request_base_t, request_t
    class(request_base_t), intent(inout) :: req

```

```

        type(request_t), intent(in) :: request
    end subroutine request_base_release_workload

    !> Handle associated callback and release workload with the information from the request cont
    !!
    !! The procedure must call the associated callback handler using the handler_id.
    !! Remark: The callback manager is quite squishy regarding a missing handler (silent failure)
    !!         The procedure has to take care whether the callback was actually successful.
    !! The further release of the workload can then be deferred to the release_workload procedure
    !! \param[in] request.
    subroutine request_base_handle_and_release_workload (req, request)
        import :: request_base_t, request_t
        class(request_base_t), intent(inout) :: req
        type(request_t), intent(in) :: request
    end subroutine request_base_handle_and_release_workload
end interface

public :: request_t, request_base_t
contains

subroutine request_group_cache_init (cache, comm)
    class(request_group_cache_t), intent(inout) :: cache
    type(MPI_COMM), intent(in) :: comm
    call MPI_COMM_DUP (comm, cache%parent_comm)
    !! Local operation.
    call MPI_COMM_GROUP (cache%parent_comm, cache%parent_group)
    cache%group = MPI_GROUP_EMPTY
    cache%comm = MPI_COMM_NULL
end subroutine request_group_cache_init

subroutine request_group_cache_reset (cache)
    class(request_group_cache_t), intent(inout) :: cache
    cache%group = MPI_GROUP_EMPTY
    cache%comm = MPI_COMM_NULL
end subroutine request_group_cache_reset

subroutine request_group_cache_update (cache, tag, rank)
    class(request_group_cache_t), intent(inout) :: cache
    integer, intent(in) :: tag
    integer, dimension(:), allocatable, intent(inout) :: rank
    type(MPI_GROUP) :: group
    integer :: result, error
    call move_alloc (rank, cache%rank)
    call MPI_GROUP_INCL (cache%parent_group, size (cache%rank), cache%rank, group)
    call MPI_GROUP_COMPARE (cache%group, group, result)
    if (result /= MPI_IDENT) then
        cache%group = group
        if (cache%comm /= MPI_COMM_NULL) call MPI_COMM_FREE (cache%comm)
        !! Group-local operation. However, time consuming.
        call MPI_COMM_CREATE_GROUP (cache%parent_comm, cache%group, tag, &
            cache%comm, error)
        if (error /= 0) then
            call msg_bug ("Error occurred during communicator creation...")
        end if
    end if
end if

```

```

! else
! call msg_message ("CACHE UPDATE: GROUPS ARE (NEARLY) IDENTICAL")
end if
end subroutine request_group_cache_update

subroutine request_group_cache_get_comm (cache, comm)
class(request_group_cache_t), intent(in) :: cache
type(MPI_COMM), intent(out) :: comm
comm = cache%comm
end subroutine request_group_cache_get_comm

logical function request_group_cache_is_master (cache) result (flag)
class(request_group_cache_t), intent(in) :: cache
integer :: rank, error
call MPI_COMM_RANK (cache%comm, rank, error)
if (error /= 0) then
call msg_bug ("Error: Could not retrieve group rank.")
end if
flag = (rank == 0)
end function request_group_cache_is_master

!! =====
!! request_base_t
!! =====

!> Initialize request base with parent communicator.
!!
!! In order to separate the communication between different parts of the request library,
!! duplicate the parent communicator using MPI_COMM_DUP, also done by cache and handler objects.
!!
!! \param[in] comm Parent MPI communicator for overall library.
subroutine request_base_init (req, comm)
class(request_base_t), intent(out) :: req
type(MPI_COMM), intent(in) :: comm
call MPI_COMM_DUP (comm, req%comm)
call MPI_COMM_DUP (comm, req%external_comm)
call req%cache%init (comm)
call req%handler%init (comm)
end subroutine request_base_init

subroutine request_base_write (req, unit)
class(request_base_t), intent(in) :: req
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit)
if (allocated (req%balancer)) then
call req%balancer%write (u)
else
write (u, "(A)") "[BALANCER]"
write (u, "(A)") "=> Not allocated"
end if
call req%handler%write (u)
end subroutine request_base_write

```



```

!> Check whether current worker is master rank in object communicator.
!!
!! Do not confuse with a group's master !!!
!! Proof: rank == 0
logical function request_base_is_master (req) result (flag)
  class(request_base_t), intent(in) :: req
  integer :: rank, ierr
  call MPI_COMM_RANK (req%comm, rank, ierr)
  if (ierr /= 0) then
    write (*, "(A,1X,I0)") "MPI Error: request_base_is_master", ierr
    stop 1
  end if
  flag = (rank == 0)
end function request_base_is_master

!> Provide external communicator.
!!
!! The external communicator is just a duplicate of request%comm,
!! in order to provide the same group of workers to external communication,
!! however, in a different context, such that communication from outside does not interfere with
subroutine request_base_get_external_comm (req, comm)
  class(request_base_t), intent(in) :: req
  type(MPI_COMM), intent(out) :: comm
  comm = req%external_comm
end subroutine request_base_get_external_comm

!> Add balancer to request.
!!
!! \param[inout] balancer
subroutine request_base_add_balancer (req, balancer)
  class(request_base_t), intent(inout) :: req
  class(balancer_base_t), allocatable, intent(inout) :: balancer
  if (allocated (req%balancer)) deallocate (req%balancer)
  call move_alloc (balancer, req%balancer)
end subroutine request_base_add_balancer

!> Add request handler with handler_id.
!!
!! \param[in] handler_id
!! \param[in] handler Pointer to handler object.
subroutine request_base_add_handler (req, handler_id, handler)
  class(request_base_t), intent(inout) :: req
  integer, intent(in) :: handler_id
  class(request_handler_t), pointer, intent(in) :: handler
  call req%handler%add (handler_id, handler)
end subroutine request_base_add_handler

!> Reset request.
!! Clear handler manager from associated callbacks,
!! deallocate balancer, iff allocated, and reset communicator cache.
subroutine request_base_reset (req, deallocate_balancer)
  class(request_base_t), intent(inout) :: req
  logical, intent(in), optional :: deallocate_balancer
  logical :: flag

```

```

        flag = .false.; if (present (deallocate_balancer)) &
            flag = deallocate_balancer
        if (flag .and. allocated (req%balancer)) then
            deallocate (req%balancer)
        end if
        call req%handler%clear ()
        call req%cache%reset ()
    end subroutine request_base_reset

    !> Call handler for master communication for handler_id.
    !!
    !! \param[in] handler_id The associated key of the callback object.
    !! \param[in] source_rank The rank of the result's source.
    subroutine request_base_call_handler (req, handler_id, source_rank)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: handler_id
        integer, intent(in) :: source_rank
        call req%handler%callback (handler_id, source_rank)
    end subroutine request_base_call_handler

    !> Call handler for slave communication for handler_id.
    !!
    !! \param[in] handler_id The associated key of the callback object.
    subroutine request_base_call_client_handler (req, handler_id)
        class(request_base_t), intent(inout) :: req
        integer, intent(in) :: handler_id
        call req%handler%client_callback (handler_id, 0)
    end subroutine request_base_call_client_handler

    !> Wait on all handler in request handler manager to finish communication.
    subroutine request_base_await_handler (req)
        class(request_base_t), intent(inout) :: req
        call req%handler%waitall ()
    end subroutine request_base_await_handler

    subroutine request_base_barrier (req)
        class(request_base_t), intent(in) :: req
        integer :: error
        call MPI_BARRIER (req%comm, error)
        if (error /= MPI_SUCCESS) then
            call msg_fatal ("Request: Error occurred during MPI_BARRIER synchronisation.")
        end if
    end subroutine request_base_barrier
end module request_base

```

20.15.2 Request Simple

We implement a local request scheme, without any additional communication, except the callback communication.

```

(request_simple.f90)≡
<File header>
module request_simple
    use io_units

```

```

use diagnostics

use array_list

use balancer_base
use balancer_simple
use request_base

use mpi_f08 !NODEP!

implicit none

private

type, extends (request_base_t) :: request_simple_t
    integer :: n_workers = 0
    integer :: n_channels = 0
    logical, dimension(:), allocatable :: parallel_grid
contains
    procedure :: init => request_simple_init
    procedure :: write => request_simple_write
    procedure :: has_workers => request_simple_has_workers
    procedure :: update => request_simple_update
    procedure :: get_request_master => request_simple_get_request_master
    !! deferred.
    procedure :: request_workload => request_simple_request_workload
    procedure :: release_workload => request_simple_release_workload
    procedure :: handle_and_release_workload => request_simple_handle_and_release_workload
end type request_simple_t

public :: request_simple_t
contains
    subroutine request_simple_init (req, comm, n_channels)
        class(request_simple_t), intent(out) :: req
        type(MPI_COMM), intent(in) :: comm
        integer, intent(in) :: n_channels
        integer :: n_workers
        call req%base_init (comm)
        call MPI_COMM_SIZE (req%comm, req%n_workers)
        req%n_channels = n_channels
        allocate (req%parallel_grid (n_channels), source = .false.)
        call allocate_balancer ()
contains
        subroutine allocate_balancer ()
            class(balancer_base_t), allocatable :: balancer
            allocate (balancer_simple_t :: balancer)
            select type (balancer)
            type is (balancer_simple_t)
                call balancer%init (n_workers = req%n_workers, n_resources = req%n_channels)
            end select
            call req%add_balancer (balancer)
        end subroutine allocate_balancer
    end subroutine request_simple_init

```

```

!!> Update number of channels and parallel grids.
!!
!! The simple request object does not utilize the request balancer, as the complexity of the req
!! The simple approach assigns each worker several channel by a modular mapping from the set of
!! Vetoing on those channel which have a parallel grid (check the definition in vegas.f90), when
!!
!!  $w = \phi(c) = (c - 1) \bmod N$ , if not  $P(c)$ , else forall  $w$  to  $c$ .
!!
!! The information is stored in a dynamic-sized array list, which is filled, reversed and then u
!! Assigned and finished channels are then moved to the finished stack.
subroutine request_simple_update (req, parallel_grid)
  class(request_simple_t), intent(inout) :: req
  logical, dimension(:), intent(in) :: parallel_grid
  integer :: me, worker
  call req%reset ()
  call MPI_COMM_RANK (req%comm, me)
  worker = SHIFT_RANK_TO_WORKER(me)
  select type (balancer => req%balancer)
  type is (balancer_simple_t)
    call balancer%update_state (worker, parallel_grid)
  end select
  req%parallel_grid = parallel_grid
end subroutine request_simple_update

subroutine request_simple_write (req, unit)
  class(request_simple_t), intent(in) :: req
  integer, intent(in), optional :: unit
  integer :: u, n_size
  u = given_output_unit (unit)
  write (u, "(A)") "[REQUEST_SIMPLE]"
  write (u, "(A,1X,I0)") "N_CHANNELS", req%n_channels
  write (u, "(A,1X,I0)") "N_WORKERS", req%n_workers
  n_size = min (25, req%n_channels)
  write (u, "(A,25(1X,L1))") "PARALLEL_GRID", req%parallel_grid(:n_size)
  call req%base_write (u)
end subroutine request_simple_write

logical function request_simple_has_workers (req) result (flag)
  class(request_simple_t), intent(in) :: req
  flag = (req%n_workers > 1)
end function request_simple_has_workers

integer function request_simple_get_request_master (req, channel) &
  result (rank)
  class(request_simple_t), intent(in) :: req
  integer, intent(in) :: channel
  if (.not. allocated (req%balancer)) then
    call msg_bug ("Error: Balancer is not allocated.")
  end if
  rank = shift_worker_to_rank (req%balancer%get_resource_master (channel))
  !! "Caveat emptor" hits here:
  !! The balancer returns either a valid worker id or (-1) depending on the associated resource
  !! We have to check whether returned worker index is plausible.
end function request_simple_get_request_master

```

```

!> Request workload.
!!
!! Depending on parallel_grid, we fill the request object differently.
!! First, we do not set commuicator for .not. parallel_grid (group and group master are set to
!! And the callback needs to be executed.
!! Second, for parallel_grid, we set req%comm to the associated communicator and set group to .t
!! However, the overall master has the grid's result, therefore, only the master needs to the ca
!! Remark: We can actually intercept the callback for the master to himself; the results are alr
subroutine request_simple_request_workload (req, request)
  class(request_simple_t), intent(inout) :: req
  type(request_t), intent(out) :: request
  integer :: rank, worker_id
  call MPI_COMM_RANK (req%comm, rank)
  worker_id = shift_rank_to_worker (rank)
  if (.not. req%balancer%is_pending () &
      .or. .not. req%balancer%is_assignable (worker_id)) then
    request%terminate = .true.
    return
  end if
  call req%balancer%assign_worker (worker_id, request%handler_id)
  associate (channel => request%handler_id)
    if (req%parallel_grid (channel)) then
      request%comm = req%external_comm
      request%group = .true.
      !! The object communicator is master.
      request%group_master = &
        (req%get_request_master (channel) == rank)
      request%callback = req%is_master ()
    else
      request%comm = req%external_comm
      request%group = .false.
      request%group_master = .true.
      request%callback = .true.
    end if
  end associate
end subroutine request_simple_request_workload

subroutine request_simple_release_workload (req, request)
  class(request_simple_t), intent(inout) :: req
  type(request_t), intent(in) :: request
  integer :: rank, worker_id
  call MPI_COMM_RANK (req%comm, rank)
  worker_id = shift_rank_to_worker (rank)
  call req%balancer%free_worker (worker_id, request%handler_id)
end subroutine request_simple_release_workload

subroutine request_simple_handle_and_release_workload (req, request)
  class(request_simple_t), intent(inout) :: req
  type(request_t), intent(in) :: request
  call req%call_client_handler (request%handler_id)
  call req%release_workload (request)
end subroutine request_simple_handle_and_release_workload
end module request_simple

```

20.15.3 Request Caller

We implement an global queue approach, requiring permanent communication between a governor and the worker.

```
(request_caller.f90)≡
  <File header>
  module request_caller
    use kinds, only: default
    use io_units
    use diagnostics

    use request_base
    use balancer_base
    use balancer_channel
    use request_state
    use request_callback

    use mpi_f08 !NODEP!

    implicit none

    private

    type, extends (request_base_t) :: request_caller_t
      private
      integer :: n_channels = 0
      integer :: n_workers = 0
      type(request_state_t) :: state
    contains
      procedure :: init => request_caller_init
      procedure :: write => request_caller_write
      procedure :: has_workers => request_caller_has_workers
      procedure :: update_balancer => request_caller_update_balancer
      procedure :: handle_workload => request_caller_handle_workload
      procedure :: request_workload => request_caller_request_workload
      procedure :: release_workload => request_caller_release_workload
      procedure :: handle_and_release_workload => request_caller_handle_and_release_workload
      procedure :: request_terminate => request_caller_request_terminate
    end type request_caller_t

    public :: request_caller_t
  contains

    subroutine request_caller_init (req, comm, n_channels)
      class(request_caller_t), intent(out) :: req
      type(MPI_COMM), intent(in) :: comm
      integer, intent(in) :: n_channels
      call req%base_init (comm)
      call MPI_COMM_SIZE (req%comm, req%n_workers)
      !! Exclude master rank (0) from set of workers.
      req%n_workers = req%n_workers - 1
      if (.not. req%has_workers ()) then
        call msg_warning ("Must not handle less than 3 ranks in a master/slave global queue.")
        call MPI_ABORT (req%comm, 1)
      end if
    end subroutine request_caller_init
```

```

end if
req%n_channels = n_channels
call req%state%init (comm, req%n_workers)
if (req%is_master ()) then
    call allocate_balancer ()
end if
contains
subroutine allocate_balancer ()
    class(balancer_base_t), allocatable :: balancer
    allocate (balancer_channel_t :: balancer)
    select type (balancer)
    type is (balancer_channel_t)
        call balancer%init (n_workers = req%n_workers, n_resources = req%n_channels)
    end select
    call req%add_balancer (balancer)
end subroutine allocate_balancer
end subroutine request_caller_init

subroutine request_caller_write (req, unit)
    class(request_caller_t), intent(in) :: req
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(A)") "[REQUEST_CALLER]"
    call req%base_write (u)
    if (req%is_master ()) &
        call req%state%write (u)
end subroutine request_caller_write

logical function request_caller_has_workers (req) result (flag)
    class(request_caller_t), intent(in) :: req
    !! n_workers excludes the master rank.
    flag = (req%n_workers > 1)
end function request_caller_has_workers

subroutine request_caller_update_balancer (req, weight, parallel_grid)
    class(request_caller_t), intent(inout) :: req
    real(default), dimension(:), intent(in) :: weight
    logical, dimension(:), intent(in) :: parallel_grid
    !! \note bug if not allocated?
    if (.not. allocated (req%balancer)) return
    call req%state%reset ()
    call req%reset ()
    select type (balancer => req%balancer)
    type is (balancer_channel_t)
        call balancer%update_state(weight, parallel_grid)
    end select
end subroutine request_caller_update_balancer

subroutine request_caller_handle_workload (req)
    class(request_caller_t), intent(inout) :: req
    integer :: handler, tag, source, worker_id
    if (.not. allocated (req%balancer)) then
        call msg_warning ("Request: Error occured, load balancer not allocated.&

```

```

        & Terminate all workers.")
    !! We postpone to stop the program here so we can terminate all workers gracefully.
    !! First, we receive their requests, then we overwrite their "original" tag to MPI_TAG_TERMINATE
    !! Second, we iterate this, until all workers are terminated and return without doing any b
end if
call req%state%init_request ()
call req%state%receive_request ()
do while (.not. req%state%is_terminated ())
    call req%state%await_request ()
    do while (req%state%has_request ())
        call req%state%get_request (source, tag, handler)
        !! Formally differentiate between worker_id and source.
        worker_id = source
        if (.not. allocated (req%balancer)) tag = MPI_TAG_TERMINATE
        select case (tag)
        case (MPI_TAG_REQUEST)
            if (req%balancer%is_assignable (worker_id)) then
                call req%balancer%assign_worker (worker_id, handler)
                if (.not. req%balancer%has_resource_group (handler)) then
                    call req%state%update_request (source, MPI_TAG_ASSIGN_SINGLE, handler)
                else
                    call req%state%update_request (source, MPI_TAG_ASSIGN_GROUP, handler)
                    call provide_request_group (handler, source)
                end if
            end if
        else
            call req%state%terminate (source)
        end if
        case (MPI_TAG_HANDLER_AND_RELEASE)
            call req%call_handler (handler, source_rank = source)
            call req%balancer%free_worker (worker_id, handler)
        case (MPI_TAG_RELEASE)
            call req%balancer%free_worker (worker_id, handler)
        case (MPI_TAG_TERMINATE)
            call req%state%terminate (source)
        case (MPI_TAG_CLIENT_TERMINATE)
            !! Allow workers to request their own termination.
            call req%state%terminate (source)
        case default
            call msg_warning ()
        end select
    end do
    call req%state%receive_request ()
end do
!! If we are here, there should be no leftover communication.
!! Hence, we must check whether there is no left-over communication call (from server-side).
call req%state%free_request ()
contains
subroutine provide_request_group (handler_id, dest_rank)
    integer, intent(in) :: handler_id
    integer, intent(in) :: dest_rank
    integer, dimension(:), allocatable :: rank
    !! Rank indices and worker indices are identical, as we skip the master worker deliberately,
    !! we can reuse the worker indices as rank indices.
    call req%balancer%get_resource_group (handler_id, rank)

```



```

        call req%state%provide_request_group (dest_rank, rank)
    end subroutine provide_request_group
end subroutine request_caller_handle_workload

subroutine request_caller_request_workload (req, request)
    class(request_caller_t), intent(inout) :: req
    type(request_t), intent(out) :: request
    type(MPI_STATUS) :: status
    call req%state%client_serve (request%handler_id, status)
    request%terminate = .false.
    request%group = .false.
    request%callback = .false.
    request%comm = MPI_COMM_NULL
    select case (status%MPI_TAG)
    case (MPI_TAG_ASSIGN_SINGLE)
        !! Default to req's communicator.
        request%comm = req%external_comm
        request%group_master = .true.
        request%callback = .true.
    case (MPI_TAG_ASSIGN_GROUP)
        request%group = .true.
        call retrieve_request_group (request%handler_id)
        call req%cache%get_comm (request%comm)
        request%group_master = req%cache%is_master ()
        request%callback = req%cache%is_master ()
    case (MPI_TAG_TERMINATE)
        request%terminate = status%MPI_TAG == MPI_TAG_TERMINATE
    end select
contains
    subroutine retrieve_request_group (handler_id)
        integer, intent(in) :: handler_id
        integer, dimension(:), allocatable :: rank
        !! Here, worker and rank indices are interchangeable.
        call req%state%retrieve_request_group (rank)
        call req%cache%update (handler_id, rank)
    end subroutine retrieve_request_group
end subroutine request_caller_request_workload

subroutine request_caller_release_workload (req, request)
    class(request_caller_t), intent(inout) :: req
    type(request_t), intent(in) :: request
    call req%state%client_free (request%handler_id, has_callback = request%group_master)
end subroutine request_caller_release_workload

subroutine request_caller_handle_and_release_workload (req, request)
    class(request_caller_t), intent(inout) :: req
    type(request_t), intent(in) :: request
    if (.not. req%handler%has_handler (request%handler_id)) then
        call msg_bug ("Request: Handler is not registered for this worker.")
    end if
    call req%release_workload (request)
    call req%call_client_handler (request%handler_id)
end subroutine request_caller_handle_and_release_workload

```

```

subroutine request_caller_request_terminate (req)
  class(request_caller_t), intent(inout) :: req
  if (req%is_master ()) return
  call req%state%client_terminate ()
end subroutine request_caller_request_terminate
end module request_caller

```

Request Caller State

We implement the complete communication for `request_caller` into a state (or in WK's nomenclature, instance) object.

```

(request_state.f90)≡
<File header>
module request_state
  use, intrinsic :: iso_fortran_env, only: ERROR_UNIT
  use iterator
  use diagnostics

  use mpi_f08 !NODEP!

  implicit none

  private

  integer, parameter, public :: MPI_EMPTY_HANDLER = 0

  integer, parameter, public :: MPI_TAG_NULL = 0, &
    MPI_TAG_REQUEST = 1, &
    MPI_TAG_RELEASE = 2, &
    MPI_TAG_HANDLER_AND_RELEASE = 4, &
    MPI_TAG_TERMINATE = 8, &
    MPI_TAG_CLIENT_TERMINATE = 16, &
    MPI_TAG_ASSIGN_SINGLE = 32, &
    MPI_TAG_ASSIGN_GROUP = 64, &
    MPI_TAG_COMMUNICATOR_GROUP = 128

  integer, parameter :: MPI_STATE_ERR = 1

  type :: request_state_t
    private
    type(MPI_COMM) :: comm
    integer :: n_workers = 0
    integer :: n_workers_done = 0
    !! From MPI-3.1 book
    !! i \in {1, N_workes_done}, max size = N_workers
    type(MPI_Request), dimension(:), allocatable :: request
    type(MPI_Status), dimension(:), allocatable :: status
    integer, dimension(:), allocatable :: indices
    !! i \in {1, N_workers}
    integer, dimension(:), allocatable :: handler
    logical, dimension(:), allocatable :: terminated
    type(iterator_t) :: request_iterator
  contains

```

```

    procedure :: init => request_state_init
    procedure :: write => request_state_write
    procedure :: reset => request_state_reset
    procedure :: is_terminated => request_state_is_terminated
    procedure, private :: set_terminated => request_state_set_terminated
    procedure :: terminate => request_state_terminate
    procedure :: client_terminate => request_state_client_terminate
    procedure :: init_request => request_state_init_request
    procedure :: receive_request => request_state_receive_request
    procedure :: await_request => request_state_await_request
    procedure :: has_request => request_state_has_request
    procedure :: get_request => request_state_get_request
    procedure :: update_request => request_state_update_request
    procedure :: free_request => request_state_free_request
    procedure :: provide_request_group => request_state_provide_request_group
    procedure :: retrieve_request_group => request_state_retrieve_request_group
    procedure :: client_serve => request_state_client_serve
    procedure :: client_free => request_state_client_free
end type request_state_t

public :: request_state_t
contains
  subroutine request_state_init (state, comm, n_workers)
    class(request_state_t), intent(out) :: state
    type(MPI_COMM), intent(in) :: comm
    integer, intent(in) :: n_workers
    integer :: rank
    call MPI_COMM_DUP (comm, state%comm)
    state%n_workers = n_workers
    state%n_workers_done = n_workers
    call state%request_iterator%init (1, n_workers)
    allocate (state%request(state%n_workers), source = MPI_REQUEST_NULL)
    allocate (state%status(state%n_workers), source = MPI_STATUS_IGNORE)
    allocate (state%handler(state%n_workers), source = MPI_EMPTY_HANDLER)
    allocate (state%indices(state%n_workers), source = 0)
    allocate (state%terminated(state%n_workers), source = .false.)
    state%indices = [(rank, rank = 1, n_workers)]
  end subroutine request_state_init

  subroutine request_state_write (state, unit)
    class(request_state_t), intent(in) :: state
    integer, intent(in), optional :: unit
    integer :: u, i
    u = ERROR_UNIT; if (present (unit)) u = unit
    write (u, "(A)") "[REQUEST_STATE]"
    write (u, "(A,1X,I0)") "N_WORKERS", state%n_workers
    write (u, "(A,1X,I0)") "N_WORKERS_DONE", state%n_workers_done
    write (u, "(A)") "RANK | SOURCE | TAG | ERROR | REQUEST_NULL"
    do i = 1, state%n_workers_done
      write (u, "(A,4(1X,I0),1X,L1)") "REQUEST", state%indices(i), &
        state%status(i)%MPI_SOURCE, &
        state%status(i)%MPI_TAG, &
        state%status(i)%MPI_ERROR, &
        (state%request(i) == MPI_REQUEST_NULL)
    end do
  end subroutine request_state_write

```

```

end do
write (u, "(A,999(1X,I0))") "HANDLER", state%handler
write (u, "(A,999(1X,L1))") "TERMINATED", state%terminated
end subroutine request_state_write

subroutine request_state_reset (state)
class(request_state_t), intent(inout) :: state
integer :: rank
state%n_workers_done = state%n_workers
call state%request_iterator%init (1, state%n_workers)
state%handler = MPI_EMPTY_HANDLER
state%indices = [(rank, rank = 1, state%n_workers)]
state%terminated = .false.
end subroutine request_state_reset

! pure function request_state_is_terminated (state) result (flag)
function request_state_is_terminated (state) result (flag)
class(request_state_t), intent(in) :: state
logical :: flag
flag = all (state%terminated)
end function request_state_is_terminated

!> Set rank to be terminated (however, do not communicate it).
!!
!! This is an EVIL procedure, as it operates only locally on the master
!! and does not communicate its purpose.
!! However, in order to allow termination requests from client-side
!! we need to manipulate the specific rank states.
subroutine request_state_set_terminated (state, rank)
class(request_state_t), intent(inout) :: state
integer, intent(in) :: rank
state%terminated(rank) = .true.
end subroutine request_state_set_terminated

subroutine request_state_terminate (state, rank)
class(request_state_t), intent(inout) :: state
integer, intent(in) :: rank
integer :: error
call MPI_SEND (MPI_EMPTY_HANDLER, 1, MPI_INTEGER, &
rank, MPI_TAG_TERMINATE, state%comm, error)
if (error /= 0) then
write (msg_buffer, "(A,1X,I3)") "Request: Error occurred during terminate, RANK", rank
call msg_bug ()
end if
call state%set_terminated (rank)
end subroutine request_state_terminate

subroutine request_state_client_terminate (state)
class(request_state_t), intent(in) :: state
integer :: error
call MPI_SEND (MPI_EMPTY_HANDLER, 1, MPI_INTEGER, &
0, MPI_TAG_CLIENT_TERMINATE, state%comm, error)
if (error /= 0) then
write (msg_buffer, "(A,1X,I3)") "Request: Error occurred during client-sided terminate"

```

```

        call msg_bug ()
    end if
end subroutine request_state_client_terminate

!> Init persistent requests.
!!
!! Must be called before first receive_request.
!! Free_request must be called after is_terminated returns true.
subroutine request_state_init_request (state)
    class(request_state_t), intent(inout) :: state
    integer :: i, rank, error
    do i = 1, state%n_workers_done
        rank = state%indices(i)
        call MPI_RECV_INIT (state%handler(rank), 1, MPI_INTEGER, &
            rank, MPI_ANY_TAG, state%comm, state%request(rank), error)
        if (error /= 0) then
            write (msg_buffer, "(A,2(A,1X,I0))") "Request: Error occurred during receive init, &
                & RANK", rank, "HANDLER", state%handler(rank)
            call msg_message ()
            call MPI_ABORT (state%comm, MPI_STATE_ERR)
        end if
    end do
end subroutine request_state_init_request

!> Receive requests from non-terminated workers.
!!
!! Before receiving new requests, sanitize arrays of received ranks from terminated ones.
subroutine request_state_receive_request (state)
    class(request_state_t), intent(inout) :: state
    integer :: i, rank
    integer :: error
    if (state%is_terminated ()) return
    call sanitize_from_terminated_ranks ()
    !! Receive new requests from (still active) workers.
    do i = 1, state%n_workers_done
        rank = state%indices(i)
        call MPI_START (state%request(rank), error)
        if (error /= 0) then
            write (msg_buffer, "(A,2(A,1X,I6))") "Request: Error occurred during receive request, &
                & RANK", rank, "HANDLER", state%handler(rank)
            call msg_message ()
            call MPI_ABORT (state%comm, MPI_STATE_ERR)
        end if
    end do
contains
    subroutine sanitize_from_terminated_ranks ()
        integer :: n_workers_done
        integer, dimension(:), allocatable :: indices
        !! Remove terminated ranks from done workers.
        indices = pack(state%indices(:state%n_workers_done), &
            .not. state%terminated(state%indices(:state%n_workers_done)))
        state%n_workers_done = size (indices)
        state%indices(:state%n_workers_done) = indices
    end subroutine sanitize_from_terminated_ranks

```

```

end subroutine request_state_receive_request

subroutine request_state_await_request (state)
  class(request_state_t), intent(inout) :: state
  integer :: error
  if (state%is_terminated ()) return
  !! We verify that we have active handles associated with request state.
  call MPI_TESTSOME (state%n_workers, state%request, state%n_workers_done, &
    state%indices, state%status, error)
  if (error /= 0) then
    write (ERROR_UNIT, "(A)") "Error occurred during await (testing) request..."
    call state%write (ERROR_UNIT)
    call MPI_ABORT (state%comm, MPI_STATE_ERR)
  else if (state%n_workers_done == MPI_UNDEFINED) then
    write (ERROR_UNIT, "(A)") "TEST_WAITSOME returned with MPI_UNDEFINED."
    call state%write (ERROR_UNIT)
    call MPI_ABORT (state%comm, MPI_STATE_ERR)
  end if
  !! Wait a little bit...
  if (state%n_workers_done == 0) then
    !! Proof: REQUEST(i), i \in {1, N_workers}, i is equivalent to rank.
    !! Proof: INDICES(j), STATUS(j), j \in {1, N_workers_done}
    !! Proof: INDICES(j) -> i, injectiv.
    call MPI_WAITSOME (state%n_workers, state%request, state%n_workers_done, &
      state%indices, state%status, error)
    if (error /= 0) then
      write (ERROR_UNIT, "(A)") "Error occurred during await request..."
      call state%write (ERROR_UNIT)
      call MPI_ABORT (state%comm, MPI_STATE_ERR)
    end if
  endif
  call state%request_iterator%init (1, state%n_workers_done)
end subroutine request_state_await_request

pure function request_state_has_request (state) result (flag)
  class(request_state_t), intent(in) :: state
  logical :: flag
  flag = state%request_iterator%is_iterable ()
end function request_state_has_request

subroutine request_state_get_request (state, rank, tag, handler)
  class(request_state_t), intent(inout) :: state
  integer, intent(out) :: rank
  integer, intent(out) :: tag
  integer, intent(out) :: handler
  integer :: ndx
  if (.not. state%has_request ()) then
    call msg_bug ("Request: Cannot access missing request.")
  end if
  ndx = state%request_iterator%next ()
  rank = state%indices(ndx)
  if (rank /= state%status(ndx)%MPI_SOURCE) then
    write (msg_buffer, "(A,2(1X,I3))") &
      "Request: RANK and SOURCE mismatch", rank, state%status(ndx)%MPI_SOURCE
  end if
end subroutine request_state_get_request

```

```

        call msg_bug ()
    end if
    tag = state%status(ndx)%MPI_TAG
    handler = state%handler(rank)
end subroutine request_state_get_request

subroutine request_state_update_request (state, rank, tag, handler)
    class(request_state_t), intent(inout) :: state
    integer, intent(in) :: rank
    integer, intent(in) :: tag
    integer, intent(in) :: handler
    integer :: error
    state%handler(rank) = handler
    call MPI_SEND (handler, 1, MPI_INTEGER, &
        rank, tag, state%comm, error)
    if (error /= 0) then
        write (msg_buffer, "(A,3(A,1X,I3))") "Request: Error occurred during update, &
            &RANK", rank, "TAG", tag, "HANDLER", handler
        call msg_bug ()
    end if
end subroutine request_state_update_request

subroutine request_state_free_request (state)
    class(request_state_t), intent(inout) :: state
    integer :: rank
    do rank = 1, state%n_workers
        if (state%request(rank) == MPI_REQUEST_NULL) cycle
        call MPI_REQUEST_FREE (state%request(rank))
    end do
end subroutine request_state_free_request

subroutine request_state_provide_request_group (state, dest_rank, worker)
    class(request_state_t), intent(in) :: state
    integer, intent(in) :: dest_rank
    integer, dimension(:), intent(in) :: worker
    call MPI_SEND (worker, size (worker), MPI_INTEGER, &
        dest_rank, MPI_TAG_COMMUNICATOR_GROUP, state%comm)
end subroutine request_state_provide_request_group

subroutine request_state_retrieve_request_group (state, worker)
    class(request_state_t), intent(inout) :: state
    integer, dimension(:), allocatable, intent(out) :: worker
    type(MPI_STATUS) :: status
    integer :: n_workers
    call MPI_PROBE (0, MPI_TAG_COMMUNICATOR_GROUP, state%comm, status)
    call MPI_GET_COUNT(status, MPI_INTEGER, n_workers)
    allocate (worker (n_workers), source = 0)
    call MPI_RECV (worker, n_workers, MPI_INTEGER, &
        0, MPI_TAG_COMMUNICATOR_GROUP, state%comm, status)
end subroutine request_state_retrieve_request_group

!> Query for a request (send an request tag, then receive a handler).
subroutine request_state_client_serve (state, handler_id, status)
    class(request_state_t), intent(in) :: state

```

```

integer, intent(out) :: handler_id
type(MPI_STATUS), intent(out) :: status
call MPI_SEND (MPI_EMPTY_HANDLER, 1, MPI_INTEGER, &
               0, MPI_TAG_REQUEST, state%comm)
call MPI_RECV (handler_id, 1, MPI_INTEGER, &
               0, MPI_ANY_TAG, state%comm, status)
end subroutine request_state_client_serve

!> Free handler from worker.
subroutine request_state_client_free (state, handler_id, has_callback)
  class(request_state_t), intent(in) :: state
  integer, intent(in) :: handler_id
  logical, intent(in) :: has_callback
  integer :: tag
  tag = merge (MPI_TAG_HANDLER_AND_RELEASE, MPI_TAG_RELEASE, has_callback)
  call MPI_SEND (handler_id, 1, MPI_INTEGER, &
                 0, tag, state%comm)
end subroutine request_state_client_free
end module request_state

```

20.15.4 Balancer Base

Balancer Base Base type for usage for extensions of `request_base`.

```

(balancer_base.f90)≡
module balancer_base
  use io_units
  use diagnostics
  use array_list

  implicit none

  private

  type :: worker_t
    private
    integer :: resource = 0
    integer :: state = 0
    integer :: n_resources = 0
    logical :: assigned = .false.
  contains
    procedure :: write => worker_write
    procedure :: is_assigned => worker_is_assigned
    procedure :: get_resource => worker_get_resource
    procedure :: get_state => worker_get_state
    procedure :: add_resource => worker_add_resource
    procedure :: free => worker_free
  end type worker_t

  type :: resource_t
    private
    integer :: resource_id = 0
    logical :: active = .false.
    integer :: n_assigned_workers = 0

```



```

contains
  procedure :: write => resource_write
  procedure :: is_active => resource_is_active
  procedure :: set_active => resource_set_active
  procedure :: set_inactive => resource_set_inactive
end type resource_t

integer, parameter, public :: STATE_SINGLE = 1, &
  STATE_ALL = 2

type :: resource_state_t
  integer :: n_workers = 0
  integer :: mode = 0
  type(array_list_t) :: resource_stack
  type(array_list_t) :: finished_stack
contains
  procedure :: write => resource_state_write
  procedure :: init => resource_state_init
  procedure :: add_resource => resource_state_add_resource
  procedure :: freeze => resource_state_freeze
  procedure :: clear => resource_state_clear
  procedure :: has_resource => resource_state_has_resource
  procedure :: assign_resource => resource_state_assign_resource
  procedure :: free_resource => resource_state_free_resource
end type resource_state_t

!> Dynamic load balancer.
!!
!! We organize resources and workers in a transparent way using indices.
!! These indices replace pointer magic.
!!
!! The balancer aggregates a dynamic state, however, we allow the state by
!! the use of a pointer, to access the static fields of the balancer.
type, abstract :: balancer_base_t
  integer :: n_workers = 0
  integer :: n_resources = 0
  integer :: n_states = 0
  type(worker_t), dimension(:), allocatable :: worker
  type(resource_t), dimension(:), allocatable :: resource
  type(resource_state_t), dimension(:), allocatable :: state
contains
  procedure :: base_init => balancer_base_base_init
  procedure :: base_write => balancer_base_write
  procedure(balancer_base_deferred_write), deferred :: write
  procedure :: add_state => balancer_base_add_state
  procedure, private :: link_worker_and_state => balancer_base_link_worker_and_state
  procedure :: is_assignable => balancer_base_is_assignable
  procedure :: is_worker_pending => balancer_base_is_worker_pending
  procedure :: is_pending => balancer_base_is_pending
  procedure(balancer_base_has_resource_group), deferred :: has_resource_group
  procedure(balancer_base_get_resource_group), deferred :: get_resource_group
  procedure(balancer_base_get_resource_master), deferred :: get_resource_master
  procedure(balancer_base_assign_worker), deferred :: assign_worker
  procedure(balancer_base_free_worker), deferred :: free_worker

```

```

end type balancer_base_t

abstract interface
  subroutine balancer_base_deferred_write (balancer, unit)
    import :: balancer_base_t
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in), optional :: unit
  end subroutine balancer_base_deferred_write

  !> Has resource an associated resource group.
  !!
  !! \note .true. only on an active resource, else .false.
  pure logical function balancer_base_has_resource_group (balancer, resource_id) &
    result (flag)
    import :: balancer_base_t
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
  end function balancer_base_has_resource_group

  !> Get resource group.
  !!
  !! \note Implementation must check against group existence.
  !! \return group (allocated|NOT allocated for (inactive|non-group) resource)
  pure subroutine balancer_base_get_resource_group (balancer, resource_id, group)
    import :: balancer_base_t
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer, dimension(:), allocatable, intent(out) :: group
  end subroutine balancer_base_get_resource_group

  !> Get resource master (worker).
  !!
  !! Return worker as given, however, if extended type is used in a non-local
  !! or in combination with a communicative request type, then check on activation status of as
  !!
  !! \return worker Valid worker index (\in {1, ..., N}) only on active resource*, else -1.
  pure integer function balancer_base_get_resource_master (balancer, resource_id) &
    result (worker)
    import :: balancer_base_t
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
  end function balancer_base_get_resource_master

  !> Assign resource to a given worker or retrieve current assigned resource.
  !!
  !! If worker has already a resource assigned, return resource.
  !! If worker has not been assigned a resource, retrieve new resource from state.
  !!
  !! \note Each call must check if a worker is assignable, if not, the procedure must return re
  subroutine balancer_base_assign_worker (balancer, worker_id, resource_id)
    import :: balancer_base_t
    class(balancer_base_t), intent(inout) :: balancer
    integer, intent(in) :: worker_id
    integer, intent(out) :: resource_id

```

```

end subroutine balancer_base_assign_worker

!> Free assignment of worker.
!!
!! If worker is not assigned, this procedure is idempotent.
!! If worker is assigned, alter state correspondingly.
!! \note In order to correctly free a worker from a resource, we have to explicitly keep track of the resource.
!! This feature is mostly relevant for resources with a worker group.
! The resource may be disassociated from their worker by earlier calls or the former worker may be freed.
!! In the latter case, we are not allowed to free them (as the new resource is still active).
!! Therefore, each call must check if a worker and resource are still associated and the resource is still active.
!! Only, in this case, disassociating workers and resource is allowed.
subroutine balancer_base_free_worker (balancer, worker_id, resource_id)
  import :: balancer_base_t
  class(balancer_base_t), intent(inout) :: balancer
  integer, intent(in) :: worker_id
  integer, intent(in) :: resource_id
end subroutine balancer_base_free_worker
end interface

public :: balancer_base_t, resource_state_t
public :: shift_rank_to_worker, shift_worker_to_rank
contains
!> Shift rank index to worker index.
!! Proof: rank \in {0, ..., N - 1}, worker \in {1, ..., N}
elemental integer function shift_rank_to_worker (rank) result (worker)
  integer, intent(in) :: rank
  worker = rank + 1
end function shift_rank_to_worker

!> Shift worker index to rank index.
!! Proof: rank \in {0, ..., N - 1}, worker \in {1, ..., N}
elemental integer function shift_worker_to_rank (worker) result (rank)
  integer, intent(in) :: worker
  rank = worker - 1
end function shift_worker_to_rank

subroutine worker_write (worker, unit)
  class(worker_t), intent(in) :: worker
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(3(A,1X,I3,1X),A,1X,L1)") "RESOURCE", worker%resource, &
    "STATE", worker%state, &
    "N_RESOURCES", worker%n_resources, &
    "ASSIGNED", worker%assigned
end subroutine worker_write

elemental logical function worker_is_assigned (worker) result (flag)
  class(worker_t), intent(in) :: worker
  flag = worker%assigned
end function worker_is_assigned

elemental integer function worker_get_resource (worker) result (resource_id)

```

```

        class(worker_t), intent(in) :: worker
        resource_id = worker%resource
    end function worker_get_resource

    elemental integer function worker_get_state (worker) result (i_state)
        class(worker_t), intent(in) :: worker
        i_state = worker%state
    end function worker_get_state

    elemental subroutine worker_add_resource (worker, resource_id)
        class(worker_t), intent(inout) :: worker
        integer, intent(in) :: resource_id
        worker%n_resources = worker%n_resources + 1
        worker%assigned = .true.
        worker%resource = resource_id
    end subroutine worker_add_resource

    elemental subroutine worker_free (worker)
        class(worker_t), intent(inout) :: worker
        worker%assigned = .false.
        worker%resource = 0
    end subroutine worker_free

    subroutine resource_write (resource, unit)
        class(resource_t), intent(in) :: resource
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(A,1X,I3,1X,A,1X,L1,1X,A,1X,I3)") &
            "RESOURCE_ID", resource%resource_id, &
            "ACTIVE", resource%active, &
            "N_ASSIGNED_WORKERS", resource%n_assigned_workers
    end subroutine resource_write

    elemental logical function resource_is_active (resource) result (flag)
        class(resource_t), intent(in) :: resource
        flag = resource%active
    end function resource_is_active

    subroutine resource_set_active (resource, n_workers)
        class(resource_t), intent(inout) :: resource
        integer, intent(in) :: n_workers
        resource%active = .true.
        resource%n_assigned_workers = n_workers
    end subroutine resource_set_active

    subroutine resource_set_inactive (resource)
        class(resource_t), intent(inout) :: resource
        resource%active = .false.
    end subroutine resource_set_inactive

    subroutine resource_state_write (state, unit)
        class(resource_state_t), intent(in) :: state
        integer, intent(in), optional :: unit

```

```

integer :: u
u = given_output_unit (unit)
write (u, "(A,1X,10)") "N_STATE_WORKERS", state%n_workers
select case (state%mode)
case (STATE_SINGLE)
    write (u, "(A)") "MODE ONE-TO-ONE"
case (STATE_ALL)
    write (u, "(A)") "MODE ALL-TO-ONE"
case default
    write (u, "(A)") "UNSUPPORTED MODE"
end select
write (u, "(A)") "RESOURCE"
call state%resource_stack%write (u)
write (u, "(A)") "FINISHED"
call state%finished_stack%write (u)
end subroutine resource_state_write

subroutine resource_state_init (state, mode, n_workers)
    class(resource_state_t), intent(out) :: state
    integer, intent(in) :: mode
    integer, intent(in) :: n_workers
    state%mode = mode
    state%n_workers = n_workers
    call state%resource_stack%init ()
    call state%finished_stack%init ()
end subroutine resource_state_init

subroutine resource_state_add_resource (state, i_resource)
    class(resource_state_t), intent(inout) :: state
    integer, intent(in) :: i_resource
    call state%resource_stack%add (i_resource)
end subroutine resource_state_add_resource

subroutine resource_state_freeze (state)
    class(resource_state_t), intent(inout) :: state
    call state%resource_stack%sort ()
    call state%resource_stack %reverse_order ()
end subroutine resource_state_freeze

subroutine resource_state_clear (state)
    class(resource_state_t), intent(inout) :: state
    call state%resource_stack%clear ()
    call state%finished_stack%clear ()
end subroutine resource_state_clear

elemental function resource_state_has_resource (state) result (flag)
    class(resource_state_t), intent(in) :: state
    logical :: flag
    flag = .not. state%resource_stack%is_empty ()
end function resource_state_has_resource

function resource_state_assign_resource (state) result (i_resource)
    class(resource_state_t), intent(inout) :: state
    integer :: i_resource

```

```

    if (state%resource_stack%is_empty ()) then
        i_resource = 0
        call msg_bug ("Error: No leftover resource on stack.")
        return
    end if
    i_resource = state%resource_stack%remove () !! Pop last element from stack.
end function resource_state_assign_resource

subroutine resource_state_free_resource (state, i_resource)
    class(resource_state_t), intent(inout) :: state
    integer, intent(in) :: i_resource
    if (state%resource_stack%is_element (i_resource)) then
        call msg_bug ("Error: Cannot free resource, still on resource stack.")
    end if
    call state%finished_stack%add (i_resource)
end subroutine resource_state_free_resource

subroutine balancer_base_write (balancer, unit)
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(A)") "[REQUEST BALANCER]"
    write (u, "(3(A,1X,I3,1X))") "N_WORKERS", balancer%n_workers, &
        "N_RESOURCES", balancer%n_resources, &
        "N_STATES", balancer%n_states
    write (u, "(A)") "[WORKER]"
    do i = 1, balancer%n_workers
        call balancer%worker(i)%write (u)
    end do
    write (u, "(A)") "[RESOURCE]"
    do i = 1, balancer%n_resources
        call balancer%resource(i)%write (u)
    end do
    write (u, "(A)") "[STATES]"
    do i = 1, balancer%n_states
        call balancer%state(i)%write (u)
    end do
end subroutine balancer_base_write

subroutine balancer_base_base_init (balancer, n_workers, n_resources)
    class(balancer_base_t), intent(out) :: balancer
    integer, intent(in) :: n_workers
    integer, intent(in) :: n_resources
    balancer%n_workers = n_workers
    balancer%n_resources = n_resources
    allocate (balancer%worker (n_workers))
    allocate (balancer%resource (n_resources))
    call init_resource ()
contains
    subroutine init_resource ()
        integer :: i
        do i = 1, balancer%n_resources
            balancer%resource(i)%resource_id = i
        end do
    end subroutine
end subroutine

```

```

        end do
    end subroutine init_resource
end subroutine balancer_base_base_init

!> Add partition of workers and link with workers.
!! We move the allocated partition object into the balancer.
!! We then assign each partition its respective number of workers in a incrementing linear fashi
!! However, we postpone the linking of the resources to the partition, which can be either done
subroutine balancer_base_add_state (balancer, state)
    class(balancer_base_t), intent(inout) :: balancer
    type(resource_state_t), dimension(:), allocatable, intent(inout) :: state
    balancer%n_states = size (state)
    call move_alloc (state, balancer%state)
    call balancer%link_worker_and_state ()
end subroutine balancer_base_add_state

subroutine balancer_base_link_worker_and_state (balancer)
    class(balancer_base_t), intent(inout) :: balancer
    integer :: i, j, i_worker
    if (.not. allocated (balancer%state)) &
        call msg_bug ("Error: resource state not allocated.")
    !! Link worker to a state.
    i_worker = 1
    do i = 1, balancer%n_states
        do j = 1, balancer%state(i)%n_workers
            if (i_worker > balancer%n_workers) then
                call msg_bug ("Balancer: Number of state workers&
                    & exceeding global number of workers")
            end if
            associate (worker => balancer%worker(i_worker))
                worker%state = i
                !! Reset worker attributes.
                worker%resource = 0
                worker%n_resources = 0
                worker%assigned = .false.
            end associate
            i_worker = i_worker + 1
        end do
    end do
end subroutine balancer_base_link_worker_and_state

!> Is a worker unassigned, or is a worker assigned, but already assigned to an active resource?
!!
!! \note Fence for assign_worker TBP.
!! The assign_worker TPB must call is_assignable in order to retrieve the worker status.
!! \param[in] worker_id
!! \return flag If worker is NOT assigned, return .true. if state has resources.
!!             If worker is assigned, return .true. if associated resource is active.
pure logical function balancer_base_is_assignable (balancer, worker_id) result (flag)
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in) :: worker_id
    integer :: i_state, resource_id
    flag = .false.
    if (balancer%worker(worker_id)%assigned) then

```

```

        resource_id = balancer%worker(worker_id)%resource
        flag = balancer%resource(resource_id)%is_active ()
    else
        i_state = balancer%worker(worker_id)%get_state ()
        flag = balancer%state(i_state)%has_resource ()
    end if
end function balancer_base_is_assignable

!> Is a worker still pending.
!!
!! Test worker assignment, and if there is a (valid) resource and if it is still active.
pure logical function balancer_base_is_worker_pending (balancer, worker_id) result (flag)
    class(balancer_base_t), intent(in) :: balancer
    integer, intent(in) :: worker_id
    integer :: resource_id
    flag = balancer%worker(worker_id)%assigned
    if (flag) then
        resource_id = balancer%worker(worker_id)%get_resource ()
        flag = balancer%resource(resource_id)%is_active ()
    end if
end function balancer_base_is_worker_pending

logical function balancer_base_is_pending (balancer) result (flag)
    class(balancer_base_t), intent(in) :: balancer
    flag = all (balancer%state%has_resource ())
end function balancer_base_is_pending

end module balancer_base

```

20.15.5 Balancer Simple

```

(balancer_simple.f90)≡
<File header>
module balancer_simple
    use io_units
    use diagnostics

    use balancer_base

    implicit none

    private

    integer, parameter :: N_BALANCER_SIMPLE_STATES = 1, &
        BALANCER_SIMPLE_CHANNEL = 1

    !> Simple balancer.
    !!
    !! The simple balancer distribute the channel among the N workers using a modulo prescription.
    !! However, it does assign all workers to a channel capable of grid with parallelizable structure.
    !!
    !! The balancer use local, non-communicative approach; each worker allocates an own instance of
    !! and fills it with the respecting resources.
    !!

```



```

!! We defer possible checks (or sentinels) to the request module, e.g. such as checking whether
type, extends (balancer_base_t) :: balancer_simple_t
    logical, dimension(:), allocatable :: parallel_grid
contains
    procedure :: init => balancer_simple_init
    procedure :: write => balancer_simple_write
    procedure :: update_state => balancer_simple_update_state
    procedure :: has_resource_group => balancer_simple_has_resource_group
    procedure :: get_resource_group => balancer_simple_get_resource_group
    procedure :: get_resource_master => balancer_simple_get_resource_master
    procedure, private :: map_channel_to_worker => balancer_simple_map_channel_to_worker
    procedure :: assign_worker => balancer_simple_assign_worker
    procedure :: free_worker => balancer_simple_free_worker
end type balancer_simple_t

public :: balancer_simple_t
contains
    subroutine balancer_simple_init (balancer, n_workers, n_resources)
        class(balancer_simple_t), intent(out) :: balancer
        integer, intent(in) :: n_workers
        integer, intent(in) :: n_resources
        type(resource_state_t), dimension(:), allocatable :: state
        call balancer%base_init (n_workers, n_resources)
        allocate (balancer%parallel_grid(n_resources), source = .false.)
        allocate (state (N_BALANCER_SIMPLE_STATES))
        call state(BALANCER_SIMPLE_CHANNEL)%init ( &
            mode = STATE_SINGLE, &
            n_workers = balancer%n_workers)
        call balancer%add_state (state)
    end subroutine balancer_simple_init

    subroutine balancer_simple_write (balancer, unit)
        class(balancer_simple_t), intent(in) :: balancer
        integer, intent(in), optional :: unit
        integer :: u, n_size
        u = given_output_unit (unit)
        call balancer%base_write (u)
        n_size = min (25, size (balancer%parallel_grid))
        write (u, "(A,25(1X,L1))") "Parallel Grids:", balancer%parallel_grid(:n_size)
    end subroutine balancer_simple_write

!> Update balancer state.
!!
!! Each worker update its own balancer state requiring information about the worker_id.
subroutine balancer_simple_update_state (balancer, worker_id, parallel_grid)
    class(balancer_simple_t), intent(inout) :: balancer
    integer, intent(in) :: worker_id
    logical, dimension(:), intent(in) :: parallel_grid
    integer :: ch, worker
    balancer%parallel_grid = parallel_grid
    if (.not. allocated (balancer%state)) then
        call msg_bug ("Error: balancer state not allocated.")
    end if
    associate (state => balancer%state(BALANCER_SIMPLE_CHANNEL))

```

```

    call state%clear ()
    do ch = 1, balancer%n_resources
        if (parallel_grid(ch)) then
            call state%add_resource (ch)
        else
            worker = balancer%map_channel_to_worker (ch)
            if (worker == worker_id) then
                call state%add_resource (ch)
            end if
        end if
    end do
    call state%freeze ()
end associate
end subroutine balancer_simple_update_state

pure logical function balancer_simple_has_resource_group (balancer, resource_id) &
    result (flag)
    class(balancer_simple_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    if (.not. balancer%resource(resource_id)%is_active ()) then
        flag = .false.
        return
    end if
    flag = balancer%parallel_grid (resource_id)
end function balancer_simple_has_resource_group

pure subroutine balancer_simple_get_resource_group (balancer, resource_id, group)
    class(balancer_simple_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer, dimension(:), allocatable, intent(out) :: group
    integer :: i
    if (.not. balancer%has_resource_group (resource_id)) return
    group = pack ([(i, i=1,balancer%n_workers)], &
        mask = balancer%worker%get_resource () == resource_id)
end subroutine balancer_simple_get_resource_group

!> Retrieve resource master holding the results to be communicated.
!!
!! As the simple balancer operates locally on each worker, we do not need to check whether a res
!! All the resources (and their respective order) is fixed at each update of the balancer.
pure integer function balancer_simple_get_resource_master (balancer, resource_id) &
    result (worker_id)
    class(balancer_simple_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    !! \note Do NOT check on resource activation (see interface prescription).
    if (balancer%parallel_grid(resource_id)) then
        worker_id = 1
    else
        worker_id = balancer%map_channel_to_worker (resource_id)
    end if
end function balancer_simple_get_resource_master

pure integer function balancer_simple_map_channel_to_worker (balancer, channel) &
    result (worker)

```

```

class(balancer_simple_t), intent(in) :: balancer
integer, intent(in) :: channel
!! Proof: channel \in {1, N_c}, number of workers N, rank \in {0, ..., N - 1}
!! Proof: worker \in {1, ..., N}
!! a = b mod c, then 0 <= a < c
worker = mod (channel - 1, balancer%n_workers) + 1
end function balancer_simple_map_channel_to_worker

subroutine balancer_simple_assign_worker (balancer, worker_id, resource_id)
class(balancer_simple_t), intent(inout) :: balancer
integer, intent(in) :: worker_id
integer, intent(out) :: resource_id
integer :: i
if (.not. balancer%is_assignable (worker_id)) then
    resource_id = -1
    RETURN
end if
if (balancer%worker(worker_id)%is_assigned ()) then
    resource_id = balancer%worker(worker_id)%get_resource ()
    RETURN
end if
associate (state => balancer%state(BALANCER_SIMPLE_CHANNEL))
    if (.not. state%has_resource ()) then
        resource_id = 0
        return
    end if
    resource_id = state%assign_resource ()
    if (balancer%parallel_grid(resource_id)) then
        do i = 1, balancer%n_workers
            if (balancer%is_worker_pending (i)) then
                write (msg_buffer, "(A,1X,I0,1X,A,1X,I0,1X,A)") "WORKER", i, "ASSIGNED"
                call msg_bug ()
            end if
            call balancer%worker(i)%add_resource (resource_id)
        end do
        call balancer%resource(resource_id)%set_active (n_workers = balancer%n_workers)
    else
        call balancer%worker(worker_id)%add_resource (resource_id)
        call balancer%resource(resource_id)%set_active (n_workers = 1)
    end if
end associate
end subroutine balancer_simple_assign_worker

subroutine balancer_simple_free_worker (balancer, worker_id, resource_id)
class(balancer_simple_t), intent(inout) :: balancer
integer, intent(in) :: worker_id
integer, intent(in) :: resource_id
integer :: i
if (.not. balancer%worker(worker_id)%is_assigned ()) return
if (.not. resource_id == balancer%worker(worker_id)%get_resource ()) then
    call msg_bug ("Balancer simple: resource and associated resource do not match.")
end if
associate (state => balancer%state(BALANCER_SIMPLE_CHANNEL))
    call balancer%resource(resource_id)%set_inactive ()
end associate

```

```

        call state%free_resource (resource_id)
        if (balancer%parallel_grid(resource_id)) then
            do i = 1, balancer%n_workers
                call balancer%worker(i)%free ()
            end do
        else
            call balancer%worker(worker_id)%free ()
        end if
    end associate
end subroutine balancer_simple_free_worker
end module balancer_simple

```

20.15.6 Balancer Channel

```

<balancer_channel.f90>≡
<File header>
module balancer_channel
    use kinds, only: default
    use io_units
    use diagnostics

    use balancer_base

    implicit none

    private

    real(default), parameter :: BETA = 1.5_default

    integer, parameter :: N_BALANCER_CHANNEL_STATE = 2, &
        CHANNEL_STATE = 1, &
        GRID_STATE = 2

    type, extends(balancer_base_t) :: balancer_channel_t
        private
        integer :: n_parallel_grids = 0
        integer :: n_parallel_channels = 0
        integer :: n_grid_workers = 0
        integer :: n_channel_workers = 0
        logical, dimension(:), allocatable :: parallel_grid
    contains
        procedure :: init => balancer_channel_init
        procedure :: write => balancer_channel_write
        procedure :: update_state => balancer_channel_update_state
        procedure :: has_resource_group => balancer_channel_has_resource_group
        procedure :: get_resource_group => balancer_channel_get_resource_group
        procedure :: get_resource_master => balancer_channel_get_resource_master
        procedure :: assign_worker => balancer_channel_assign_worker
        procedure :: free_worker => balancer_channel_free_worker
    end type balancer_channel_t

    public :: balancer_channel_t
contains
    subroutine balancer_channel_init (balancer, n_workers, n_resources)

```

```

class(balancer_channel_t), intent(out), target :: balancer
integer, intent(in) :: n_workers
integer, intent(in) :: n_resources
call balancer%base_init (n_workers, n_resources)
allocate (balancer%parallel_grid(n_resources), source = .false.)
end subroutine balancer_channel_init

subroutine balancer_channel_write (balancer, unit)
class(balancer_channel_t), intent(in) :: balancer
integer, intent(in), optional :: unit
integer :: u, n_size
u = given_output_unit (unit)
write (u, "(A)") "Channel Balancer."
write (u, "(A,1X,I3)") "Parallel grids: ", balancer%n_parallel_grids
write (u, "(A,1X,I3)") "Parallel channels: ", balancer%n_parallel_channels
write (u, "(A,1X,I3)") "Grid workers: ", balancer%n_grid_workers
write (u, "(A,1X,I3)") "Channel workers: ", balancer%n_channel_workers
n_size = min (25, size (balancer%parallel_grid))
write (u, "(A,25(1X,L1))") "Parallel Grids:", balancer%parallel_grid(:n_size)
call balancer%base_write (u)
end subroutine balancer_channel_write

subroutine balancer_channel_update_state (balancer, weight, parallel_grid)
class(balancer_channel_t), intent(inout) :: balancer
real(default), dimension(:), intent(in) :: weight
logical, dimension(:), intent(in) :: parallel_grid
real(default) :: min_parallel_weight
balancer%parallel_grid = parallel_grid
min_parallel_weight = balancer%n_resources** (1._default - 1_default / BETA) &
/ balancer%n_workers**BETA
balancer%parallel_grid = &
balancer%parallel_grid .and. (weight >= min_parallel_weight)
if (balancer%n_resources >= balancer%n_workers) then
!! Apply full multi-channel parallelization.
balancer%n_parallel_grids = 0
balancer%n_parallel_channels = balancer%n_resources
balancer%parallel_grid = .false.
balancer%n_grid_workers = 0
balancer%n_channel_workers = balancer%n_workers
else
if (count (balancer%parallel_grid) == balancer%n_resources) then
!! Apply full VEGAS parallelization.
balancer%n_parallel_grids = balancer%n_resources
balancer%n_parallel_channels = 0
balancer%n_grid_workers = balancer%n_workers
balancer%n_channel_workers = 0
else
!! Apply mixed mode.
balancer%n_parallel_grids = count (balancer%parallel_grid)
balancer%n_parallel_channels = balancer%n_resources - balancer%n_parallel_grids
call compute_mixed_mode (weight)
end if
end if
if (allocated (balancer%state)) then

```

```

        deallocate (balancer%state)
    end if
    call allocate_state ()
contains
    subroutine compute_mixed_mode (weight)
        real(default), dimension(:), intent(in) :: weight
        real(default) :: weight_parallel_grids, &
            ratio_weight, &
            ratio_n_channels, &
            ratio
        !! Apply mixed mode.
        weight_parallel_grids = sum (weight, balancer%parallel_grid)
        !! Overall normalization of weight,  $\alpha_{\text{grids}}$  +
        !!  $\alpha_{\text{channels}}$  = 1.
        !!  $\alpha_{\text{channels}}$  = 1 -  $\alpha_{\text{grids}}$ 
        ratio_weight = weight_parallel_grids / (1 - weight_parallel_grids)
        ratio_n_channels = real (balancer%n_parallel_grids, default) &
            / (balancer%n_resources - balancer%n_parallel_grids)
        !! The average computation of channel is proportional to its weight.
        !! Reweight number of channels (per mode) by their summed weights.
        !!  $R = w * N / (w * N + w' * N')$ ; primed refer to parallel grid entities.
        !!  $= 1 / (1 + w' / w * N' / N)$ 
        ratio = 1 / (1 + ratio_weight * ratio_n_channels)
        ratio = min (max (ratio, 0.0_default), 1.0_default) !! Safe-guard ratio computation.
        !! In the case of small numbers of workers and a very small ratio,
        !! nint can assign no worker to channel/grid parallelization,
        !! which is still requested by n_parallel_channels/grids.
        !! In that case, we have to enforce: n_worker = n_channel_worker + n_grid_worker
        balancer%n_channel_workers = nint (ratio * balancer%n_workers)
        balancer%n_grid_workers = nint ((1 - ratio) * balancer%n_workers)
        !! In the case of small numbers of workers and a very small ratio,
        !! nint can assign no worker to channel/grid parallelization,
        !! which is still requested by n_parallel_channels/grids.
        !! In that case, we have to enforce: n_worker = n_channel_worker + n_grid_worker
        if (balancer%n_workers >= 2 &
            .AND. (balancer%n_parallel_channels > 0 .and. balancer%n_channel_workers < 1)) then
            balancer%n_channel_workers = 1
            balancer%n_grid_workers = balancer%n_grid_workers - 1
        end if
        !! The grid resources will only be increased to N = 2
        !! if more than 3 workers are present.
        if (balancer%n_workers >= 3 &
            .AND. (balancer%n_parallel_grids > 0 .and. balancer%n_grid_workers < 2)) then
            balancer%n_grid_workers = 2
            balancer%n_channel_workers = balancer%n_channel_workers - 2
        end if
    end subroutine compute_mixed_mode

    subroutine allocate_state ()
        type(resource_state_t), dimension(:), allocatable :: state
        integer :: ch
        allocate (state(N_BALANCER_CHANNEL_STATE))
        call state(CHANNEL_STATE)%init ( &
            mode = STATE_SINGLE, &

```

```

        n_workers = balancer%n_channel_workers)
    call state(GRID_STATE)%init ( &
        mode = STATE_ALL, &
        n_workers = balancer%n_grid_workers)
    do ch = 1, balancer%n_resources
        if (balancer%parallel_grid(ch)) then
            call state(GRID_STATE)%add_resource (ch)
        else
            call state(CHANNEL_STATE)%add_resource (ch)
        end if
    end do
    call state(CHANNEL_STATE)%freeze ()
    call state(GRID_STATE)%freeze ()
    call balancer%add_state (state)
end subroutine allocate_state
end subroutine balancer_channel_update_state

pure function balancer_channel_has_resource_group (balancer, resource_id) &
    result (flag)
    class(balancer_channel_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    logical :: flag
    if (.not. balancer%resource(resource_id)%is_active ()) then
        flag = .false.
        return
    end if
    flag = balancer%parallel_grid(resource_id)
end function balancer_channel_has_resource_group

pure subroutine balancer_channel_get_resource_group (balancer, resource_id, group)
    class(balancer_channel_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer, dimension(:), allocatable, intent(out) :: group
    integer :: i
    if (.not. balancer%has_resource_group (resource_id)) return
    group = pack ([i, i = 1, balancer%n_workers]), &
        mask = balancer%worker%get_resource () == resource_id
end subroutine balancer_channel_get_resource_group

pure integer function balancer_channel_get_resource_master (balancer, resource_id) &
    result (worker_id)
    class(balancer_channel_t), intent(in) :: balancer
    integer, intent(in) :: resource_id
    integer :: i
    if (.not. balancer%resource(resource_id)%is_active ()) then
        worker_id = -1
        return
    end if
    !! Linear search.
    !! First element in worker group is defined as master.
    associate (worker => balancer%worker)
        do i = 1, balancer%n_workers
            if (worker(i)%get_resource () == resource_id) then
                worker_id = i
            end if
        end do
    end associate
end function balancer_channel_get_resource_master

```

```

        exit
    end if
end do
end associate
end function balancer_channel_get_resource_master

subroutine balancer_channel_assign_worker (balancer, worker_id, resource_id)
class(balancer_channel_t), intent(inout) :: balancer
integer, intent(in) :: worker_id
integer, intent(out) :: resource_id
integer :: i_state
if (.not. balancer%is_assignable (worker_id)) then
    resource_id = -1
    return
end if
if (balancer%worker(worker_id)%is_assigned ()) then
    resource_id = balancer%worker(worker_id)%get_resource ()
    return
end if
associate (state => balancer%state)
    i_state = balancer%worker(worker_id)%get_state ()
    if (.not. state(i_state)%has_resource ()) then
        resource_id = 0
        return
    end if
    resource_id = state(i_state)%assign_resource ()
    select case (state(i_state)%mode)
    case (STATE_SINGLE)
        call balancer%worker(worker_id)%add_resource (resource_id)
        call balancer%resource(resource_id)%set_active (n_workers = 1)
    case (STATE_ALL)
        call fill_resource_group (i_state, resource_id)
    end select
end associate
contains
subroutine fill_resource_group (i_state, resource_id)
integer, intent(in) :: i_state
integer, intent(in) :: resource_id
integer :: i, n_workers
n_workers = 0
do i = 1, balancer%n_workers
    if (.not. balancer%worker(i)%get_state () == i_state) cycle
    if (balancer%is_worker_pending (i)) then
        write (msg_buffer, "(A,1X,I0,1X,A,1X,I0,1X,A)") "WORKER", i, "STATE", i_state, "ASSIGN"
        call msg_bug ()
    end if
    call balancer%worker(i)%add_resource (resource_id)
    n_workers = n_workers + 1
end do
if (n_workers /= balancer%state(i_state)%n_workers) then
    call msg_bug ("Number of assigned workers unequal to number of state workers.")
end if
call balancer%resource(resource_id)%set_active (n_workers = n_workers)
end subroutine fill_resource_group

```



```

end subroutine balancer_channel_assign_worker

!> Free worker from associated resource.
!!
!! Idempotent. Depending on state association, given resource must equal worker's resource (checked)
!! For all state, the *current* resource of the worker may differ (grouping behavior!), only in case of error
!! Else, free all worker from resource group.
subroutine balancer_channel_free_worker (balancer, worker_id, resource_id)
  class(balancer_channel_t), intent(inout) :: balancer
  integer, intent(in) :: worker_id
  integer, intent(in) :: resource_id
  integer :: i, i_state
  if (.not. balancer%worker(worker_id)%is_assigned ()) return
  associate (state => balancer%state)
    i_state = balancer%worker(worker_id)%get_state ()
    select case (state(i_state)%mode)
    case (STATE_SINGLE)
      if (.not. resource_id == balancer%worker(worker_id)%get_resource ()) then
        call msg_bug ("Channel balancer: resource and associated resource do not match.")
      end if
      call balancer%resource(resource_id)%set_inactive ()
      call state(i_state)%free_resource (resource_id)
      call balancer%worker(worker_id)%free ()
    case (STATE_ALL)
      if (resource_id /= balancer%worker(worker_id)%get_resource ()) then
        if (balancer%resource(resource_id)%is_active ()) then
          msg_buffer = "Channel balancer: resource is still active,&
            & but worker is assigned to another resource."
          call msg_bug ()
        else
          !! Special case: Worker was already freed from (now inactive) resource_id (by another worker)
          !! and in the mean time assigned to a new resource. So, nothing to do.
          return
        end if
      end if
      call balancer%resource(resource_id)%set_inactive ()
      call state(i_state)%free_resource (resource_id)
    do i = 1, balancer%n_workers
      if (.not. balancer%worker(i)%get_state () == i_state) cycle
      call balancer%worker(i)%free ()
    end do
  end select
end associate
end subroutine balancer_channel_free_worker
end module balancer_channel

```

20.15.7 Request Callback

request handler Base type and interface for providing two-sided communication in a callback fashion.

request handler manager Manages handler with a binary tree.

(request_callback.f90)≡

```

module request_callback
  use, intrinsic :: iso_fortran_env, only: ERROR_UNIT
  use binary_tree
  use diagnostics

  use mpi_f08 !NODEP!

  implicit none

  private

  !> Request handler.
  !!
  !! A request handler allows to dispatch an object for communication a priori
  !! for a slave and a master.
  !! Typically, each slave register its own request handles, whereas the master
  !! requests all possible requests handles matching those of the slaves.
  !! The requests can then be used later on, e.g. during a computation, a slave
  !! may add a request to the master worker and starts sending an object.
  !! The master worker looks up the appropriate request handler, which then
  !! closes the communication, i.e. by a receive call.
  !! Most important: Only a pointer to the buffer object is stored, therefore, the calling function
  !! has to ensure, that the communication object (buffer) will not be changed
  !! during a request handle (receive or send).
  !!
  !! Remark: The handler allows for a tag offset which allows to unify the the communication.
  !! The problem occurs when multiple callback need to be handled simultaneously and MPI needs
  !! Each message has a tuple of (source, tag, comm) associated, we can unify this tuple
  !! tag = tag_offset + {1, ..., N_requests} where tag_offsets are multiple of N_requests.
  !! The latter condition should be checked by a modulo.
  !! What happens if the communication is out of order (is this a problem? check with standard)?
  type, abstract :: request_handler_t
    integer :: n_requests = 0
    integer :: tag_offset = 0
    type(MPI_REQUEST), dimension(:), allocatable :: request
    type(MPI_STATUS), dimension(:), allocatable :: status
    logical :: activated = .false.
    logical :: finished = .false.
  contains
    procedure :: base_write => request_handler_base_write
    procedure(request_handler_write), deferred :: write
    !! \todo{sbrass} implement initialization procedure.
    procedure(request_handler_handle), deferred :: handle
    procedure(request_handler_client_handle), deferred :: client_handle
    procedure :: allocate => request_handler_allocate
    procedure :: get_status => request_handler_get_status
    procedure :: testall => request_handler_testall
    procedure :: waitall => request_handler_waitall
    procedure :: free => request_handler_free
  end type request_handler_t

  type :: request_handler_manager_t
    private
    type(MPI_COMM) :: comm

```

```

    type(binary_tree_t) :: tree
contains
    procedure :: init => request_handler_manager_init
    procedure :: write => request_handler_manager_write
    procedure :: add => request_handler_manager_add
    procedure :: clear => request_handler_manager_clear
    procedure :: has_handler => request_handler_manager_has_handler
    procedure :: test => request_handler_manager_test
    procedure :: wait => request_handler_manager_wait
    procedure :: waitall => request_handler_manager_waitall
    procedure, private :: fill_status => request_handler_manager_fill_status
    procedure, private :: handler_at => request_handler_manager_handler_at
    procedure :: callback => request_handler_manager_callback
    procedure :: client_callback => request_handler_manager_client_callback
end type request_handler_manager_t

abstract interface
    subroutine request_handler_write (handler, unit)
        import :: request_handler_t
        class(request_handler_t), intent(in) :: handler
        integer, intent(in), optional :: unit
    end subroutine request_handler_write

    !!> Handle a request from server side.
    !!
    !! The message tag can be used in order to unify the respective messages between master and slave.
    !! E.g. by explicitly setting it, or by using it in a computation  $i * N_R + j$ ,  $i \in \{1, \dots, N_R\}$ ,  $j \in \{1, \dots, N_S\}$ .
    !!
    !! Must set *activated* to .true. when called.
    !! \param[in] source Integer rank of the source in comm.
    !! \param[in] tag Specify the message tag.
    !! \param[in] comm MPI communicator.
    subroutine request_handler_handle (handler, source_rank, comm)
        import :: request_handler_t, MPI_COMM
        class(request_handler_t), intent(inout) :: handler
        integer, intent(in) :: source_rank
        type(MPI_COMM), intent(in) :: comm
    end subroutine request_handler_handle

    !!> Handle a request from client side.
    !!
    !! Must set *activated* to .true. when called.
    !! \param[in] rank Integer of the receiver in comm.
    !! \param[in] tag Specify the message tag.
    !! \param[in] comm MPI communicator.
    subroutine request_handler_client_handle (handler, dest_rank, comm)
        import :: request_handler_t, MPI_COMM
        class(request_handler_t), intent(inout) :: handler
        integer, intent(in) :: dest_rank
        type(MPI_COMM), intent(in) :: comm
    end subroutine request_handler_client_handle
end interface

public :: request_handler_t, request_handler_manager_t

```

```

contains
!!
!! Request handler.
!!
subroutine request_handler_base_write (handler, unit)
  class(request_handler_t), intent(in) :: handler
  integer, intent(in), optional :: unit
  integer :: u, i
  u = ERROR_UNIT; if (present (unit)) u = unit
  write (u, "(A,1X,IO)") "N_REQUESTS", handler%n_requests
  write (u, "(A,1X,IO)") "TAG_OFFSET", handler%tag_offset
  write (u, "(A,1X,L1)") "FINISHED", handler%finished
  write (u, "(A,1X,L1)") "ACTIVATED", handler%activated
  write (u, "(A)") "I | SOURCE | TAG | ERROR | REQUEST_NULL"
  do i = 1, handler%n_requests
    write (u, "(A,4(1X,IO),1X,L1)") "REQUEST", i, &
      handler%status(i)%MPI_SOURCE, &
      handler%status(i)%MPI_TAG, &
      handler%status(i)%MPI_ERROR, &
      (handler%request(i) == MPI_REQUEST_NULL)
  end do
end subroutine request_handler_base_write

!> Allocate MPI request and status object.
!!
!! Must be called during or after object-initialization.
!!
!! \param[inout] handler Handler must be intent inout, as the calling function may already manip
!! \param[in] n_requests Number of MPI requests the objects needs to be able to handle.
!! \param[in] tag_offset First tag to be used, all other must follow in an increasing manner unt
!! Proof: tag \in {tag_offset, tag_offset + n_requests}.
subroutine request_handler_allocate (handler, n_requests, tag_offset)
  class(request_handler_t), intent(inout) :: handler
  integer, intent(in) :: n_requests
  integer, intent(in) :: tag_offset
  allocate (handler%request(n_requests), source = MPI_REQUEST_NULL)
  allocate (handler%status(n_requests))
  handler%n_requests = n_requests
  if (mod (tag_offset, n_requests) /= 0) &
    call msg_bug ("Error during handler allocate, tag_offset is not a multiple of n_requests.
!! What is the max.-allowed MPI_TAG?
  handler%tag_offset = tag_offset
  handler%activated = .false.
  handler%finished = .false.
end subroutine request_handler_allocate

!> Get status from request objects in a non-destructive way.
subroutine request_handler_get_status (handler)
  class(request_handler_t), intent(inout) :: handler
  integer :: i
  logical :: flag
  if (.not. handler%activated) return
  handler%finished = .true.
  do i = 1, handler%n_requests

```

```

        call MPI_REQUEST_GET_STATUS (handler%request(i), flag, &
            handler%status(i))
        handler%finished = handler%finished .and. flag
    end do
end subroutine request_handler_get_status

!> Call MPI_WAITALL and raise finished flag.
subroutine request_handler_waitall (handler)
    class(request_handler_t), intent(inout) :: handler
    integer :: error
    if (.not. handler%activated .or. handler%finished) return
    call MPI_WAITALL (handler%n_requests, handler%request, handler%status, error)
    if (error /= 0) then
        call msg_bug ("Request: Error occurred during waitall on handler.")
    end if
    handler%finished = .true.
end subroutine request_handler_waitall

logical function request_handler_testall (handler) result (flag)
    class(request_handler_t), intent(inout) :: handler
    integer :: error
    if (.not. handler%activated .or. .not. handler%finished) then
        call MPI_TESTALL (handler%n_requests, handler%request, handler%finished, &
            handler%status, error)
        ! call print_status ()
        if (error /= 0) then
            call msg_bug ("Request: Error occurred during testall on handler.")
        end if
    end if
    flag = handler%finished
contains
    subroutine print_status ()
        integer :: i
        do i = 1, handler%n_requests
            associate (status => handler%status(i))
                write (ERROR_UNIT, *) status%MPI_SOURCE, status%MPI_TAG, status%MPI_ERROR
            end associate
        end do
    end subroutine print_status
end function request_handler_testall

subroutine request_handler_free (handler)
    class(request_handler_t), intent(inout) :: handler
    integer :: i, error
    do i = 1, handler%n_requests
        if (handler%request(i) == MPI_REQUEST_NULL) cycle
        call MPI_REQUEST_FREE (handler%request(i), error)
        if (error /= 0) then
            call msg_bug ("Request: Error occurred during free request on handler.")
        end if
    end do
end subroutine request_handler_free

!!

```

```

!! Request handler manager.
!!
subroutine request_handler_manager_init (rhmm, comm)
  class(request_handler_manager_t), intent(out) :: rhmm
  type(MPI_COMM), intent(in) :: comm
  call MPI_COMM_DUP (comm, rhmm%comm)
end subroutine request_handler_manager_init

subroutine request_handler_manager_write (rhmm, unit)
  class(request_handler_manager_t), intent(in) :: rhmm
  integer, intent(in), optional :: unit
  integer :: u
  u = ERROR_UNIT; if (present (unit)) u = unit
  write (u, "(A)") "[REQUEST_CALLBACK_MANAGER]"
  call rhmm%tree%write (u)
end subroutine request_handler_manager_write

subroutine request_handler_manager_add (rhmm, handler_id, handler)
  class(request_handler_manager_t), intent(inout) :: rhmm
  integer, intent(in) :: handler_id
  class(request_handler_t), pointer, intent(in) :: handler
  class(*), pointer :: obj
  obj => handler
  call rhmm%tree%insert (handler_id, obj)
end subroutine request_handler_manager_add

subroutine request_handler_manager_clear (rhmm)
  class(request_handler_manager_t), intent(inout) :: rhmm
  call rhmm%tree%clear ()
end subroutine request_handler_manager_clear

!> Get status (in a non-destructive way) for all associated handler.
subroutine request_handler_manager_fill_status (rhmm)
  class(request_handler_manager_t), intent(inout) :: rhmm
  type(binary_tree_iterator_t) :: iterator
  integer :: handler_id
  class(request_handler_t), pointer :: handler
  call iterator%init (rhmm%tree)
  do while (iterator%is_iterable ())
    call iterator%next (handler_id)
    call rhmm%handler_at (handler_id, handler)
    call handler%get_status ()
  end do
end subroutine request_handler_manager_fill_status

logical function request_handler_manager_test (rhmm, handler_id) result (flag)
  class(request_handler_manager_t), intent(inout) :: rhmm
  integer, intent(in) :: handler_id
  class(request_handler_t), pointer :: handler
  call rhmm%handler_at (handler_id, handler)
  flag = handler%testall ()
end function request_handler_manager_test

subroutine request_handler_manager_wait (rhmm, handler_id)

```

```

class(request_handler_manager_t), intent(inout) :: rhm
integer, intent(in) :: handler_id
class(request_handler_t), pointer :: handler
call rhm%handler_at (handler_id, handler)
call handler%waitall ()
end subroutine request_handler_manager_wait

subroutine request_handler_manager_waitall (rhm)
class(request_handler_manager_t), intent(inout) :: rhm
type(binary_tree_iterator_t) :: iterator
integer :: handler_id
call iterator%init (rhm%tree)
do while (iterator%is_iterable ())
    call iterator%next (handler_id)
    !! Test handler (destructive test on request handler).
    if (.not. rhm%test (handler_id)) &
        call rhm%wait (handler_id)
end do
end subroutine request_handler_manager_waitall

subroutine request_handler_manager_handler_at (rhm, handler_id, handler)
class(request_handler_manager_t), intent(in) :: rhm
integer, intent(in) :: handler_id
class(request_handler_t), pointer, intent(out) :: handler
class(*), pointer :: obj
call rhm%tree%search (handler_id, obj)
select type (obj)
class is (request_handler_t)
    handler => obj
class default
    call msg_bug ("Object is not derived from request_handler_t.")
end select
end subroutine request_handler_manager_handler_at

function request_handler_manager_has_handler (rhm, handler_id) result (flag)
class(request_handler_manager_t), intent(inout) :: rhm
integer, intent(in) :: handler_id
logical :: flag
flag = rhm%tree%has_key (handler_id)
end function request_handler_manager_has_handler

!> Call server-sided procedure of callback with handler_id.
!!
!! \param[in] handler_id
!! \param[in] source
subroutine request_handler_manager_callback (rhm, handler_id, source_rank)
class(request_handler_manager_t), intent(inout) :: rhm
integer, intent(in) :: handler_id
integer, intent(in) :: source_rank
class(request_handler_t), pointer :: handler
if (.not. rhm%tree%has_key (handler_id)) return
call rhm%handler_at (handler_id, handler)
call handler%handle (source_rank = source_rank, comm = rhm%comm)
end subroutine request_handler_manager_callback

```

```

!> Call client-sided procedure of callback with handler_id.
!!
!! \param[in] handler_id
!! \param[in] source Destination rank.
subroutine request_handler_manager_client_callback (rhm, handler_id, dest_rank)
    class(request_handler_manager_t), intent(inout) :: rhm
    integer, intent(in) :: handler_id
    integer, intent(in) :: dest_rank
    class(request_handler_t), pointer :: handler
    if (.not. rhm%tree%has_key (handler_id)) return
    call rhm%handler_at (handler_id, handler)
    call handler%client_handle (dest_rank = dest_rank, comm = rhm%comm)
end subroutine request_handler_manager_client_callback
end module request_callback

```


Chapter 21

Multi-Channel Integration

The abstract representation of multi-channel Monte Carlo algorithms for integration and event generation.

Module `mci_base`: The abstract types and their methods. It provides a test integrator that is referenced in later unit tests.

iterations Container for defining integration call and pass settings.

integration_results This module handles results from integrating processes. It records passes and iterations, calculates statistical averages, and provides the user output of integration results.

These are the implementations:

Module `mci_midpoint`: A simple integrator that uses the midpoint rule to sample the integrand uniformly over the unit hypercube. There is only one integration channel, so this can be matched only to single-channel phase space.

Module `mci_vamp`: Interface for the VAMP package.

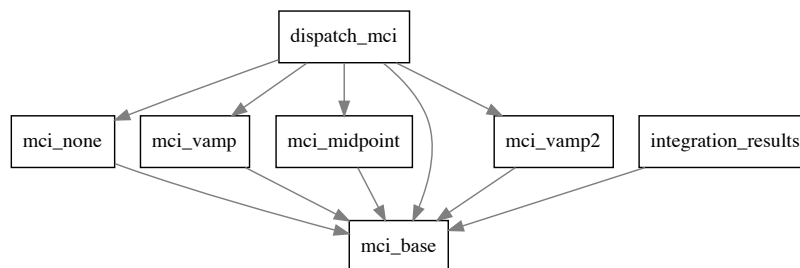


Figure 21.1: Module dependencies in `src/mci`.

21.1 Generic Integrator

This module provides a multi-channel integrator (MCI) base type, a corresponding configuration type, and methods for integration and event generation.

```
<mci_base.f90>≡  
  <File header>  
  
  module mci_base  
  
    use kinds  
    use io_units  
    use format_utils, only: pac_fmt  
    use format_defs, only: FMT_14, FMT_17  
    use diagnostics  
    use cputime  
    use phs_base  
    use rng_base  
  
    <Standard module head>  
  
    <MCI base: public>  
  
    <MCI base: types>  
  
    <MCI base: interfaces>  
  
    contains  
  
    <MCI base: procedures>  
  
  end module mci_base
```

21.1.1 MCI: integrator

The MCI object contains the methods for integration and event generation. For the actual work and data storage, it spawns an MCI instance object.

The base object contains the number of integration dimensions and the number of channels as configuration data. Further configuration data are stored in the concrete extensions.

The MCI sum contains all relevant information about the integrand. It can be used for comparing the current configuration against a previous one. If they match, we can skip an actual integration. (Implemented only for the VAMP version.)

There is a random-number generator (its state with associated methods) available as `rng`. It may or may not be used for integration. It will be used for event generation.

```
<MCI base: public>≡  
  public :: mci_t  
  
<MCI base: types>≡  
  type, abstract :: mci_t  
    integer :: n_dim = 0
```

```

integer :: n_channel = 0
integer :: n_chain = 0
integer, dimension(:), allocatable :: chain
real(default), dimension(:), allocatable :: chain_weights
character(32) :: md5sum = ""
logical :: integral_known = .false.
logical :: error_known = .false.
logical :: efficiency_known = .false.
real(default) :: integral = 0
real(default) :: error = 0
real(default) :: efficiency = 0
logical :: use_timer = .false.
type(timer_t) :: timer
class(rng_t), allocatable :: rng
contains
  <MCI base: mci: TBP>
end type mci_t

```

Finalizer: the random-number generator may need one.

```

<MCI base: mci: TBP>≡
  procedure :: base_final => mci_final
  procedure (mci_final), deferred :: final

<MCI base: procedures>≡
  subroutine mci_final (object)
    class(mci_t), intent(inout) :: object
    if (allocated (object%rng)) call object%rng%final ()
  end subroutine mci_final

```

Output: basic and extended output.

```

<MCI base: mci: TBP>+≡
  procedure :: base_write => mci_write
  procedure (mci_write), deferred :: write

<MCI base: procedures>+≡
  subroutine mci_write (object, unit, pacify, md5sum_version)
    class(mci_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    logical, intent(in), optional :: md5sum_version
    logical :: md5sum_ver
    integer :: u, i, j
    character(len=7) :: fmt
    call pac_fmt (fmt, FMT_17, FMT_14, pacify)
    u = given_output_unit (unit)
    md5sum_ver = .false.
    if (present (md5sum_version)) md5sum_ver = md5sum_version
    if (object%use_timer .and. .not. md5sum_ver) then
      write (u, "(2x)", advance="no")
      call object%timer%write (u)
    end if
    if (object%integral_known) then
      write (u, "(3x,A," // fmt // ")") &
        "Integral" = ", object%integral

```

```

end if
if (object%error_known) then
  write (u, "(3x,A," // fmt // ")") &
    "Error" = ", object%error
end if
if (object%efficiency_known) then
  write (u, "(3x,A," // fmt // ")") &
    "Efficiency" = ", object%efficiency
end if
write (u, "(3x,A,I0)") "Number of channels" = ", object%n_channel
write (u, "(3x,A,I0)") "Number of dimensions" = ", object%n_dim
if (object%n_chain > 0) then
  write (u, "(3x,A,I0)") "Number of chains" = ", object%n_chain
  write (u, "(3x,A)") "Chains:"
  do i = 1, object%n_chain
    write (u, "(5x,I0,':')", advance = "no") i
    do j = 1, object%n_channel
      if (object%chain(j) == i) &
        write (u, "(1x,I0)", advance = "no") j
      end do
      write (u, "(A)")
    end do
  end do
end if
end subroutine mci_write

```

Print an informative message when starting integration.

```

<MCI base: mci: TBP>+≡
  procedure (mci_startup_message), deferred :: startup_message
  procedure :: base_startup_message => mci_startup_message

<MCI base: procedures>+≡
  subroutine mci_startup_message (mci, unit, n_calls)
    class(mci_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
    if (mci%n_chain > 0) then
      write (msg_buffer, "(A,3(1x,I0,1x,A))") &
        "Integrator:", mci%n_chain, "chains,", &
        mci%n_channel, "channels,", &
        mci%n_dim, "dimensions"
    else
      write (msg_buffer, "(A,3(1x,I0,1x,A))") &
        "Integrator:", &
        mci%n_channel, "channels,", &
        mci%n_dim, "dimensions"
    end if
    call msg_message (unit = unit)
  end subroutine mci_startup_message

```

Dump type-specific info to a logfile.

```

<MCI base: mci: TBP>+≡
  procedure(mci_write_log_entry), deferred :: write_log_entry

<MCI base: interfaces>≡
  abstract interface

```

```

subroutine mci_write_log_entry (mci, u)
  import
  class(mci_t), intent(in) :: mci
  integer, intent(in) :: u
end subroutine mci_write_log_entry
end interface

```

In order to avoid dependencies on definite MCI implementations, we introduce a MD5 sum calculator.

```

⟨MCI base: mci: TBP⟩+≡
  procedure(mci_compute_md5sum), deferred :: compute_md5sum
⟨MCI base: interfaces⟩+≡
  abstract interface
    subroutine mci_compute_md5sum (mci, pacify)
      import
      class(mci_t), intent(inout) :: mci
      logical, intent(in), optional :: pacify
    end subroutine mci_compute_md5sum
  end interface

```

Record the index of the MCI object within a process. For multi-component processes with more than one integrator, the integrator should know about its own index, so file names can be unique, etc. The default implementation does nothing, however.

```

⟨MCI base: mci: TBP⟩+≡
  procedure :: record_index => mci_record_index
⟨MCI base: procedures⟩+≡
  subroutine mci_record_index (mci, i_mci)
    class(mci_t), intent(inout) :: mci
    integer, intent(in) :: i_mci
  end subroutine mci_record_index

```

There is no Initializer for the abstract type, but a generic setter for the number of channels and dimensions. We make two aliases available, to be able to override it.

```

⟨MCI base: mci: TBP⟩+≡
  procedure :: set_dimensions => mci_set_dimensions
  procedure :: base_set_dimensions => mci_set_dimensions
⟨MCI base: procedures⟩+≡
  subroutine mci_set_dimensions (mci, n_dim, n_channel)
    class(mci_t), intent(inout) :: mci
    integer, intent(in) :: n_dim
    integer, intent(in) :: n_channel
    mci%n_dim = n_dim
    mci%n_channel = n_channel
  end subroutine mci_set_dimensions

```

Declare particular dimensions as flat. This information can be used to simplify integration. When generating events, the flat dimensions should be sampled with uniform and uncorrelated distribution. It depends on the integrator what to do with that information.

```

<MCI base: mci: TBP>+≡
  procedure (mci_declare_flat_dimensions), deferred :: declare_flat_dimensions

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_declare_flat_dimensions (mci, dim_flat)
      import
      class(mci_t), intent(inout) :: mci
      integer, dimension(:), intent(in) :: dim_flat
    end subroutine mci_declare_flat_dimensions
  end interface

```

Declare particular channels as equivalent, possibly allowing for permutations or reflections of dimensions. We use the information stored in the `phs_channel_t` object array that the phase-space module provides.

(We do not test this here, deferring the unit test to the `mci_vamp` implementation where we actually use this feature.)

```

<MCI base: mci: TBP>+≡
  procedure (mci_declare_equivalences), deferred :: declare_equivalences

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_declare_equivalences (mci, channel, dim_offset)
      import
      class(mci_t), intent(inout) :: mci
      type(phs_channel_t), dimension(:), intent(in) :: channel
      integer, intent(in) :: dim_offset
    end subroutine mci_declare_equivalences
  end interface

```

Declare particular channels as chained together. The implementation may use this array for keeping their weights equal to each other, etc.

The chain array is an array sized by the number of channels. For each channel, there is an integer entry that indicates the corresponding chains. The total number of chains is the maximum value of this entry.

```

<MCI base: mci: TBP>+≡
  procedure :: declare_chains => mci_declare_chains

<MCI base: procedures>+≡
  subroutine mci_declare_chains (mci, chain)
    class(mci_t), intent(inout) :: mci
    integer, dimension(:), intent(in) :: chain
    allocate (mci%chain (size (chain)))
    mci%n_chain = maxval (chain)
    allocate (mci%chain_weights (mci%n_chain), source = 0._default)
    mci%chain = chain
  end subroutine mci_declare_chains

```

Collect channel weights according to chains and store them in the `chain_weights` for output. We sum up the weights for all channels that share the same `chain` index and store the results in the `chain_weights` array.

```

(MCI base: mci: TBP)+≡
  procedure :: collect_chain_weights => mci_collect_chain_weights

(MCI base: procedures)+≡
  subroutine mci_collect_chain_weights (mci, weight)
    class(mci_t), intent(inout) :: mci
    real(default), dimension(:), intent(in) :: weight
    integer :: i, c
    if (allocated (mci%chain)) then
      mci%chain_weights = 0
      do i = 1, size (mci%chain)
        c = mci%chain(i)
        mci%chain_weights(c) = mci%chain_weights(c) + weight(i)
      end do
    end if
  end subroutine mci_collect_chain_weights

```

Check if there are chains.

```

(MCI base: mci: TBP)+≡
  procedure :: has_chains => mci_has_chains

(MCI base: procedures)+≡
  function mci_has_chains (mci) result (flag)
    class(mci_t), intent(in) :: mci
    logical :: flag
    flag = allocated (mci%chain)
  end function mci_has_chains

```

Output of the chain weights, kept separate from the main `write` method.

[The formatting will work as long as the number of chains is less than 10^{10} ...]

```

(MCI base: mci: TBP)+≡
  procedure :: write_chain_weights => mci_write_chain_weights

(MCI base: procedures)+≡
  subroutine mci_write_chain_weights (mci, unit)
    class(mci_t), intent(in) :: mci
    integer, intent(in), optional :: unit
    integer :: u, i, n, n_digits
    character(4) :: ifmt
    u = given_output_unit (unit)
    if (allocated (mci%chain_weights)) then
      write (u, "(1x,A)") "Weights of channel chains (groves):"
      n_digits = 0
      n = size (mci%chain_weights)
      do while (n > 0)
        n = n / 10
        n_digits = n_digits + 1
      end do
      write (ifmt, "(A1,I1)") "I", n_digits
      do i = 1, size (mci%chain_weights)
        write (u, "(3x," // ifmt // ",F13.10)") i, mci%chain_weights(i)
      end do
    end if
  end subroutine mci_write_chain_weights

```

```

        end do
    end if
end subroutine mci_write_chain_weights

```

Set the MD5 sum, independent of initialization.

```

<MCI base: mci: TBP>+≡
    procedure :: set_md5sum => mci_set_md5sum

<MCI base: procedures>+≡
    subroutine mci_set_md5sum (mci, md5sum)
        class(mci_t), intent(inout) :: mci
        character(32), intent(in) :: md5sum
        mci%md5sum = md5sum
    end subroutine mci_set_md5sum

```

Initialize a new integration pass. This is not necessarily meaningful, so we provide an empty base method. The `mci_vamp` implementation overrides this.

```

<MCI base: mci: TBP>+≡
    procedure :: add_pass => mci_add_pass

<MCI base: procedures>+≡
    subroutine mci_add_pass (mci, adapt_grids, adapt_weights, final_pass)
        class(mci_t), intent(inout) :: mci
        logical, intent(in), optional :: adapt_grids
        logical, intent(in), optional :: adapt_weights
        logical, intent(in), optional :: final_pass
    end subroutine mci_add_pass

```

Allocate an instance with matching type. This must be deferred.

```

<MCI base: mci: TBP>+≡
    procedure (mci_allocate_instance), deferred :: allocate_instance

<MCI base: interfaces>+≡
    abstract interface
        subroutine mci_allocate_instance (mci, mci_instance)
            import
            class(mci_t), intent(in) :: mci
            class(mci_instance_t), intent(out), pointer :: mci_instance
        end subroutine mci_allocate_instance
    end interface

```

Import a random-number generator. We transfer the allocation of an existing generator state into the object. The generator state may already be initialized, or we can reset it by its `init` method.

```

<MCI base: mci: TBP>+≡
    procedure :: import_rng => mci_import_rng

<MCI base: procedures>+≡
    subroutine mci_import_rng (mci, rng)
        class(mci_t), intent(inout) :: mci
        class(rng_t), intent(inout), allocatable :: rng
        call move_alloc (rng, mci%rng)
    end subroutine mci_import_rng

```


Activate or deactivate the timer.

```

<MCI base: mci: TBP>+≡
  procedure :: set_timer => mci_set_timer

<MCI base: procedures>+≡
  subroutine mci_set_timer (mci, active)
    class(mci_t), intent(inout) :: mci
    logical, intent(in) :: active
    mci%use_timer = active
  end subroutine mci_set_timer

```

Start and stop signal for the timer, if active. The elapsed time can then be retrieved from the MCI record.

```

<MCI base: mci: TBP>+≡
  procedure :: start_timer => mci_start_timer
  procedure :: stop_timer => mci_stop_timer

<MCI base: procedures>+≡
  subroutine mci_start_timer (mci)
    class(mci_t), intent(inout) :: mci
    if (mci%use_timer) call mci%timer%start ()
  end subroutine mci_start_timer

  subroutine mci_stop_timer (mci)
    class(mci_t), intent(inout) :: mci
    if (mci%use_timer) call mci%timer%stop ()
  end subroutine mci_stop_timer

```

Sampler test. Evaluate the sampler a given number of times. Results are discarded, so we don't need the MCI instance which would record them.

The evaluation channel is iterated, and the *x* parameters are randomly chosen.

```

<MCI base: mci: TBP>+≡
  procedure :: sampler_test => mci_sampler_test

<MCI base: procedures>+≡
  subroutine mci_sampler_test (mci, sampler, n_calls)
    class(mci_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_calls
    real(default), dimension(:), allocatable :: x_in, f
    real(default), dimension(:,:), allocatable :: x_out
    real(default) :: val
    integer :: i, c
    allocate (x_in (mci%n_dim))
    allocate (f (mci%n_channel))
    allocate (x_out (mci%n_dim, mci%n_channel))
    do i = 1, n_calls
      c = mod (i, mci%n_channel) + 1
      call mci%rng%generate_array (x_in)
      call sampler%evaluate (c, x_in, val, x_out, f)
    end do
  end subroutine mci_sampler_test

```

Integrate: this depends on the implementation. We foresee a pacify flag to take care of small numerical noise on different platforms.

```

(MCI base: mci: TBP)+≡
  procedure (mci_integrate), deferred :: integrate

(MCI base: interfaces)+≡
  abstract interface
    subroutine mci_integrate (mci, instance, sampler, &
      n_it, n_calls, results, pacify)
    import
    class(mci_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: pacify
    class(mci_results_t), intent(inout), optional :: results
  end subroutine mci_integrate
end interface

```

Event generation. Depending on the implementation, event generation may or may not require a previous integration pass.

Instead of a black-box `simulate` method, we require an initializer, a finalizer, and procedures for generating a single event. This allows us to interface simulation event by event from the outside, and it facilitates the further processing of an event after successful generation. For integration, this is not necessary.

The initializer has `intent(inout)` for the `mci` passed object. The reason is that the initializer can read integration results and grids from file, where the results can modify the `mci` record.

```

(MCI base: mci: TBP)+≡
  procedure (mci_prepare_simulation), deferred :: prepare_simulation

(MCI base: interfaces)+≡
  abstract interface
    subroutine mci_prepare_simulation (mci)
    import
    class(mci_t), intent(inout) :: mci
  end subroutine mci_prepare_simulation
end interface

```

The generated event will reside in in the `instance` object (overall results and weight) and in the `sampler` object (detailed data). In the real application, we can subsequently call methods of the `sampler` in order to further process the generated event.

The `target` attributes are required by the VAMP implementation, which uses pointers to refer to the instance and sampler objects from within the integration function.

```

(MCI base: mci: TBP)+≡
  procedure (mci_generate), deferred :: generate_weighted_event
  procedure (mci_generate), deferred :: generate_unweighted_event

```

```

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_generate (mci, instance, sampler)
      import
      class(mci_t), intent(inout) :: mci
      class(mci_instance_t), intent(inout), target :: instance
      class(mci_sampler_t), intent(inout), target :: sampler
    end subroutine mci_generate
  end interface

```

This is analogous, but we rebuild the event from the information stored in `state` instead of generating it.

Note: currently unused outside of tests, might be deleted later.

```

<MCI base: mci: TBP>+≡
  procedure (mci_rebuild), deferred :: rebuild_event

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_rebuild (mci, instance, sampler, state)
      import
      class(mci_t), intent(inout) :: mci
      class(mci_instance_t), intent(inout) :: instance
      class(mci_sampler_t), intent(inout) :: sampler
      class(mci_state_t), intent(in) :: state
    end subroutine mci_rebuild
  end interface

```

Pacify: reduce numerical noise. The base implementation does nothing.

```

<MCI base: mci: TBP>+≡
  procedure :: pacify => mci_pacify

<MCI base: procedures>+≡
  subroutine mci_pacify (object, efficiency_reset, error_reset)
    class(mci_t), intent(inout) :: object
    logical, intent(in), optional :: efficiency_reset, error_reset
  end subroutine mci_pacify

```

Return the value of the integral, error, efficiency, and time per call.

```

<MCI base: mci: TBP>+≡
  procedure :: get_integral => mci_get_integral
  procedure :: get_error => mci_get_error
  procedure :: get_efficiency => mci_get_efficiency
  procedure :: get_time => mci_get_time

<MCI base: procedures>+≡
  function mci_get_integral (mci) result (integral)
    class(mci_t), intent(in) :: mci
    real(default) :: integral
    if (mci%integral_known) then
      integral = mci%integral
    else
      call msg_bug ("The integral is unknown. This is presumably a" // &
        "WHIZARD bug.")
    end if
  end function

```

```

        end if
    end function mci_get_integral

function mci_get_error (mci) result (error)
    class(mci_t), intent(in) :: mci
    real(default) :: error
    if (mci%error_known) then
        error = mci%error
    else
        error = 0
    end if
end function mci_get_error

function mci_get_efficiency (mci) result (efficiency)
    class(mci_t), intent(in) :: mci
    real(default) :: efficiency
    if (mci%efficiency_known) then
        efficiency = mci%efficiency
    else
        efficiency = 0
    end if
end function mci_get_efficiency

function mci_get_time (mci) result (time)
    class(mci_t), intent(in) :: mci
    real(default) :: time
    if (mci%use_timer) then
        time = mci%timer
    else
        time = 0
    end if
end function mci_get_time

```

Return the MD5 sum of the configuration. This may be overridden in an extension, to return a different MD5 sum.

```

<MCI base: mci: TBP>+≡
    procedure :: get_md5sum => mci_get_md5sum

<MCI base: procedures>+≡
    pure function mci_get_md5sum (mci) result (md5sum)
        class(mci_t), intent(in) :: mci
        character(32) :: md5sum
        md5sum = mci%md5sum
    end function mci_get_md5sum

```

21.1.2 MCI instance

The base type contains an array of channel weights. The value `mci_weight` is the combined MCI weight that corresponds to a particular sampling point.

For convenience, we also store the `x` and Jacobian values for this sampling point.

```

<MCI base: public>+≡

```

```

    public :: mci_instance_t
<MCI base: types>+≡
    type, abstract :: mci_instance_t
        logical :: valid = .false.
        real(default), dimension(:), allocatable :: w
        real(default), dimension(:), allocatable :: f
        real(default), dimension(:,:), allocatable :: x
        integer :: selected_channel = 0
        real(default) :: mci_weight = 0
        real(default) :: integrand = 0
        logical :: negative_weights = .false.
        integer :: n_dropped = 0
    contains
        <MCI base: mci instance: TBP>
    end type mci_instance_t

```

Output: deferred

```

<MCI base: mci instance: TBP>≡
    procedure (mci_instance_write), deferred :: write
<MCI base: interfaces>+≡
    abstract interface
        subroutine mci_instance_write (object, unit, pacify)
            import
            class(mci_instance_t), intent(in) :: object
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: pacify
        end subroutine mci_instance_write
    end interface

```

A finalizer, just in case.

```

<MCI base: mci instance: TBP>+≡
    procedure (mci_instance_final), deferred :: final
<MCI base: interfaces>+≡
    abstract interface
        subroutine mci_instance_final (object)
            import
            class(mci_instance_t), intent(inout) :: object
        end subroutine mci_instance_final
    end interface

```

Init: basic initializer for the arrays, otherwise deferred. Assigning the mci object is also deferred, because it depends on the concrete type.

The weights are initialized with an uniform normalized value.

```

<MCI base: mci instance: TBP>+≡
    procedure (mci_instance_base_init), deferred :: init
    procedure :: base_init => mci_instance_base_init
<MCI base: procedures>+≡
    subroutine mci_instance_base_init (mci_instance, mci)
        class(mci_instance_t), intent(out) :: mci_instance
        class(mci_t), intent(in), target :: mci

```

```

allocate (mci_instance%w (mci%n_channel))
allocate (mci_instance%f (mci%n_channel))
allocate (mci_instance%x (mci%n_dim, mci%n_channel))
if (mci%n_channel > 0) then
  call mci_instance%set_channel_weights &
    (spread (1._default, dim=1, ncopies=mci%n_channel))
end if
mci_instance%f = 0
mci_instance%x = 0
end subroutine mci_instance_base_init

```

Explicitly set the array of channel weights.

(MCI base: mci instance: TBP)+≡

```

procedure :: set_channel_weights => mci_instance_set_channel_weights

```

(MCI base: procedures)+≡

```

subroutine mci_instance_set_channel_weights (mci_instance, weights, sum_non_zero)
  class(mci_instance_t), intent(inout) :: mci_instance
  real(default), dimension(:), intent(in) :: weights
  logical, intent(out), optional :: sum_non_zero
  real(default) :: wsum
  wsum = sum (weights)
  if (wsum /= 0) then
    mci_instance%w = weights / wsum
    if (present (sum_non_zero)) sum_non_zero = .true.
  else
    if (present (sum_non_zero)) sum_non_zero = .false.
    call msg_warning ("MC sampler initialization:&
      & sum of channel weights is zero")
  end if
end subroutine mci_instance_set_channel_weights

```

Compute the overall weight factor for a configuration of x values and Jacobians f . The x values come in $n_channel$ rows with n_dim entries each. The f factors constitute an array with $n_channel$ entries.

We assume that the x and f arrays are already stored inside the MC instance. The result is also stored there.

(MCI base: mci instance: TBP)+≡

```

procedure (mci_instance_compute_weight), deferred :: compute_weight

```

(MCI base: interfaces)+≡

```

abstract interface
  subroutine mci_instance_compute_weight (mci, c)
    import
    class(mci_instance_t), intent(inout) :: mci
    integer, intent(in) :: c
  end subroutine mci_instance_compute_weight
end interface

```

Record the integrand as returned by the sampler. Depending on the implementation, this may merely copy the value, or do more complicated things.

We may need the MCI weight for the actual computations, so this should be called after the previous routine.

```

<MCI base: mci_instance: TBP>+≡
  procedure (mci_instance_record_integrand), deferred :: record_integrand

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_instance_record_integrand (mci, integrand)
      import
      class(mci_instance_t), intent(inout) :: mci
      real(default), intent(in) :: integrand
    end subroutine mci_instance_record_integrand
  end interface

```

Sample a point directly: evaluate the sampler, then compute the weight and the weighted integrand. Finally, record the integrand within the MCI instance.

If a signal (interrupt) was raised recently, we abort the calculation before entering the sampler. Thus, a previous calculation will have completed and any data are already recorded, but any new point can be discarded. If the `abort` flag is present, we may delay the interrupt, so we can do some cleanup.

```

<MCI base: mci_instance: TBP>+≡
  procedure :: evaluate => mci_instance_evaluate

<MCI base: procedures>+≡
  subroutine mci_instance_evaluate (mci, sampler, c, x)
    class(mci_instance_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x
    real(default) :: val
    call sampler%evaluate (c, x, val, mci%x, mci%f)
    mci%valid = sampler%is_valid ()
    if (mci%valid) then
      call mci%compute_weight (c)
      call mci%record_integrand (val)
    end if
  end subroutine mci_instance_evaluate

```

Initiate and terminate simulation. In contrast to integration, we implement these as methods of the process instance, since the `mci` configuration object is unchanged.

The safety factor reduces the acceptance probability for unweighted events. The implementation of this feature depends on the concrete type.

```

<MCI base: mci_instance: TBP>+≡
  procedure (mci_instance_init_simulation), deferred :: init_simulation
  procedure (mci_instance_final_simulation), deferred :: final_simulation

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_instance_init_simulation (instance, safety_factor)
      import
      class(mci_instance_t), intent(inout) :: instance
      real(default), intent(in), optional :: safety_factor
    end subroutine mci_instance_init_simulation
  end interface

```

```

        end subroutine mci_instance_init_simulation
    end interface

    abstract interface
        subroutine mci_instance_final_simulation (instance)
            import
            class(mci_instance_t), intent(inout) :: instance
        end subroutine mci_instance_final_simulation
    end interface

```

Assuming that the sampler is in a completely defined state, just extract the data that `evaluate` would compute. Also record the integrand.

```

⟨MCI base: mci instance: TBP⟩+≡
    procedure :: fetch => mci_instance_fetch

⟨MCI base: procedures⟩+≡
    subroutine mci_instance_fetch (mci, sampler, c)
        class(mci_instance_t), intent(inout) :: mci
        class(mci_sampler_t), intent(in) :: sampler
        integer, intent(in) :: c
        real(default) :: val
        mci%valid = sampler%is_valid ()
        if (mci%valid) then
            call sampler%fetch (val, mci%x, mci%f)
            call mci%compute_weight (c)
            call mci%record_integrand (val)
        end if
    end subroutine mci_instance_fetch

```

The value, i.e., the weighted integrand, is the integrand (which should be taken as-is from the sampler) multiplied by the MCI weight.

```

⟨MCI base: mci instance: TBP⟩+≡
    procedure :: get_value => mci_instance_get_value

⟨MCI base: procedures⟩+≡
    function mci_instance_get_value (mci) result (value)
        class(mci_instance_t), intent(in) :: mci
        real(default) :: value
        if (mci%valid) then
            value = mci%integrand * mci%mci_weight
        else
            value = 0
        end if
    end function mci_instance_get_value

```

This is an extra routine. By default, the event weight is equal to the value returned by the previous routine. However, if we select a channel for event generation not just based on the channel weights, the event weight has to account for this bias, so the event weight that applies to event generation is different. In that case, we should override the default routine.

```

⟨MCI base: mci instance: TBP⟩+≡
    procedure :: get_event_weight => mci_instance_get_value

```


Excess weight can occur during unweighted event generation, if the assumed maximum value of the integrand is too small. This excess should be normalized in the same way as the event weight above (which for unweighted events becomes unity).

```

<MCI base: mci_instance: TBP>+≡
  procedure (mci_instance_get_event_excess), deferred :: get_event_excess

<MCI base: interfaces>+≡
  abstract interface
    function mci_instance_get_event_excess (mci) result (excess)
      import
      class(mci_instance_t), intent(in) :: mci
      real(default) :: excess
    end function mci_instance_get_event_excess
  end interface

```

Dropped events (i.e., events with zero weight that are not retained) are counted within the `mci_instance` object.

```

<MCI base: mci_instance: TBP>+≡
  procedure :: get_n_event_dropped => mci_instance_get_n_event_dropped
  procedure :: reset_n_event_dropped => mci_instance_reset_n_event_dropped
  procedure :: record_event_dropped => mci_instance_record_event_dropped

<MCI base: procedures>+≡
  function mci_instance_get_n_event_dropped (mci) result (n_dropped)
    class(mci_instance_t), intent(in) :: mci
    integer :: n_dropped
    n_dropped = mci%n_dropped
  end function mci_instance_get_n_event_dropped

  subroutine mci_instance_reset_n_event_dropped (mci)
    class(mci_instance_t), intent(inout) :: mci
    mci%n_dropped = 0
  end subroutine mci_instance_reset_n_event_dropped

  subroutine mci_instance_record_event_dropped (mci)
    class(mci_instance_t), intent(inout) :: mci
    mci%n_dropped = mci%n_dropped + 1
  end subroutine mci_instance_record_event_dropped

```

21.1.3 MCI state

This object can hold the relevant information that allows us to reconstruct the MCI instance without re-evaluating the sampler completely.

We store the `x_in` MC input parameter set, which coincides with the section of the complete `x` array that belongs to a particular channel. We also store the MC function value. When we want to reconstruct the state, we can use the input array to recover the complete `x` and `f` arrays (i.e., the kinematics), but do not need to recompute the MC function value (the dynamics).

The `mci_state_t` may be extended, to allow storing/recalling more information. In that case, we would override the type-bound procedures. However, the

base type is also a concrete type and self-contained.

```

<MCI base: public>+≡
    public :: mci_state_t

<MCI base: types>+≡
    type :: mci_state_t
        integer :: selected_channel = 0
        real(default), dimension(:), allocatable :: x_in
        real(default) :: val
    contains
        <MCI base: mci state: TBP>
    end type mci_state_t

```

Output:

```

<MCI base: mci state: TBP>≡
    procedure :: write => mci_state_write

<MCI base: procedures>+≡
    subroutine mci_state_write (object, unit)
        class(mci_state_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "MCI state:"
        write (u, "(3x,A,I0)") "Channel   = ", object%selected_channel
        write (u, "(3x,A,999(1x,F12.10))") "x (in)   =", object%x_in
        write (u, "(3x,A,ES19.12)") "Integrand = ", object%val
    end subroutine mci_state_write

```

To store the object, we take the relevant section of the **x** array. The channel used for storing data is taken from the **instance** object, but it could be arbitrary in principle.

```

<MCI base: mci instance: TBP>+≡
    procedure :: store => mci_instance_store

<MCI base: procedures>+≡
    subroutine mci_instance_store (mci, state)
        class(mci_instance_t), intent(in) :: mci
        class(mci_state_t), intent(out) :: state
        state%selected_channel = mci%selected_channel
        allocate (state%x_in (size (mci%x, 1)))
        state%x_in = mci%x(:,mci%selected_channel)
        state%val = mci%integrand
    end subroutine mci_instance_store

```

Recalling the state, we must consult the sampler in order to fully reconstruct the **x** and **f** arrays. The integrand value is known, and we also give it to the sampler, bypassing evaluation.

The final steps are equivalent to the **evaluate** method above.

```

<MCI base: mci instance: TBP>+≡
    procedure :: recall => mci_instance_recall

```

```

<MCI base: procedures>+≡
  subroutine mci_instance_recall (mci, sampler, state)
    class(mci_instance_t), intent(inout) :: mci
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
    if (size (state%x_in) == size (mci%x, 1) &
        .and. state%selected_channel <= size (mci%x, 2)) then
      call sampler%rebuild (state%selected_channel, &
        state%x_in, state%val, mci%x, mci%f)
      call mci%compute_weight (state%selected_channel)
      call mci%record_integrand (state%val)
    else
      call msg_fatal ("Recalling event: mismatch in channel or dimension")
    end if
  end subroutine mci_instance_recall

```

21.1.4 MCI sampler

A sampler is an object that implements a multi-channel parameterization of the unit hypercube. Specifically, it is able to compute, given a channel and a set of x MC parameter values, the complete set of x values and associated Jacobian factors f for all channels.

Furthermore, the sampler should return a single real value, the integrand, for the given point in the hypercube.

It must implement a method `evaluate` for performing the above computations.

```

<MCI base: public>+≡
  public :: mci_sampler_t

<MCI base: types>+≡
  type, abstract :: mci_sampler_t
  contains
  <MCI base: mci sampler: TBP>
  end type mci_sampler_t

```

Output, deferred to the implementation.

```

<MCI base: mci sampler: TBP>≡
  procedure (mci_sampler_write), deferred :: write

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_sampler_write (object, unit, testflag)
      import
      class(mci_sampler_t), intent(in) :: object
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: testflag
    end subroutine mci_sampler_write
  end interface

```

The evaluation routine. Input is the channel index `c` and the one-dimensional parameter array `x_in`. Output are the integrand value `val`, the two-dimensional parameter array `x` and the Jacobian array `f`.

```

(MCI base: mci_sampler: TBP)+≡
  procedure (mci_sampler_evaluate), deferred :: evaluate

(MCI base: interfaces)+≡
  abstract interface
    subroutine mci_sampler_evaluate (sampler, c, x_in, val, x, f)
      import
      class(mci_sampler_t), intent(inout) :: sampler
      integer, intent(in) :: c
      real(default), dimension(:), intent(in) :: x_in
      real(default), intent(out) :: val
      real(default), dimension(:, :), intent(out) :: x
      real(default), dimension(:), intent(out) :: f
    end subroutine mci_sampler_evaluate
  end interface

```

Query the validity of the sampling point. Can be called after `evaluate`.

```

(MCI base: mci_sampler: TBP)+≡
  procedure (mci_sampler_is_valid), deferred :: is_valid

(MCI base: interfaces)+≡
  abstract interface
    function mci_sampler_is_valid (sampler) result (valid)
      import
      class(mci_sampler_t), intent(in) :: sampler
      logical :: valid
    end function mci_sampler_is_valid
  end interface

```

The shortcut. Again, the channel index `c` and the parameter array `x_in` are input. However, we also provide the integrand value `val`, and we just require that the complete parameter array `x` and Jacobian array `f` are recovered.

```

(MCI base: mci_sampler: TBP)+≡
  procedure (mci_sampler_rebuild), deferred :: rebuild

(MCI base: interfaces)+≡
  abstract interface
    subroutine mci_sampler_rebuild (sampler, c, x_in, val, x, f)
      import
      class(mci_sampler_t), intent(inout) :: sampler
      integer, intent(in) :: c
      real(default), dimension(:), intent(in) :: x_in
      real(default), intent(in) :: val
      real(default), dimension(:, :), intent(out) :: x
      real(default), dimension(:), intent(out) :: f
    end subroutine mci_sampler_rebuild
  end interface

```

This routine should extract the important data from a sampler that has been filled by other means. We fetch the integrand value `val`, the two-dimensional parameter array `x` and the Jacobian array `f`.

```

<MCI base: mci_sampler: TBP>+≡
  procedure (mci_sampler_fetch), deferred :: fetch

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_sampler_fetch (sampler, val, x, f)
      import
      class(mci_sampler_t), intent(in) :: sampler
      real(default), intent(out) :: val
      real(default), dimension(:,:), intent(out) :: x
      real(default), dimension(:), intent(out) :: f
    end subroutine mci_sampler_fetch
  end interface

```

21.1.5 Results record

This is an abstract type which allows us to implement callback: each integration results can optionally be recorded to an instance of this object. The actual object may store a new result, average results, etc. It may also display a result on-line or otherwise, whenever the `record` method is called.

```

<MCI base: public>+≡
  public :: mci_results_t

<MCI base: types>+≡
  type, abstract :: mci_results_t
  contains
    <MCI base: mci_results: TBP>
  end type mci_results_t

```

The output routine is deferred. We provide an extra `verbose` flag, which could serve any purpose.

```

<MCI base: mci_results: TBP>≡
  procedure (mci_results_write), deferred :: write
  procedure (mci_results_write_verbose), deferred :: write_verbose

<MCI base: interfaces>+≡
  abstract interface
    subroutine mci_results_write (object, unit, suppress)
      import
      class(mci_results_t), intent(in) :: object
      integer, intent(in), optional :: unit
      logical, intent(in), optional :: suppress
    end subroutine mci_results_write

    subroutine mci_results_write_verbose (object, unit)
      import
      class(mci_results_t), intent(in) :: object
      integer, intent(in), optional :: unit
    end subroutine mci_results_write_verbose

```

```
end interface
```

This is the generic `record` method, which can be called directly from the integrator. The `record_extended` procedure store additionally the valid calls, positive and negative efficiency.

```
<MCI base: mci results: TBP>+=
  generic :: record => record_simple, record_extended
  procedure (mci_results_record_simple), deferred :: record_simple
  procedure (mci_results_record_extended), deferred :: record_extended

<MCI base: interfaces>+=
  abstract interface
    subroutine mci_results_record_simple (object, n_it, &
      n_calls, integral, error, efficiency, chain_weights, suppress)
      import
      class(mci_results_t), intent(inout) :: object
      integer, intent(in) :: n_it
      integer, intent(in) :: n_calls
      real(default), intent(in) :: integral
      real(default), intent(in) :: error
      real(default), intent(in) :: efficiency
      real(default), dimension(:), intent(in), optional :: chain_weights
      logical, intent(in), optional :: suppress
    end subroutine mci_results_record_simple

    subroutine mci_results_record_extended (object, n_it, n_calls,&
      & n_calls_valid, integral, error, efficiency, efficiency_pos,&
      & efficiency_neg, chain_weights, suppress)
      import
      class(mci_results_t), intent(inout) :: object
      integer, intent(in) :: n_it
      integer, intent(in) :: n_calls
      integer, intent(in) :: n_calls_valid
      real(default), intent(in) :: integral
      real(default), intent(in) :: error
      real(default), intent(in) :: efficiency
      real(default), intent(in) :: efficiency_pos
      real(default), intent(in) :: efficiency_neg
      real(default), dimension(:), intent(in), optional :: chain_weights
      logical, intent(in), optional :: suppress
    end subroutine mci_results_record_extended
  end interface
```

21.1.6 Unit tests

Test module, followed by the corresponding implementation module.

```
<mci_base.ut.f90>=
  <File header>

  module mci_base_ut
    use unit_tests
    use mci_base_util
```

```

    <Standard module head>

    <MCI base: public test>

    <MCI base: public test auxiliary>

contains

    <MCI base: test driver>

end module mci_base_ut
<mci_base_uti.f90>≡
    <File header>

module mci_base_uti

    <Use kinds>
    use io_units
    use diagnostics
    use phs_base
    use rng_base

    use mci_base

    use rng_base_ut, only: rng_test_t

    <Standard module head>

    <MCI base: public test auxiliary>

    <MCI base: test declarations>

    <MCI base: test types>

contains

    <MCI base: tests>

end module mci_base_uti
API: driver for the unit tests below.
<MCI base: public test>≡
    public :: mci_base_test
<MCI base: test driver>≡
    subroutine mci_base_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <MCI base: execute tests>
    end subroutine mci_base_test

```

Test implementation of the configuration type

The concrete type contains the number of requested calls and the integral result, to be determined.

The `max_factor` entry is set for the actual test integration, where the integrand is not unity but some other constant value. This value should be set here, such that the actual maximum of the integrand is known when vetoing unweighted events.

(MCI base: public test auxiliary)≡

```
public :: mci_test_t
```

(MCI base: test types)≡

```
type, extends (mci_t) :: mci_test_t
  integer :: divisions = 0
  integer :: tries = 0
  real(default) :: max_factor = 1
contains
  procedure :: final => mci_test_final
  procedure :: write => mci_test_write
  procedure :: startup_message => mci_test_startup_message
  procedure :: write_log_entry => mci_test_write_log_entry
  procedure :: compute_md5sum => mci_test_compute_md5sum
  procedure :: declare_flat_dimensions => mci_test_ignore_flat_dimensions
  procedure :: declare_equivalences => mci_test_ignore_equivalences
  procedure :: set_divisions => mci_test_set_divisions
  procedure :: set_max_factor => mci_test_set_max_factor
  procedure :: allocate_instance => mci_test_allocate_instance
  procedure :: integrate => mci_test_integrate
  procedure :: prepare_simulation => mci_test_ignore_prepare_simulation
  procedure :: generate_weighted_event => mci_test_generate_weighted_event
  procedure :: generate_unweighted_event => &
    mci_test_generate_unweighted_event
  procedure :: rebuild_event => mci_test_rebuild_event
end type mci_test_t
```

Finalizer: base version is sufficient

(MCI base: tests)≡

```
subroutine mci_test_final (object)
  class(mci_test_t), intent(inout) :: object
  call object%base_final ()
end subroutine mci_test_final
```

Output: trivial

(MCI base: tests)+≡

```
subroutine mci_test_write (object, unit, pacify, md5sum_version)
  class(mci_test_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  logical, intent(in), optional :: md5sum_version
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Test integrator:"
  call object%base_write (u, pacify, md5sum_version)
```



```

        if (object%divisions /= 0) then
            write (u, "(3x,A,I0)") "Number of divisions = ", object%divisions
        end if
        if (allocated (object%rng)) call object%rng%write (u)
    end subroutine mci_test_write

```

Short version.

```

<MCI base: tests>+≡
subroutine mci_test_startup_message (mci, unit, n_calls)
    class(mci_test_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
    call mci%base_startup_message (unit = unit, n_calls = n_calls)
    write (msg_buffer, "(A,1x,I0,1x,A)") &
        "Integrator: Test:", mci%divisions, "divisions"
    call msg_message (unit = unit)
end subroutine mci_test_startup_message

```

Log entry: nothing.

```

<MCI base: tests>+≡
subroutine mci_test_write_log_entry (mci, u)
    class(mci_test_t), intent(in) :: mci
    integer, intent(in) :: u
end subroutine mci_test_write_log_entry

```

Compute MD5 sum: nothing.

```

<MCI base: tests>+≡
subroutine mci_test_compute_md5sum (mci, pacify)
    class(mci_test_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
end subroutine mci_test_compute_md5sum

```

This is a no-op for the test integrator.

```

<MCI base: tests>+≡
subroutine mci_test_ignore_flat_dimensions (mci, dim_flat)
    class(mci_test_t), intent(inout) :: mci
    integer, dimension(:), intent(in) :: dim_flat
end subroutine mci_test_ignore_flat_dimensions

```

Ditto.

```

<MCI base: tests>+≡
subroutine mci_test_ignore_equivalences (mci, channel, dim_offset)
    class(mci_test_t), intent(inout) :: mci
    type(phs_channel_t), dimension(:), intent(in) :: channel
    integer, intent(in) :: dim_offset
end subroutine mci_test_ignore_equivalences

```

Set the number of divisions to a nonzero value.

```

<MCI base: tests>+≡
subroutine mci_test_set_divisions (object, divisions)
    class(mci_test_t), intent(inout) :: object

```

```

        integer, intent(in) :: divisions
        object%divisions = divisions
    end subroutine mci_test_set_divisions

```

Set the maximum factor (default is 1).

```

<MCI base: tests>+≡
    subroutine mci_test_set_max_factor (object, max_factor)
        class(mci_test_t), intent(inout) :: object
        real(default), intent(in) :: max_factor
        object%max_factor = max_factor
    end subroutine mci_test_set_max_factor

```

Allocate instance with matching type.

```

<MCI base: tests>+≡
    subroutine mci_test_allocate_instance (mci, mci_instance)
        class(mci_test_t), intent(in) :: mci
        class(mci_instance_t), intent(out), pointer :: mci_instance
        allocate (mci_test_instance_t :: mci_instance)
    end subroutine mci_test_allocate_instance

```

Integrate: sample at the midpoints of uniform bits and add the results. We implement this for one and for two dimensions. In the latter case, we scan over two channels and multiply with the channel weights.

The arguments `n_it` and `n_calls` are ignored in this implementations.

The test integrator does not set error or efficiency, so those will remain undefined.

```

<MCI base: tests>+≡
    subroutine mci_test_integrate (mci, instance, sampler, &
        n_it, n_calls, results, pacify)
        class(mci_test_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
        logical, intent(in), optional :: pacify
        class(mci_results_t), intent(inout), optional :: results
        real(default), dimension(:), allocatable :: integral
        real(default), dimension(:), allocatable :: x
        integer :: i, j, c
        select type (instance)
        type is (mci_test_instance_t)
            allocate (integral (mci%n_channel))
            integral = 0
            allocate (x (mci%n_dim))
            select case (mci%n_dim)
            case (1)
                do c = 1, mci%n_channel
                    do i = 1, mci%divisions
                        x(1) = (i - 0.5_default) / mci%divisions
                        call instance%evaluate (sampler, c, x)
                        integral(c) = integral(c) + instance%get_value ()
                    end do
                end do
            end select
        end select
    end subroutine mci_test_integrate

```

```

        end do
        mci%integral = dot_product (instance%w, integral) &
            / mci%divisions
        mci%integral_known = .true.
    case (2)
        do c = 1, mci%n_channel
            do i = 1, mci%divisions
                x(1) = (i - 0.5_default) / mci%divisions
            do j = 1, mci%divisions
                x(2) = (j - 0.5_default) / mci%divisions
                call instance%evaluate (sampler, c, x)
                integral(c) = integral(c) + instance%get_value ()
            end do
        end do
        end do
        mci%integral = dot_product (instance%w, integral) &
            / mci%divisions / mci%divisions
        mci%integral_known = .true.
    end select
    if (present (results)) then
        call results%record (n_it, n_calls, &
            mci%integral, mci%error, &
            efficiency = 0._default)
    end if
end select
end subroutine mci_test_integrate

```

Simulation initializer and finalizer: nothing to do here.

```

<MCI base: tests>+≡
subroutine mci_test_ignore_prepare_simulation (mci)
    class(mci_test_t), intent(inout) :: mci
end subroutine mci_test_ignore_prepare_simulation

```

Event generator. We use mock random numbers for first selecting the channel and then setting the x values. The results reside in the state of `instance` and `sampler`.

```

<MCI base: tests>+≡
subroutine mci_test_generate_weighted_event (mci, instance, sampler)
    class(mci_test_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    real(default) :: r
    real(default), dimension(:), allocatable :: x
    integer :: c
    select type (instance)
    type is (mci_test_instance_t)
        allocate (x (mci%n_dim))
        select case (mci%n_channel)
        case (1)
            c = 1
            call mci%rng%generate (x(1))
        case (2)
            call mci%rng%generate (r)

```

```

        if (r < instance%w(1)) then
            c = 1
        else
            c = 2
        end if
        call mci%rng%generate (x)
    end select
    call instance%evaluate (sampler, c, x)
end select
end subroutine mci_test_generate_weighted_event

```

For unweighted events, we generate weighted events and apply a simple rejection step to the relative event weight, until an event passes.

(This might result in an endless loop if we happen to be in sync with the mock random generator cycle. Therefore, limit the number of tries.)

(MCI base: tests)+≡

```

subroutine mci_test_generate_unweighted_event (mci, instance, sampler)
    class(mci_test_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    real(default) :: r
    integer :: i
    select type (instance)
    type is (mci_test_instance_t)
        mci%tries = 0
        do i = 1, 10
            call mci%generate_weighted_event (instance, sampler)
            mci%tries = mci%tries + 1
            call mci%rng%generate (r)
            if (r < instance%rel_value) exit
        end do
    end select
end subroutine mci_test_generate_unweighted_event

```

Here, we rebuild the event from the state without consulting the rng.

(MCI base: tests)+≡

```

subroutine mci_test_rebuild_event (mci, instance, sampler, state)
    class(mci_test_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
    select type (instance)
    type is (mci_test_instance_t)
        call instance%recall (sampler, state)
    end select
end subroutine mci_test_rebuild_event

```

Instance of the test MCI type

This instance type simulates the VAMP approach. We implement the VAMP multi-channel formula, but keep the channel-specific probability functions g_i

smooth and fixed. We also keep the weights fixed.

The setup is as follows: we have n mappings of the unit hypercube

$$x = x(x^{(k)}) \quad \text{where } x = (x_1, \dots). \quad (21.1)$$

The Jacobian factors are the determinants

$$f^{(k)}(x^{(k)}) = \left| \frac{\partial x}{\partial x^{(k)}} \right| \quad (21.2)$$

We introduce arbitrary probability functions

$$g^{(k)}(x^{(k)}) \quad \text{with} \quad \int dx^{(k)} g^{(k)}(x^{(k)}) = 1 \quad (21.3)$$

and weights

$$w_k \quad \text{with} \quad \sum_k w_k = 1 \quad (21.4)$$

and construct the joint probability function

$$g(x) = \sum_k w_k \frac{g^{(k)}(x^{(k)}(x))}{f^{(k)}(x^{(k)}(x))} \quad (21.5)$$

which also satisfies

$$\int g(x) dx = 1. \quad (21.6)$$

The algorithm implements a resolution of unity as follows

$$\begin{aligned} 1 &= \int dx = \int \frac{g(x)}{g(x)} dx \\ &= \sum_k w_k \int \frac{g^{(k)}(x^{(k)}(x))}{f^{(k)}(x^{(k)}(x))} \frac{dx}{g(x)} \\ &= \sum_k w_k \int g^{(k)}(x^{(k)}) \frac{dx^{(k)}}{g(x^{(k)})} \end{aligned} \quad (21.7)$$

where each of the integrals in the sum is evaluated using the channel-specific variables $x^{(k)}$.

We provide two examples: (1) trivial with one channel, one dimension, and all functions unity and (2) two channels and two dimensions with

$$\begin{aligned} x(x^{(1)}) &= (x_1^{(1)}, x_2^{(1)}) \\ x(x^{(2)}) &= (x_1^{(2)2}, x_2^{(2)}) \end{aligned} \quad (21.8)$$

hence

$$f^{(1)} \equiv 1, \quad f^{(2)}(x^{(2)}) = 2x_1^{(2)} \quad (21.9)$$

The probability functions are

$$g^{(1)} \equiv 1, \quad g^{(2)}(x^{(2)}) = 2x_2^{(2)} \quad (21.10)$$

In the concrete implementation of the integrator instance we store values for the channel probabilities g_i and the accumulated probability g .

We also store the result (product of integrand and MCI weight), the expected maximum for the result in each channel.

```
<XXX MCI base: public>≡
  public :: mci_test_instance_t
```

```

<MCI base: test types>+≡
type, extends (mci_instance_t) :: mci_test_instance_t
  type(mci_test_t), pointer :: mci => null ()
  real(default) :: g = 0
  real(default), dimension(:), allocatable :: gi
  real(default) :: value = 0
  real(default) :: rel_value = 0
  real(default), dimension(:), allocatable :: max
contains
  procedure :: write => mci_test_instance_write
  procedure :: final => mci_test_instance_final
  procedure :: init => mci_test_instance_init
  procedure :: compute_weight => mci_test_instance_compute_weight
  procedure :: record_integrand => mci_test_instance_record_integrand
  procedure :: init_simulation => mci_test_instance_init_simulation
  procedure :: final_simulation => mci_test_instance_final_simulation
  procedure :: get_event_excess => mci_test_instance_get_event_excess
end type mci_test_instance_t

```

Output: trivial

```

<MCI base: tests>+≡
subroutine mci_test_instance_write (object, unit, pacify)
  class(mci_test_instance_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  integer :: u, c
  u = given_output_unit (unit)
  write (u, "(1x,A,ES13.7)") "Result value = ", object%value
  write (u, "(1x,A,ES13.7)") "Rel. weight = ", object%rel_value
  write (u, "(1x,A,ES13.7)") "Integrand = ", object%integrand
  write (u, "(1x,A,ES13.7)") "MCI weight = ", object%mci_weight
  write (u, "(3x,A,I0)") "c = ", object%selected_channel
  write (u, "(3x,A,ES13.7)") "g = ", object%g
  write (u, "(1x,A)") "Channel parameters:"
  do c = 1, object%mci%n_channel
    write (u, "(1x,I0,A,4(1x,ES13.7))") c, ": w/f/g/m =", &
      object%w(c), object%f(c), object%gi(c), object%max(c)
    write (u, "(4x,A,9(1x,F9.7))") "x =", object%x(:,c)
  end do
end subroutine mci_test_instance_write

```

The finalizer is empty.

```

<MCI base: tests>+≡
subroutine mci_test_instance_final (object)
  class(mci_test_instance_t), intent(inout) :: object
end subroutine mci_test_instance_final

```

Initializer. We make use of the analytical result that the maximum of the weighted integrand, in each channel, is equal to 1 (one-dimensional case) and 2 (two-dimensional case), respectively.

```

<MCI base: tests>+≡
subroutine mci_test_instance_init (mci_instance, mci)

```

```

class(mci_test_instance_t), intent(out) :: mci_instance
class(mci_t), intent(in), target :: mci
call mci_instance%base_init (mci)
select type (mci)
type is (mci_test_t)
    mci_instance%mci => mci
end select
allocate (mci_instance%gi (mci%n_channel))
mci_instance%gi = 0
allocate (mci_instance%max (mci%n_channel))
select case (mci%n_channel)
case (1)
    mci_instance%max = 1._default
case (2)
    mci_instance%max = 2._default
end select
end subroutine mci_test_instance_init

```

Compute weight: we implement the VAMP multi-channel formula. The channel probabilities *gi* are predefined functions.

(MCI base: tests)+≡

```

subroutine mci_test_instance_compute_weight (mci, c)
class(mci_test_instance_t), intent(inout) :: mci
integer, intent(in) :: c
integer :: i
mci%selected_channel = c
select case (mci%mci%n_dim)
case (1)
    mci%gi(1) = 1
case (2)
    mci%gi(1) = 1
    mci%gi(2) = 2 * mci%x(2,2)
end select
mci%g = 0
do i = 1, mci%mci%n_channel
    mci%g = mci%g + mci%w(i) * mci%gi(i) / mci%f(i)
end do
mci%mci_weight = mci%gi(c) / mci%g
end subroutine mci_test_instance_compute_weight

```

Record the integrand. Apply the Jacobian weight to get the absolute value. Divide by the channel maximum and by any overall factor to get the value relative to the maximum.

(MCI base: tests)+≡

```

subroutine mci_test_instance_record_integrand (mci, integrand)
class(mci_test_instance_t), intent(inout) :: mci
real(default), intent(in) :: integrand
mci%integrand = integrand
mci%value = mci%integrand * mci%mci_weight
mci%rel_value = mci%value / mci%max(mci%selected_channel) &
    / mci%mci%max_factor
end subroutine mci_test_instance_record_integrand

```

Nothing to do here.

```

<MCI base: tests>+≡
  subroutine mci_test_instance_init_simulation (instance, safety_factor)
    class(mci_test_instance_t), intent(inout) :: instance
    real(default), intent(in), optional :: safety_factor
  end subroutine mci_test_instance_init_simulation

  subroutine mci_test_instance_final_simulation (instance)
    class(mci_test_instance_t), intent(inout) :: instance
  end subroutine mci_test_instance_final_simulation

```

Return always zero.

```

<MCI base: tests>+≡
  function mci_test_instance_get_event_excess (mci) result (excess)
    class(mci_test_instance_t), intent(in) :: mci
    real(default) :: excess
    excess = 0
  end function mci_test_instance_get_event_excess

```

Test sampler

The test sampler implements a fixed configuration, either trivial (one-channel, one-dimension), or slightly nontrivial (two-channel, two-dimension). In the second channel, the first parameter is mapped according to $x_1 = x_1^{(2)2}$, so we have $f^{(2)}(x^{(2)}) = 2x_1^{(2)}$.

For display purposes, we store the return values inside the object. This is not strictly necessary.

```

<MCI base: test types>+≡
  type, extends (mci_sampler_t) :: test_sampler_t
    real(default) :: integrand = 0
    integer :: selected_channel = 0
    real(default), dimension(:, :), allocatable :: x
    real(default), dimension(:), allocatable :: f
  contains
    procedure :: init => test_sampler_init
    procedure :: write => test_sampler_write
    procedure :: compute => test_sampler_compute
    procedure :: is_valid => test_sampler_is_valid
    procedure :: evaluate => test_sampler_evaluate
    procedure :: rebuild => test_sampler_rebuild
    procedure :: fetch => test_sampler_fetch
  end type test_sampler_t

```

```

<MCI base: tests>+≡
  subroutine test_sampler_init (sampler, n)
    class(test_sampler_t), intent(out) :: sampler
    integer, intent(in) :: n
    allocate (sampler%x (n, n))
    allocate (sampler%f (n))
  end subroutine test_sampler_init

```


Output

(MCI base: tests)+≡

```
subroutine test_sampler_write (object, unit, testflag)
  class(test_sampler_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u, c
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Test sampler:"
  write (u, "(3x,A,ES13.7)") "Integrand = ", object%integrand
  write (u, "(3x,A,I0)") "Channel = ", object%selected_channel
  do c = 1, size (object%f)
    write (u, "(1x,I0,':',1x,A,ES13.7)") c, "f = ", object%f(c)
    write (u, "(4x,A,9(1x,F9.7))") "x =", object%x(:,c)
  end do
end subroutine test_sampler_write
```

Compute x and Jacobians, given the input parameter array. This is called both by `evaluate` and `rebuild`.

(MCI base: tests)+≡

```
subroutine test_sampler_compute (sampler, c, x_in)
  class(test_sampler_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  sampler%selected_channel = c
  select case (size (sampler%f))
  case (1)
    sampler%x(:,1) = x_in
    sampler%f = 1
  case (2)
    select case (c)
    case (1)
      sampler%x(:,1) = x_in
      sampler%x(1,2) = sqrt (x_in(1))
      sampler%x(2,2) = x_in(2)
    case (2)
      sampler%x(1,1) = x_in(1) ** 2
      sampler%x(2,1) = x_in(2)
      sampler%x(:,2) = x_in
    end select
    sampler%f(1) = 1
    sampler%f(2) = 2 * sampler%x(1,2)
  end select
end subroutine test_sampler_compute
```

The point is always valid.

(MCI base: tests)+≡

```
function test_sampler_is_valid (sampler) result (valid)
  class(test_sampler_t), intent(in) :: sampler
  logical :: valid
  valid = .true.
end function test_sampler_is_valid
```

The integrand is always equal to 1.

```

(MCI base: tests)+≡
subroutine test_sampler_evaluate (sampler, c, x_in, val, x, f)
  class(test_sampler_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default), intent(out) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  call sampler%compute (c, x_in)
  sampler%integrand = 1
  val = sampler%integrand
  x = sampler%x
  f = sampler%f
end subroutine test_sampler_evaluate

```

Construct kinematics from the input x array. Set the integrand instead of evaluating it.

```

(MCI base: tests)+≡
subroutine test_sampler_rebuild (sampler, c, x_in, val, x, f)
  class(test_sampler_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default), intent(in) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  call sampler%compute (c, x_in)
  sampler%integrand = val
  x = sampler%x
  f = sampler%f
end subroutine test_sampler_rebuild

```

Recall contents.

```

(MCI base: tests)+≡
subroutine test_sampler_fetch (sampler, val, x, f)
  class(test_sampler_t), intent(in) :: sampler
  real(default), intent(out) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  val = sampler%integrand
  x = sampler%x
  f = sampler%f
end subroutine test_sampler_fetch

```

Test results object

This mock object just stores and displays the current result.

```

(MCI base: test types)+≡
type, extends (mci_results_t) :: mci_test_results_t
  integer :: n_it = 0
  integer :: n_calls = 0

```

```

    real(default) :: integral = 0
    real(default) :: error = 0
    real(default) :: efficiency = 0
contains
  <MCI base: mci test results: TBP>
end type mci_test_results_t

```

Output.

```

<MCI base: mci test results: TBP>≡
  procedure :: write => mci_test_results_write
  procedure :: write_verbose => mci_test_results_write_verbose

<MCI base: tests>+≡
  subroutine mci_test_results_write (object, unit, suppress)
    class(mci_test_results_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: suppress
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A,1x,I0)") "Iterations = ", object%n_it
    write (u, "(3x,A,1x,I0)") "Calls      = ", object%n_calls
    write (u, "(3x,A,1x,F12.10)") "Integral  = ", object%integral
    write (u, "(3x,A,1x,F12.10)") "Error     = ", object%error
    write (u, "(3x,A,1x,F12.10)") "Efficiency = ", object%efficiency
  end subroutine mci_test_results_write

  subroutine mci_test_results_write_verbose (object, unit)
    class(mci_test_results_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A,1x,I0)") "Iterations = ", object%n_it
    write (u, "(3x,A,1x,I0)") "Calls      = ", object%n_calls
    write (u, "(3x,A,1x,F12.10)") "Integral  = ", object%integral
    write (u, "(3x,A,1x,F12.10)") "Error     = ", object%error
    write (u, "(3x,A,1x,F12.10)") "Efficiency = ", object%efficiency
  end subroutine mci_test_results_write_verbose

```

Record result.

```

<MCI base: mci test results: TBP>+≡
  procedure :: record_simple => mci_test_results_record_simple
  procedure :: record_extended => mci_test_results_record_extended

<MCI base: tests>+≡
  subroutine mci_test_results_record_simple (object, n_it, n_calls, &
    integral, error, efficiency, chain_weights, suppress)
    class(mci_test_results_t), intent(inout) :: object
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    real(default), intent(in) :: integral
    real(default), intent(in) :: error
    real(default), intent(in) :: efficiency
    real(default), dimension(:), intent(in), optional :: chain_weights
    logical, intent(in), optional :: suppress

```

```

object%n_it = n_it
object%n_calls = n_calls
object%integral = integral
object%error = error
object%efficiency = efficiency
end subroutine mci_test_results_record_simple

subroutine mci_test_results_record_extended (object, n_it, n_calls, &
      & n_calls_valid, integral, error, efficiency, efficiency_pos, &
      & efficiency_neg, chain_weights, suppress)
class(mci_test_results_t), intent(inout) :: object
integer, intent(in) :: n_it
integer, intent(in) :: n_calls
integer, intent(in) :: n_calls_valid
real(default), intent(in) :: integral
real(default), intent(in) :: error
real(default), intent(in) :: efficiency
real(default), intent(in) :: efficiency_pos
real(default), intent(in) :: efficiency_neg
real(default), dimension(:), intent(in), optional :: chain_weights
logical, intent(in), optional :: suppress
object%n_it = n_it
object%n_calls = n_calls
object%integral = integral
object%error = error
object%efficiency = efficiency
end subroutine mci_test_results_record_extended

```

Integrator configuration data

Construct and display a test integrator configuration object.

```

<MCI base: execute tests>≡
  call test (mci_base_1, "mci_base_1", &
    "integrator configuration", &
    u, results)

<MCI base: test declarations>≡
  public :: mci_base_1

<MCI base: tests>+≡
  subroutine mci_base_1 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

    real(default) :: integrand

    write (u, "(A)")  "* Test output: mci_base_1"
    write (u, "(A)")  "* Purpose: initialize and display &
      &test integrator"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator"

```

```

write (u, "(A)")

allocate (mci_test_t :: mci)
call mci%set_dimensions (2, 2)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_t :: sampler)
select type (sampler)
type is (test_sampler_t)
    call sampler%init (2)
end select

write (u, "(A)")  "* Evaluate sampler for given point and channel"
write (u, "(A)")

call sampler%evaluate (1, [0.25_default, 0.8_default], &
    integrand, mci_instance%x, mci_instance%f)

call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute MCI weight"
write (u, "(A)")

call mci_instance%compute_weight (1)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Get integrand and compute weight for another point"
write (u, "(A)")

call mci_instance%evaluate (sampler, 2, [0.5_default, 0.6_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recall results, again"
write (u, "(A)")

call mci_instance%final ()
deallocate (mci_instance)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

```

```

call mci_instance%fetch (sampler, 2)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Retrieve value"
write (u, "(A)")

write (u, "(1x,A,ES13.7)") "Weighted integrand = ", &
    mci_instance%get_value ()

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_1"

end subroutine mci_base_1

```

Trivial integral

Use the MCI approach to compute a trivial one-dimensional integral.

```

<MCI base: execute tests>+≡
    call test (mci_base_2, "mci_base_2", &
        "integration", &
        u, results)

<MCI base: test declarations>+≡
    public :: mci_base_2

<MCI base: tests>+≡
    subroutine mci_base_2 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler

        write (u, "(A)")  "* Test output: mci_base_2"
        write (u, "(A)")  "* Purpose: perform a test integral"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator"
        write (u, "(A)")

        allocate (mci_test_t :: mci)
        call mci%set_dimensions (1, 1)
        select type (mci)
            type is (mci_test_t)
                call mci%set_divisions (10)
            end select

        call mci%write (u)

        write (u, "(A)")

```

```

write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_t :: sampler)
select type (sampler)
type is (test_sampler_t)
    call sampler%init (1)
end select

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 0, 0)

call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_2"

end subroutine mci_base_2

```

Nontrivial integral

Use the MCI approach to compute a simple two-dimensional integral with two channels.

```

<MCI base: execute tests>+≡
    call test (mci_base_3, "mci_base_3", &
        "integration (two channels)", &
        u, results)

<MCI base: test declarations>+≡
    public :: mci_base_3

<MCI base: tests>+≡
    subroutine mci_base_3 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler

        write (u, "(A)")  "* Test output: mci_base_3"
        write (u, "(A)")  "* Purpose: perform a nontrivial test integral"
        write (u, "(A)")
    end subroutine mci_base_3

```

```

write (u, "(A)")  "* Initialize integrator"
write (u, "(A)")

allocate (mci_test_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_test_t)
    call mci%set_divisions (10)
end select

write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_t :: sampler)
select type (sampler)
type is (test_sampler_t)
    call sampler%init (2)
end select

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 0, 0)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with higher resolution"
write (u, "(A)")

select type (mci)
type is (mci_test_t)
    call mci%set_divisions (100)
end select

call mci%integrate (mci_instance, sampler, 0, 0)
call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_3"

end subroutine mci_base_3

```


Event generation

We generate “random” events, one weighted and one unweighted. The test implementation does not require an integration pass, we can generate events immediately.

```
<MCI base: execute tests>+≡
    call test (mci_base_4, "mci_base_4", &
               "event generation (two channels)", &
               u, results)

<MCI base: test declarations>+≡
    public :: mci_base_4

<MCI base: tests>+≡
    subroutine mci_base_4 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng

        write (u, "(A)")  "* Test output: mci_base_4"
        write (u, "(A)")  "* Purpose: generate events"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator, instance, sampler"
        write (u, "(A)")

        allocate (mci_test_t :: mci)
        call mci%set_dimensions (2, 2)
        select type (mci)
            type is (mci_test_t)
                call mci%set_divisions (10)
        end select

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        allocate (test_sampler_t :: sampler)
        select type (sampler)
            type is (test_sampler_t)
                call sampler%init (2)
        end select

        allocate (rng_test_t :: rng)
        call mci%import_rng (rng)

        write (u, "(A)")  "* Generate weighted event"
        write (u, "(A)")

        call mci%generate_weighted_event (mci_instance, sampler)

        call sampler%write (u)
        write (u, *)
        call mci_instance%write (u)
```

```

write (u, "(A)")
write (u, "(A)")  "* Generate unweighted event"
write (u, "(A)")

call mci%generate_unweighted_event (mci_instance, sampler)

select type (mci)
type is (mci_test_t)
  write (u, "(A,I0)")  " Success in try ", mci%tries
  write (u, "(A)")
end select

call sampler%write (u)
write (u, *)
call mci_instance%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_4"

end subroutine mci_base_4

```

Store and recall data

We generate an event and store the relevant data, i.e., the input parameters and the result value for a particular channel. Then we use those data to recover the event, as far as the MCI record is concerned.

```

<MCI base: execute tests>+≡
  call test (mci_base_5, "mci_base_5", &
    "store and recall", &
    u, results)

<MCI base: test declarations>+≡
  public :: mci_base_5

<MCI base: tests>+≡
  subroutine mci_base_5 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng
    class(mci_state_t), allocatable :: state

    write (u, "(A)")  "* Test output: mci_base_5"
    write (u, "(A)")  "* Purpose: store and recall an event"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator, instance, sampler"
    write (u, "(A)")

```

```

allocate (mci_test_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_test_t)
    call mci%set_divisions (10)
end select

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_t :: sampler)
select type (sampler)
type is (test_sampler_t)
    call sampler%init (2)
end select

allocate (rng_test_t :: rng)
call mci%import_rng (rng)

write (u, "(A)")  "* Generate weighted event"
write (u, "(A)")

call mci%generate_weighted_event (mci_instance, sampler)

call sampler%write (u)
write (u, *)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Store data"
write (u, "(A)")

allocate (state)
call mci_instance%store (state)
call mci_instance%final ()
deallocate (mci_instance)

call state%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recall data and rebuild event"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)
call mci%rebuild_event (mci_instance, sampler, state)

call sampler%write (u)
write (u, *)
call mci_instance%write (u)

call mci_instance%final ()
call mci%final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_5"

end subroutine mci_base_5

```

Chained channels

Chain channels together. In the base configuration, this just fills entries in an extra array (each channel may belong to a chain). In type implementations, this will be used for grouping equivalent channels by keeping their weights equal.

```

<MCI base: execute tests>+≡
  call test (mci_base_6, "mci_base_6", &
    "chained channels", &
    u, results)

<MCI base: test declarations>+≡
  public :: mci_base_6

<MCI base: tests>+≡
  subroutine mci_base_6 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci

    write (u, "(A)")  "* Test output: mci_base_6"
    write (u, "(A)")  "* Purpose: initialize and display &
      &test integrator with chains"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_test_t :: mci)
    call mci%set_dimensions (1, 5)

    write (u, "(A)")  "* Introduce chains"
    write (u, "(A)")

    call mci%declare_chains ([1, 2, 2, 1, 2])

    call mci%write (u)

    call mci%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: mci_base_6"

  end subroutine mci_base_6

```

Recording results

Compute a simple two-dimensional integral and record the result.

```

<MCI base: execute tests>+≡
    call test (mci_base_7, "mci_base_7", &
        "recording results", &
        u, results)

<MCI base: test declarations>+≡
    public :: mci_base_7

<MCI base: tests>+≡
    subroutine mci_base_7 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(mci_results_t), allocatable :: results

        write (u, "(A)")  "* Test output: mci_base_7"
        write (u, "(A)")  "* Purpose: perform a nontrivial test integral &
            &and record results"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator"
        write (u, "(A)")

        allocate (mci_test_t :: mci)
        call mci%set_dimensions (2, 2)
        select type (mci)
        type is (mci_test_t)
            call mci%set_divisions (10)
        end select

        write (u, "(A)")  "* Initialize instance"
        write (u, "(A)")

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        write (u, "(A)")  "* Initialize test sampler"
        write (u, "(A)")

        allocate (test_sampler_t :: sampler)
        select type (sampler)
        type is (test_sampler_t)
            call sampler%init (2)
        end select

        allocate (mci_test_results_t :: results)

        write (u, "(A)")  "* Integrate"
        write (u, "(A)")

        call mci%integrate (mci_instance, sampler, 1, 1000, results)
        call mci%write (u)

        write (u, "(A)")

```

```

write (u, "(A)")  "* Display results"
write (u, "(A)")

call results%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_7"

end subroutine mci_base_7

```

Timer

Simple checks for the embedded timer.

```

<MCI base: execute tests>+≡
  call test (mci_base_8, "mci_base_8", &
    "timer", &
    u, results)
<MCI base: test declarations>+≡
  public :: mci_base_8
<MCI base: tests>+≡
  subroutine mci_base_8 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci

    real(default) :: dummy

    write (u, "(A)")  "* Test output: mci_base_8"
    write (u, "(A)")  "* Purpose: check timer availability"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator with timer"
    write (u, "(A)")

    allocate (mci_test_t :: mci)
    call mci%set_dimensions (2, 2)
    select type (mci)
    type is (mci_test_t)
      call mci%set_divisions (10)
    end select

    call mci%set_timer (active = .true.)
    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Start timer"
    write (u, "(A)")

    call mci%start_timer ()
    call mci%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Stop timer"
write (u, "(A)")

call mci%stop_timer ()
write (u, "(A)")  " (ok)"

write (u, "(A)")
write (u, "(A)")  "* Readout"
write (u, "(A)")

dummy = mci%get_time ()
write (u, "(A)")  " (ok)"

write (u, "(A)")
write (u, "(A)")  "* Deactivate timer"
write (u, "(A)")

call mci%set_timer (active = .false.)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_base_8"

end subroutine mci_base_8

```

21.2 Iterations

This module defines a container for the list of iterations and calls, to be submitted to integration.

`<iterations.f90>`≡
<File header>

`module iterations`

<Use kinds>

<Use strings>

`use io_units`

`use diagnostics`

<Standard module head>

<Iterations: public>

<Iterations: types>

```
contains

<Iterations: procedures>

end module iterations
```

21.2.1 The iterations list

Each integration pass has a number of iterations and a number of calls per iteration. The last pass produces the end result; the previous passes are used for adaptation.

The flags `adapt_grid` and `adapt_weight` are used only if `custom_adaptation` is set. Otherwise, default settings are used that depend on the integration pass.

```
<Iterations: types>≡
  type :: iterations_spec_t
  private
    integer :: n_it = 0
    integer :: n_calls = 0
    logical :: custom_adaptation = .false.
    logical :: adapt_grids = .false.
    logical :: adapt_weights = .false.
  end type iterations_spec_t
```

We build up a list of iterations.

```
<Iterations: public>≡
  public :: iterations_list_t

<Iterations: types>+≡
  type :: iterations_list_t
  private
    integer :: n_pass = 0
    type(iterations_spec_t), dimension(:), allocatable :: pass
  contains
    <Iterations: iterations list: TBP>
  end type iterations_list_t
```

Initialize an iterations list. For each pass, we have to specify the number of iterations and calls. We may provide the adaption conventions explicitly, either as character codes or as logicals.

For passes where the adaptation conventions are not specified, we use the following default setting: adapt weights and grids for all passes except the last one.

```
<Iterations: iterations list: TBP>≡
  procedure :: init => iterations_list_init

<Iterations: procedures>≡
  subroutine iterations_list_init &
    (it_list, n_it, n_calls, adapt, adapt_code, adapt_grids, adapt_weights)
    class(iterations_list_t), intent(inout) :: it_list
    integer, dimension(:), intent(in) :: n_it, n_calls
    logical, dimension(:), intent(in), optional :: adapt
```



```

type(string_t), dimension(:), intent(in), optional :: adapt_code
logical, dimension(:), intent(in), optional :: adapt_grids, adapt_weights
integer :: i
it_list%n_pass = size (n_it)
if (allocated (it_list%pass)) deallocate (it_list%pass)
allocate (it_list%pass (it_list%n_pass))
it_list%pass%n_it = n_it
it_list%pass%n_calls = n_calls
if (present (adapt)) then
    it_list%pass%custom_adaptation = adapt
    do i = 1, it_list%n_pass
        if (adapt(i)) then
            if (verify (adapt_code(i), "wg") /= 0) then
                call msg_error ("iteration specification: " &
                    // "adaptation code letters must be 'w' or 'g'")
            end if
            it_list%pass(i)%adapt_grids = scan (adapt_code(i), "g") /= 0
            it_list%pass(i)%adapt_weights = scan (adapt_code(i), "w") /= 0
        end if
    end do
else if (present (adapt_grids) .and. present (adapt_weights)) then
    it_list%pass%custom_adaptation = .true.
    it_list%pass%adapt_grids = adapt_grids
    it_list%pass%adapt_weights = adapt_weights
end if
do i = 1, it_list%n_pass - 1
    if (.not. it_list%pass(i)%custom_adaptation) then
        it_list%pass(i)%adapt_grids = .true.
        it_list%pass(i)%adapt_weights = .true.
    end if
end do
end subroutine iterations_list_init

```

<Iterations: iterations list: TBP>+≡

```

procedure :: clear => iterations_list_clear

```

<Iterations: procedures>+≡

```

subroutine iterations_list_clear (it_list)
    class(iterations_list_t), intent(inout) :: it_list
    it_list%n_pass = 0
    deallocate (it_list%pass)
end subroutine iterations_list_clear

```

Write the list of iterations.

<Iterations: iterations list: TBP>+≡

```

procedure :: write => iterations_list_write

```

<Iterations: procedures>+≡

```

subroutine iterations_list_write (it_list, unit)
    class(iterations_list_t), intent(in) :: it_list
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(A)") char (it_list%to_string ())

```

```
end subroutine iterations_list_write
```

The output as a single-line string.

<Iterations: iterations list: TBP>+≡

```
procedure :: to_string => iterations_list_to_string
```

<Iterations: procedures>+≡

```
function iterations_list_to_string (it_list) result (buffer)
  class(iterations_list_t), intent(in) :: it_list
  type(string_t) :: buffer
  character(30) :: ibuf
  integer :: i
  buffer = "iterations = "
  if (it_list%n_pass > 0) then
    do i = 1, it_list%n_pass
      if (i > 1) buffer = buffer // ", "
      write (ibuf, "(I0,':',I0)") &
        it_list%pass(i)%n_it, it_list%pass(i)%n_calls
      buffer = buffer // trim (ibuf)
      if (it_list%pass(i)%custom_adaptation &
        .or. it_list%pass(i)%adapt_grids &
        .or. it_list%pass(i)%adapt_weights) then
        buffer = buffer // ':'
        if (it_list%pass(i)%adapt_grids) buffer = buffer // "g"
        if (it_list%pass(i)%adapt_weights) buffer = buffer // "w"
        buffer = buffer // ""
      end if
    end do
  else
    buffer = buffer // "[undefined]"
  end if
end function iterations_list_to_string
```

21.2.2 Tools

Return the total number of passes.

<Iterations: iterations list: TBP>+≡

```
procedure :: get_n_pass => iterations_list_get_n_pass
```

<Iterations: procedures>+≡

```
function iterations_list_get_n_pass (it_list) result (n_pass)
  class(iterations_list_t), intent(in) :: it_list
  integer :: n_pass
  n_pass = it_list%n_pass
end function iterations_list_get_n_pass
```

Return the number of calls for a specific pass.

<Iterations: iterations list: TBP>+≡

```
procedure :: get_n_calls => iterations_list_get_n_calls
```

```

<Iterations: procedures>+≡
function iterations_list_get_n_calls (it_list, pass) result (n_calls)
  class(iterations_list_t), intent(in) :: it_list
  integer :: n_calls
  integer, intent(in) :: pass
  if (pass <= it_list%n_pass) then
    n_calls = it_list%pass(pass)%n_calls
  else
    n_calls = 0
  end if
end function iterations_list_get_n_calls

```

```

<Iterations: iterations list: TBP>+≡
procedure :: set_n_calls => iterations_list_set_n_calls

```

```

<Iterations: procedures>+≡
subroutine iterations_list_set_n_calls (it_list, pass, n_calls)
  class(iterations_list_t), intent(inout) :: it_list
  integer, intent(in) :: pass, n_calls
  it_list%pass(pass)%n_calls = n_calls
end subroutine iterations_list_set_n_calls

```

Get the adaptation mode (automatic/custom) and, for custom adaptation, the flags for a specific pass.

```

<Iterations: iterations list: TBP>+≡
procedure :: adapt_grids => iterations_list_adapt_grids
procedure :: adapt_weights => iterations_list_adapt_weights

<Iterations: procedures>+≡
function iterations_list_adapt_grids (it_list, pass) result (flag)
  logical :: flag
  class(iterations_list_t), intent(in) :: it_list
  integer, intent(in) :: pass
  if (pass <= it_list%n_pass) then
    flag = it_list%pass(pass)%adapt_grids
  else
    flag = .false.
  end if
end function iterations_list_adapt_grids

```

```

function iterations_list_adapt_weights (it_list, pass) result (flag)
  logical :: flag
  class(iterations_list_t), intent(in) :: it_list
  integer, intent(in) :: pass
  if (pass <= it_list%n_pass) then
    flag = it_list%pass(pass)%adapt_weights
  else
    flag = .false.
  end if
end function iterations_list_adapt_weights

```

Return the total number of iterations / the iterations for a specific pass.

```

<Iterations: iterations list: TBP>+≡
procedure :: get_n_it => iterations_list_get_n_it

```

```

<Iterations: procedures>+≡
function iterations_list_get_n_it (it_list, pass) result (n_it)
  class(iterations_list_t), intent(in) :: it_list
  integer :: n_it
  integer, intent(in) :: pass
  if (pass <= it_list%n_pass) then
    n_it = it_list%pass(pass)%n_it
  else
    n_it = 0
  end if
end function iterations_list_get_n_it

```

21.2.3 Iteration Multipliers

```

<Iterations: public>+≡
public :: iteration_multipliers_t

<Iterations: types>+≡
type :: iteration_multipliers_t
  real(default) :: mult_real = 1._default
  real(default) :: mult_virt = 1._default
  real(default) :: mult_dglap = 1._default
  real(default) :: mult_threshold = 1._default
  integer, dimension(:), allocatable :: n_calls0
end type iteration_multipliers_t

```

21.2.4 Unit tests

Test module, followed by the corresponding implementation module.

```

<iterations_ut.f90>≡
<File header>

module iterations_ut
  use unit_tests
  use iterations_uti

  <Standard module head>

  <Iterations: public test>

  contains

  <Iterations: test driver>

end module iterations_ut

<iterations_uti.f90>≡
<File header>

module iterations_uti

  <Use strings>

```

```

        use iterations

        <Standard module head>

        <Iterations: test declarations>

contains

        <Iterations: tests>

    end module iterations_util

API: driver for the unit tests below.
<Iterations: public test>≡
    public :: iterations_test
<Iterations: test driver>≡
    subroutine iterations_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
        <Iterations: execute tests>
    end subroutine iterations_test

```

Empty list

```

<Iterations: execute tests>≡
    call test (iterations_1, "iterations_1", &
        "empty iterations list", &
        u, results)
<Iterations: test declarations>≡
    public :: iterations_1
<Iterations: tests>≡
    subroutine iterations_1 (u)
        integer, intent(in) :: u
        type(iterations_list_t) :: it_list

        write (u, "(A)")  "* Test output: iterations_1"
        write (u, "(A)")  "* Purpose: display empty iterations list"
        write (u, "(A)")

        call it_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: iterations_1"

    end subroutine iterations_1

```

Fill list

```

<Iterations: execute tests>+≡

```

```

call test (iterations_2, "iterations_2", &
  "create iterations list", &
  u, results)
<Iterations: test declarations>+≡
public :: iterations_2
<Iterations: tests>+≡
subroutine iterations_2 (u)
  integer, intent(in) :: u
  type(iterations_list_t) :: it_list

  write (u, "(A)")  "* Test output: iterations_2"
  write (u, "(A)")  "* Purpose: fill and display iterations list"
  write (u, "(A)")

  write (u, "(A)")  "* Minimal setup (2 passes)"
  write (u, "(A)")

  call it_list%init ([2, 4], [5000, 20000])

  call it_list%write (u)
  call it_list%clear ()

  write (u, "(A)")
  write (u, "(A)")  "* Setup with flags (3 passes)"
  write (u, "(A)")

  call it_list%init ([2, 4, 5], [5000, 20000, 400], &
    [.false., .true., .true.], &
    [var_str (""), var_str ("g"), var_str ("wg")])

  call it_list%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Extract data"
  write (u, "(A)")

  write (u, "(A,I0)")  "n_pass = ", it_list%get_n_pass ()
  write (u, "(A)")
  write (u, "(A,I0)")  "n_calls(2) = ", it_list%get_n_calls (2)
  write (u, "(A)")
  write (u, "(A,I0)")  "n_it(3) = ", it_list%get_n_it (3)

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: iterations_2"

end subroutine iterations_2

```

21.3 Integration results

We record integration results and errors in a dedicated type. This allows us to do further statistics such as weighted average, chi-squared, grouping by integration

passes, etc.

Note WHIZARD 2.2.0: This code is taken from the previous `processes` module essentially unchanged and converted into a separate module. It lacks an overhaul and, in particular, self-tests.

```
<integration_results.f90>≡
  module integration_results

    <Use kinds>
    <Use strings>
    use io_units
    use format_utils, only: mp_format, pac_fmt
    use format_defs, only: FMT_10, FMT_14
    use diagnostics
    use md5
    use os_interface
    use mci_base

    <Standard module head>

    <Integration results: public>

    <Integration results: parameters>

    <Integration results: types>

    <Integration results: interfaces>

    contains

    <Integration results: procedures>

  end module integration_results
```

21.3.1 Integration results entry

This object collects the results of an integration pass and makes them available to the outside.

The results object has to distinguish the process type:

We store the process type, the index of the integration pass and the absolute iteration index, the number of iterations contained in this result (for averages), and the integral (cross section or partial width), error estimate, efficiency.

For intermediate results, we set a flag if this result is an improvement w.r.t. previous ones.

The process type indicates decay or scattering. Dummy entries (skipped iterations) have a process type of `PRC_UNKNOWN`.

The additional information `n_calls_valid`, `efficiency_pos` and `efficiency_neg` are stored, but only used in verbose mode.

```
<Integration results: public>≡
  public :: integration_entry_t

<Integration results: types>≡
  type :: integration_entry_t
```

```

private
integer :: process_type = PRC_UNKNOWN
integer :: pass = 0
integer :: it = 0
integer :: n_it = 0
integer :: n_calls = 0
integer :: n_calls_valid = 0
logical :: improved = .false.
real(default) :: integral = 0
real(default) :: error = 0
real(default) :: efficiency = 0
real(default) :: efficiency_pos = 0
real(default) :: efficiency_neg = 0
real(default) :: chi2 = 0
real(default), dimension(:), allocatable :: chain_weights
contains
<Integration results: integration entry: TBP>
end type integration_entry_t

```

The possible values of the type indicator:

```

<Integration results: parameters>≡
integer, parameter, public :: PRC_UNKNOWN = 0
integer, parameter, public :: PRC_DECAY = 1
integer, parameter, public :: PRC_SCATTERING = 2

```

Initialize with all relevant data.

```

<Integration results: interfaces>≡
interface integration_entry_t
module procedure integration_entry_init
end interface integration_entry_t

```

```

<Integration results: procedures>≡
type(integration_entry_t) function integration_entry_init (process_type, pass,&
& it, n_it, n_calls, n_calls_valid, improved, integral, error,&
& efficiency, efficiency_pos, efficiency_neg, chi2, chain_weights)&
& result (entry)
integer, intent(in) :: process_type, pass, it, n_it, n_calls, n_calls_valid
logical, intent(in) :: improved
real(default), intent(in) :: integral, error, efficiency, efficiency_pos, efficiency_neg
real(default), intent(in), optional :: chi2
real(default), dimension(:), intent(in), optional :: chain_weights
entry%process_type = process_type
entry%pass = pass
entry%it = it
entry%n_it = n_it
entry%n_calls = n_calls
entry%n_calls_valid = n_calls_valid
entry%improved = improved
entry%integral = integral
entry%error = error
entry%efficiency = efficiency
entry%efficiency_pos = efficiency_pos

```



```

entry%efficiency_neg = efficiency_neg
if (present (chi2)) entry%chi2 = chi2
if (present (chain_weights)) then
    allocate (entry%chain_weights (size (chain_weights)))
    entry%chain_weights = chain_weights
end if
end function integration_entry_init

```

Access values, some of them computed on demand:

```

<Integration results: integration entry: TBP>≡
    procedure :: get_pass => integration_entry_get_pass
    procedure :: get_n_calls => integration_entry_get_n_calls
    procedure :: get_n_calls_valid => integration_entry_get_n_calls_valid
    procedure :: get_integral => integration_entry_get_integral
    procedure :: get_error => integration_entry_get_error
    procedure :: get_rel_error => integration_entry_get_relative_error
    procedure :: get_accuracy => integration_entry_get_accuracy
    procedure :: get_efficiency => integration_entry_get_efficiency
    procedure :: get_efficiency_pos => integration_entry_get_efficiency_pos
    procedure :: get_efficiency_neg => integration_entry_get_efficiency_neg
    procedure :: get_chi2 => integration_entry_get_chi2
    procedure :: has_improved => integration_entry_has_improved
    procedure :: get_n_groves => integration_entry_get_n_groves

<Integration results: procedures>+≡
    elemental function integration_entry_get_pass (entry) result (n)
        integer :: n
        class(integration_entry_t), intent(in) :: entry
        n = entry%pass
    end function integration_entry_get_pass

    elemental function integration_entry_get_n_calls (entry) result (n)
        integer :: n
        class(integration_entry_t), intent(in) :: entry
        n = entry%n_calls
    end function integration_entry_get_n_calls

    elemental function integration_entry_get_n_calls_valid (entry) result (n)
        integer :: n
        class(integration_entry_t), intent(in) :: entry
        n = entry%n_calls_valid
    end function integration_entry_get_n_calls_valid

    elemental function integration_entry_get_integral (entry) result (int)
        real(default) :: int
        class(integration_entry_t), intent(in) :: entry
        int = entry%integral
    end function integration_entry_get_integral

    elemental function integration_entry_get_error (entry) result (err)
        real(default) :: err
        class(integration_entry_t), intent(in) :: entry
        err = entry%error
    end function integration_entry_get_error

```

```

elemental function integration_entry_get_relative_error (entry) result (err)
  real(default) :: err
  class(integration_entry_t), intent(in) :: entry
  err = 0
  if (entry%integral /= 0) then
    err = entry%error / entry%integral
  end if
end function integration_entry_get_relative_error

elemental function integration_entry_get_accuracy (entry) result (acc)
  real(default) :: acc
  class(integration_entry_t), intent(in) :: entry
  acc = accuracy (entry%integral, entry%error, entry%n_calls)
end function integration_entry_get_accuracy

elemental function accuracy (integral, error, n_calls) result (acc)
  real(default) :: acc
  real(default), intent(in) :: integral, error
  integer, intent(in) :: n_calls
  acc = 0
  if (integral /= 0) then
    acc = error / integral * sqrt (real (n_calls, default))
  end if
end function accuracy

elemental function integration_entry_get_efficiency (entry) result (eff)
  real(default) :: eff
  class(integration_entry_t), intent(in) :: entry
  eff = entry%efficiency
end function integration_entry_get_efficiency

elemental function integration_entry_get_efficiency_pos (entry) result (eff)
  real(default) :: eff
  class(integration_entry_t), intent(in) :: entry
  eff = entry%efficiency_pos
end function integration_entry_get_efficiency_pos

elemental function integration_entry_get_efficiency_neg (entry) result (eff)
  real(default) :: eff
  class(integration_entry_t), intent(in) :: entry
  eff = entry%efficiency_neg
end function integration_entry_get_efficiency_neg

elemental function integration_entry_get_chi2 (entry) result (chi2)
  real(default) :: chi2
  class(integration_entry_t), intent(in) :: entry
  chi2 = entry%chi2
end function integration_entry_get_chi2

elemental function integration_entry_has_improved (entry) result (flag)
  logical :: flag
  class(integration_entry_t), intent(in) :: entry
  flag = entry%improved

```

```

end function integration_entry_has_improved

elemental function integration_entry_get_n_groves (entry) result (n_groves)
  integer :: n_groves
  class(integration_entry_t), intent(in) :: entry
  n_groves = 0
  if (allocated (entry%chain_weights)) then
    n_groves = size (entry%chain_weights, 1)
  end if
end function integration_entry_get_n_groves

```

This writes the standard result account into one screen line. The verbose version uses multiple lines and prints the unabridged values. Dummy entries are not written.

(Integration results: integration entry: TBP)+≡

```

  procedure :: write => integration_entry_write
  procedure :: write_verbose => integration_entry_write_verbose

```

(Integration results: procedures)+≡

```

subroutine integration_entry_write (entry, unit, verbosity, suppress)
  class(integration_entry_t), intent(in) :: entry
  integer, intent(in), optional :: unit
  integer, intent(in), optional :: verbosity
  logical, intent(in), optional :: suppress
  integer :: u
  character(1) :: star
  character(12) :: fmt
  character(7) :: fmt2
  character(120) :: buffer
  integer :: verb
  logical :: supp
  u = given_output_unit (unit); if (u < 0) return
  verb = 0; if (present (verbosity)) verb = verbosity
  supp = .false.; if (present (suppress)) supp = suppress
  if (entry%process_type /= PRC_UNKNOWN) then
    if (entry%improved .and. .not. supp) then
      star = "*"
    else
      star = " "
    end if
    call pac_fmt (fmt, FMT_14, "3x," // FMT_10 // ",1x", suppress)
    call pac_fmt (fmt2, "1x,F6.2", "2x,F5.1", suppress)
    write (buffer, "(1x,I3,1x,I10)" entry%it, entry%n_calls
    if (verb > 1) then
      write (buffer, "(A,1x,I10)" trim (buffer), entry%n_calls_valid
    end if
    write (buffer, "(A,1x," // fmt // ",1x,ES9.2,1x,F7.2," // &
      "1x,F7.2,A1," // fmt2 // ")" &
      trim (buffer), &
      entry%integral, &
      abs(entry%error), &
      abs(integration_entry_get_relative_error (entry)) * 100, &
      abs(integration_entry_get_accuracy (entry)), &
      star, &

```

```

        entry%efficiency * 100
    if (verb > 2) then
        write (buffer, "(A,1X," // fmt2 // ",1X," // fmt2 // ")") &
            trim (buffer), &
            entry%efficiency_pos * 100, &
            entry%efficiency_neg * 100
    end if
    if (entry%n_it /= 1) then
        write (buffer, "(A,1x,F7.2,1x,I3)") &
            trim (buffer), &
            entry%chi2, &
            entry%n_it
    end if
    write (u, "(A)") trim (buffer)
end if
flush (u)
end subroutine integration_entry_write

subroutine integration_entry_write_verbose (entry, unit)
    class(integration_entry_t), intent(in) :: entry
    integer, intent(in) :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, *) " process_type = ", entry%process_type
    write (u, *) "          pass = ", entry%pass
    write (u, *) "          it = ", entry%it
    write (u, *) "          n_it = ", entry%n_it
    write (u, *) "          n_calls = ", entry%n_calls
    write (u, *) " n_calls_valid = ", entry%n_calls_valid
    write (u, *) "          improved = ", entry%improved
    write (u, *) "          integral = ", entry%integral
    write (u, *) "          error = ", entry%error
    write (u, *) "          efficiency = ", entry%efficiency
    write (u, *) "efficiency_pos = ", entry%efficiency_pos
    write (u, *) "efficiency_neg = ", entry%efficiency_neg
    write (u, *) "          chi2 = ", entry%chi2
    if (allocated (entry%chain_weights)) then
        write (u, *) "          n_groves = ", size (entry%chain_weights)
        write (u, *) "chain_weights = ", entry%chain_weights
    else
        write (u, *) "          n_groves = 0"
    end if
    flush (u)
end subroutine integration_entry_write_verbose

```

Read the entry, assuming it has been written in verbose format.

(Integration results: integration entry: TBP)+≡

```
procedure :: read => integration_entry_read
```

(Integration results: procedures)+≡

```

subroutine integration_entry_read (entry, unit)
    class(integration_entry_t), intent(out) :: entry
    integer, intent(in) :: unit
    character(30) :: dummy

```

```

character :: equals
integer :: n_groves
read (unit, *) dummy, equals, entry%process_type
read (unit, *) dummy, equals, entry%pass
read (unit, *) dummy, equals, entry%it
read (unit, *) dummy, equals, entry%n_it
read (unit, *) dummy, equals, entry%n_calls
read (unit, *) dummy, equals, entry%n_calls_valid
read (unit, *) dummy, equals, entry%improved
read (unit, *) dummy, equals, entry%integral
read (unit, *) dummy, equals, entry%error
read (unit, *) dummy, equals, entry%efficiency
read (unit, *) dummy, equals, entry%efficiency_pos
read (unit, *) dummy, equals, entry%efficiency_neg
read (unit, *) dummy, equals, entry%chi2
read (unit, *) dummy, equals, n_groves
if (n_groves /= 0) then
    allocate (entry%chain_weights (n_groves))
    read (unit, *) dummy, equals, entry%chain_weights
end if
end subroutine integration_entry_read

```

Write an account of the channel weights, accumulated by groves.

<Integration results: integration entry: TBP>+≡

```

procedure :: write_chain_weights => integration_entry_write_chain_weights

```

<Integration results: procedures>+≡

```

subroutine integration_entry_write_chain_weights (entry, unit)
    class(integration_entry_t), intent(in) :: entry
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    if (allocated (entry%chain_weights)) then
        do i = 1, size (entry%chain_weights)
            write (u, "(1x,I3)", advance="no") nint (entry%chain_weights(i) * 100)
        end do
        write (u, *)
    end if
end subroutine integration_entry_write_chain_weights

```

21.3.2 Combined integration results

We collect a list of results which grows during the execution of the program. This is implemented as an array which grows if necessary; so we can easily compute averages.

We implement this as an extension of the `mci_results_t` which is defined in `mci_base` as an abstract type. We thus decouple the implementation of the integrator from the implementation of the results display, but nevertheless can record intermediate results during integration. This implies that the present extension implements a `record` method.

<Integration results: public>+≡

```

public :: integration_results_t

```

```

<Integration results: types>+≡
type, extends (mci_results_t) :: integration_results_t
  private
  integer :: process_type = PRC_UNKNOWN
  integer :: current_pass = 0
  integer :: n_pass = 0
  integer :: n_it = 0
  logical :: screen = .false.
  integer :: unit = 0
  integer :: verbosity = 0
  real(default) :: error_threshold = 0
  type(integration_entry_t), dimension(:), allocatable :: entry
  type(integration_entry_t), dimension(:), allocatable :: average
contains
  <Integration results: integration results: TBP>
end type integration_results_t

```

The array is extended in chunks of 10 entries.

```

<Integration results: parameters>+≡
integer, parameter :: RESULTS_CHUNK_SIZE = 10

<Integration results: integration results: TBP>≡
procedure :: init => integration_results_init

<Integration results: procedures>+≡
subroutine integration_results_init (results, process_type)
  class(integration_results_t), intent(out) :: results
  integer, intent(in) :: process_type
  results%process_type = process_type
  results%n_pass = 0
  results%n_it = 0
  allocate (results%entry (RESULTS_CHUNK_SIZE))
  allocate (results%average (RESULTS_CHUNK_SIZE))
end subroutine integration_results_init

```

Set verbose output of the integration results. In verbose mode, valid calls, negative as positive efficiency will be printed.

```

<Integration results: integration results: TBP>+≡
procedure :: set_verbosity => integration_results_set_verbosity

<Integration results: procedures>+≡
subroutine integration_results_set_verbosity (results, verbosity)
  class(integration_results_t), intent(inout) :: results
  integer, intent(in) :: verbosity
  results%verbosity = verbosity
end subroutine integration_results_set_verbosity

```

Set additional parameters: the `error_threshold` declares that any error value (in absolute numbers) smaller than this is to be considered zero.

```

<Integration results: integration results: TBP>+≡
procedure :: set_error_threshold => integration_results_set_error_threshold

```

```

<Integration results: procedures>+=
subroutine integration_results_set_error_threshold (results, error_threshold)
  class(integration_results_t), intent(inout) :: results
  real(default), intent(in) :: error_threshold
  results%error_threshold = error_threshold
end subroutine integration_results_set_error_threshold

```

Output (ASCII format). The `verbose` format is used for writing the header in grid files.

```

<Integration results: integration results: TBP>+=
procedure :: write => integration_results_write
procedure :: write_verbose => integration_results_write_verbose

<Integration results: procedures>+=
subroutine integration_results_write (object, unit, suppress)
  class(integration_results_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: suppress
  logical :: verb
  integer :: u, n
  u = given_output_unit (unit); if (u < 0) return
  call object%write_dline (unit)
  if (object%n_it /= 0) then
    call object%write_header (unit, logfile = .false.)
    call object%write_dline (unit)
    do n = 1, object%n_it
      if (n > 1) then
        if (object%entry(n)%pass /= object%entry(n-1)%pass) then
          call object%write_hline (unit)
          call object%average(object%entry(n-1)%pass)%write ( &
            & unit, suppress = suppress)
          call object%write_hline (unit)
        end if
      end if
      call object%entry(n)%write (unit, &
        suppress = suppress)
    end do
    call object%write_hline(unit)
    call object%average(object%n_pass)%write (unit, suppress = suppress)
  else
    call msg_message ("[WHIZARD integration results: empty]", unit)
  end if
  call object%write_dline (unit)
  flush (u)
end subroutine integration_results_write

subroutine integration_results_write_verbose (object, unit)
  class(integration_results_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u, n
  u = given_output_unit (unit); if (u < 0) return
  write (u, *) "begin(integration_results)"
  write (u, *) "  n_pass = ", object%n_pass
  write (u, *) "    n_it = ", object%n_it

```

```

if (object%n_it > 0) then
  write (u, *) "begin(integration_pass)"
  do n = 1, object%n_it
    if (n > 1) then
      if (object%entry(n)%pass /= object%entry(n-1)%pass) then
        write (u, *) "end(integration_pass)"
        write (u, *) "begin(integration_pass)"
      end if
    end if
    write (u, *) "begin(iteration)"
    call object%entry(n)%write_verbose (unit)
    write (u, *) "end(iteration)"
  end do
  write (u, *) "end(integration_pass)"
end if
write (u, *) "end(integration_results)"
flush (u)
end subroutine integration_results_write_verbose

```

Write a concise table of chain weights, i.e., the channel history where channels are collected by chains.

<Integration results: integration results: TBP>+≡

```

procedure :: write_chain_weights => &
  integration_results_write_chain_weights

```

<Integration results: procedures>+≡

```

subroutine integration_results_write_chain_weights (results, unit)
  class(integration_results_t), intent(in) :: results
  integer, intent(in), optional :: unit
  integer :: u, i, n
  u = given_output_unit (unit); if (u < 0) return
  if (allocated (results%entry(1)%chain_weights) .and. results%n_it /= 0) then
    call msg_message ("Phase-space chain (grove) weight history: " &
      // "(numbers in %)", unit)
    write (u, "(A9)", advance="no") "| chain |"
    do i = 1, integration_entry_get_n_groves (results%entry(1))
      write (u, "(1x,I3)", advance="no") i
    end do
    write (u, *)
    call results%write_dline (unit)
    do n = 1, results%n_it
      if (n > 1) then
        if (results%entry(n)%pass /= results%entry(n-1)%pass) then
          call results%write_hline (unit)
        end if
      end if
      write (u, "(1x,I6,1x,A1)", advance="no") n, "|"
      call results%entry(n)%write_chain_weights (unit)
    end do
    flush (u)
    call results%write_dline(unit)
  end if
end subroutine integration_results_write_chain_weights

```


Read the list from file. The file must be written using the `verbose` option of the writing routine.

```

<Integration results: integration results: TBP>+≡
  procedure :: read => integration_results_read

<Integration results: procedures>+≡
  subroutine integration_results_read (results, unit)
    class(integration_results_t), intent(out) :: results
    integer, intent(in) :: unit
    character(80) :: buffer
    character :: equals
    integer :: pass, it
    read (unit, *) buffer
    if (trim (adjustl (buffer)) /= "begin(integration_results)") then
      call read_err (); return
    end if
    read (unit, *) buffer, equals, results%n_pass
    read (unit, *) buffer, equals, results%n_it
    allocate (results%entry (results%n_it + RESULTS_CHUNK_SIZE))
    allocate (results%average (results%n_it + RESULTS_CHUNK_SIZE))
    it = 0
    do pass = 1, results%n_pass
      read (unit, *) buffer
      if (trim (adjustl (buffer)) /= "begin(integration_pass)") then
        call read_err (); return
      end if
      READ_ENTRIES: do
        read (unit, *) buffer
        if (trim (adjustl (buffer)) /= "begin(iteration)") then
          exit READ_ENTRIES
        end if
        it = it + 1
        call results%entry(it)%read (unit)
        read (unit, *) buffer
        if (trim (adjustl (buffer)) /= "end(iteration)") then
          call read_err (); return
        end if
      end do READ_ENTRIES
      if (trim (adjustl (buffer)) /= "end(integration_pass)") then
        call read_err (); return
      end if
      results%average(pass) = compute_average (results%entry, pass)
    end do
    read (unit, *) buffer
    if (trim (adjustl (buffer)) /= "end(integration_results)") then
      call read_err (); return
    end if
  contains
    subroutine read_err ()
      call msg_fatal ("Reading integration results from file: syntax error")
    end subroutine read_err
  end subroutine integration_results_read

```

Auxiliary output.

```

<Integration results: integration results: TBP>+≡
  procedure, private :: write_header
  procedure, private :: write_hline
  procedure, private :: write_dline

<Integration results: procedures>+≡
  subroutine write_header (results, unit, logfile)
    class(integration_results_t), intent(in) :: results
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: logfile
    character(5) :: phys_unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    select case (results%process_type)
    case (PRC_DECAY);      phys_unit = "[GeV]"
    case (PRC_SCATTERING); phys_unit = "[fb] "
    case default
      phys_unit = "    "
    end select
    write (msg_buffer, "(A, A)") &
      "It      Calls"
    if (results%verbosity > 1) then
      write (msg_buffer, "(A, A)") trim (msg_buffer), &
        "      Valid"
    end if
    write (msg_buffer, "(A, A)") trim (msg_buffer), &
      "  Integral" // phys_unit // &
      "  Error" // phys_unit // &
      "  Err[%]  Acc  Eff[%]"
    if (results%verbosity > 2) then
      write (msg_buffer, "(A, A)") trim (msg_buffer), &
        "  (+)[%]  (-)[%]"
    end if
    write (msg_buffer, "(A, A)") trim (msg_buffer), &
      "  Chi2 N[It] |"
    call msg_message (unit=u, logfile=logfile)
  end subroutine write_header

  subroutine write_hline (results, unit)
    class(integration_results_t), intent(in) :: results
    integer, intent(in), optional :: unit
    integer :: u, len
    u = given_output_unit (unit); if (u < 0) return
    len = 77
    if (results%verbosity > 1) len = len + 11
    if (results%verbosity > 2) len = len + 16
    write (u, "(A)")  "|" // (repeat("-", len)) // "|"
    flush (u)
  end subroutine write_hline

  subroutine write_dline (results, unit)
    class(integration_results_t), intent(in) :: results
    integer, intent(in), optional :: unit
    integer :: u, len
    u = given_output_unit (unit); if (u < 0) return

```

```

len = 77
if (results%verbosity > 1) len = len + 11
if (results%verbosity > 2) len = len + 16
write (u, "(A)"  "|" // (repeat ("=", len)) // "|")
flush (u)
end subroutine write_dline

```

During integration, we do not want to print all results at once, but each intermediate result as soon as we get it. Thus, the previous procedure is chopped in pieces. First piece: store the output unit and a flag whether we want to print to standard output as well. Then write the header if the results are still empty, i.e., before integration has started. The second piece writes a single result to the saved output channels. We call this from the `record` method, which can be called from the integrator directly. The third piece writes the average result, once a pass has been completed. The fourth piece writes a footer (if any), assuming that this is the final result.

```

<Integration results: integration results: TBP>+≡
  procedure :: display_init => integration_results_display_init
  procedure :: display_current => integration_results_display_current
  procedure :: display_pass => integration_results_display_pass
  procedure :: display_final => integration_results_display_final

<Integration results: procedures>+≡
  subroutine integration_results_display_init &
    (results, screen, unit)
    class(integration_results_t), intent(inout) :: results
    logical, intent(in) :: screen
    integer, intent(in), optional :: unit
    integer :: u
    if (present (unit)) results%unit = unit
    u = given_output_unit ()
    results%screen = screen
    if (results%n_it == 0) then
      if (results%screen) then
        call results%write_dline (u)
        call results%write_header (u, &
          logfile=.false.)
        call results%write_dline (u)
      end if
      if (results%unit /= 0) then
        call results%write_dline (results%unit)
        call results%write_header (results%unit, &
          logfile=.false.)
        call results%write_dline (results%unit)
      end if
    else
      if (results%screen) then
        call results%write_hline (u)
      end if
      if (results%unit /= 0) then
        call results%write_hline (results%unit)
      end if
    end if
  end subroutine

```

```

end subroutine integration_results_display_init

subroutine integration_results_display_current (results, pacify)
  class(integration_results_t), intent(in) :: results
  integer :: u
  logical, intent(in), optional :: pacify
  u = given_output_unit ()
  if (results%screen) then
    call results%entry(results%n_it)%write (u, &
      verbosity = results%verbosity, suppress = pacify)
  end if
  if (results%unit /= 0) then
    call results%entry(results%n_it)%write ( &
      results%unit, verbosity = results%verbosity, suppress = pacify)
  end if
end subroutine integration_results_display_current

subroutine integration_results_display_pass (results, pacify)
  class(integration_results_t), intent(in) :: results
  logical, intent(in), optional :: pacify
  integer :: u
  u = given_output_unit ()
  if (results%screen) then
    call results%write_hline (u)
    call results%average(results%entry(results%n_it)%pass)%write ( &
      u, verbosity = results%verbosity, suppress = pacify)
  end if
  if (results%unit /= 0) then
    call results%write_hline (results%unit)
    call results%average(results%entry(results%n_it)%pass)%write ( &
      results%unit, verbosity = results%verbosity, suppress = pacify)
  end if
end subroutine integration_results_display_pass

subroutine integration_results_display_final (results)
  class(integration_results_t), intent(inout) :: results
  integer :: u
  u = given_output_unit ()
  if (results%screen) then
    call results%write_dline (u)
  end if
  if (results%unit /= 0) then
    call results%write_dline (results%unit)
  end if
  results%screen = .false.
  results%unit = 0
end subroutine integration_results_display_final

```

Expand the list of entries if the limit has been reached:

```

<Integration results: integration results: TBP>+≡
  procedure :: expand => integration_results_expand
<Integration results: procedures>+≡
  subroutine integration_results_expand (results)

```

```

class(integration_results_t), intent(inout) :: results
type(integration_entry_t), dimension(:), allocatable :: entry_tmp
if (results%n_it == size (results%entry)) then
  allocate (entry_tmp (results%n_it))
  entry_tmp = results%entry
  deallocate (results%entry)
  allocate (results%entry (results%n_it + RESULTS_CHUNK_SIZE))
  results%entry(:results%n_it) = entry_tmp
  deallocate (entry_tmp)
end if
if (results%n_pass == size (results%average)) then
  allocate (entry_tmp (results%n_pass))
  entry_tmp = results%average
  deallocate (results%average)
  allocate (results%average (results%n_it + RESULTS_CHUNK_SIZE))
  results%average(:results%n_pass) = entry_tmp
  deallocate (entry_tmp)
end if
end subroutine integration_results_expand

```

Increment the `current_pass` counter. Must be done before each new integration pass; after integration, the recording method may use the value of this counter to define the entry.

```

<Integration results: integration results: TBP>+=
  procedure :: new_pass => integration_results_new_pass

<Integration results: procedures>+=
  subroutine integration_results_new_pass (results)
    class(integration_results_t), intent(inout) :: results
    results%current_pass = results%current_pass + 1
  end subroutine integration_results_new_pass

```

Enter results into the results list. For the error value, we may compare them with a given threshold. This guards against numerical noise, if the exact error would be zero.

```

<Integration results: integration results: TBP>+=
  procedure :: append => integration_results_append

<Integration results: procedures>+=
  subroutine integration_results_append (results, &
    n_it, n_calls, n_calls_valid, &
    integral, error, efficiency, efficiency_pos, efficiency_neg, &
    chain_weights)
    class(integration_results_t), intent(inout) :: results
    integer, intent(in) :: n_it, n_calls, n_calls_valid
    real(default), intent(in) :: integral, error, efficiency, efficiency_pos, &
      & efficiency_neg
    real(default), dimension(:), intent(in), optional :: chain_weights
    logical :: improved
    type(integration_entry_t) :: entry
    real(default) :: err_checked
    improved = .true.
    if (results%n_it /= 0) improved = abs(accuracy (integral, error, n_calls)) &

```

```

        < abs(results%entry(results%n_it)%get_accuracy ())
err_checked = 0
if (abs (error) >= results%error_threshold) err_checked = error
entry = integration_entry_t ( &
    results%process_type, results%current_pass, &
    results%n_it+1, n_it, n_calls, n_calls_valid, improved, &
    integral, err_checked, efficiency, efficiency_pos, efficiency_neg, &
    chain_weights=chain_weights)
if (results%n_it == 0) then
    results%n_it = 1
    results%n_pass = 1
else
    call results%expand ()
    if (entry%pass /= results%entry(results%n_it)%pass) &
        results%n_pass = results%n_pass + 1
    results%n_it = results%n_it + 1
end if
results%entry(results%n_it) = entry
results%average(results%n_pass) = &
    compute_average (results%entry, entry%pass)
end subroutine integration_results_append

```

Record an integration pass executed by an mci integrator object.

There is a tolerance below we treat an error (relative to the integral) as zero.

<Integration results: parameters>+≡

```
real(default), parameter, public :: INTEGRATION_ERROR_TOLERANCE = 1e-10
```

<Integration results: integration results: TBP>+≡

```
procedure :: record_simple => integration_results_record_simple
```

<Integration results: procedures>+≡

```

subroutine integration_results_record_simple &
    (object, n_it, n_calls, integral, error, efficiency, &
    chain_weights, suppress)
class(integration_results_t), intent(inout) :: object
integer, intent(in) :: n_it, n_calls
real(default), intent(in) :: integral, error, efficiency
real(default), dimension(:), intent(in), optional :: chain_weights
real(default) :: err
logical, intent(in), optional :: suppress
err = 0._default
if (abs (error) >= abs (integral) * INTEGRATION_ERROR_TOLERANCE) then
    err = error
end if
call object%append (n_it, n_calls, 0, integral, err, efficiency, 0._default,&
    & 0._default, chain_weights)
call object%display_current (suppress)
end subroutine integration_results_record_simple

```

Record extended results from integration pass.

<Integration results: integration results: TBP>+≡

```
procedure :: record_extended => integration_results_record_extended
```

(Integration results: procedures)+≡

```

subroutine integration_results_record_extended (object, n_it, n_calls,&
      & n_calls_valid, integral, error, efficiency, efficiency_pos,&
      & efficiency_neg, chain_weights, suppress)
class(integration_results_t), intent(inout) :: object
integer, intent(in) :: n_it, n_calls, n_calls_valid
real(default), intent(in) :: integral, error, efficiency, efficiency_pos,&
      & efficiency_neg
real(default), dimension(:), intent(in), optional :: chain_weights
real(default) :: err
logical, intent(in), optional :: suppress
err = 0._default
if (abs (error) >= abs (integral) * INTEGRATION_ERROR_TOLERANCE) then
      err = error
end if
call object%append (n_it, n_calls, n_calls_valid, integral, err, efficiency,&
      & efficiency_pos, efficiency_neg, chain_weights)
call object%display_current (suppress)
end subroutine integration_results_record_extended

```

Compute the average for all entries in the specified integration pass. The integrals are weighted w.r.t. their individual errors.

The quoted error of the result is the expected error, computed from the weighted average of the given individual errors.

This should be compared to the actual distribution of the results, from which we also can compute an error estimate if there is more than one iteration. The ratio of the distribution error and the averaged error, is the χ^2 value.

All error distributions are assumed Gaussian, of course. The χ^2 value is a partial check for this assumption. If it is significantly greater than unity, there is something wrong with the individual errors.

The efficiency returned is the one of the last entry in the integration pass.

If any error vanishes, averaging by this algorithm would fail. In this case, we simply average the entries and use the deviations from this average (if any) to estimate the error.

(Integration results: procedures)+≡

```

type(integration_entry_t) function compute_average (entry, pass) &
      & result (result)
type(integration_entry_t), dimension(:), intent(in) :: entry
integer, intent(in) :: pass
integer :: i
logical, dimension(size(entry)) :: mask
real(default), dimension(size(entry)) :: ivar
real(default) :: sum_ivar, variance
result%process_type = entry(1)%process_type
result%pass = pass
mask = entry%pass == pass .and. entry%process_type /= PRC_UNKNOWN
result%it = maxval (entry%it, mask)
result%n_it = count (mask)
result%n_calls = sum (entry%n_calls, mask)
result%n_calls_valid = sum (entry%n_calls_valid, mask)
if (.not. any (mask .and. entry%error == 0)) then
      where (mask)

```

```

        ivar = 1 / entry%error ** 2
    elsewhere
        ivar = 0
    end where
    sum_ivar = sum (ivar, mask)
    variance = 0
    if (sum_ivar /= 0) then
        variance = 1 / sum_ivar
    end if
    result%integral = sum (entry%integral * ivar, mask) * variance
    if (result%n_it > 1) then
        result%chi2 = &
            sum ((entry%integral - result%integral)**2 * ivar, mask) &
            / (result%n_it - 1)
    end if
else if (result%n_it /= 0) then
    result%integral = sum (entry%integral, mask) / result%n_it
    variance = 0
    if (result%n_it > 1) then
        variance = &
            sum ((entry%integral - result%integral)**2, mask) &
            / (result%n_it - 1)
    end if
    if (result%integral /= 0) then
        if (abs (variance / result%integral) &
            < 100 * epsilon (1._default)) then
            variance = 0
        end if
    end if
end if
result%chi2 = variance / result%n_it
end if
result%error = sqrt (variance)
result%efficiency = entry(last_index (mask))%efficiency
result%efficiency_pos = entry(last_index (mask))%efficiency_pos
result%efficiency_neg = entry(last_index (mask))%efficiency_neg
contains
integer function last_index (mask) result (index)
    logical, dimension(:), intent(in) :: mask
    integer :: i
    do i = size (mask), 1, -1
        if (mask(i)) exit
    end do
    index = i
end function last_index
end function compute_average

```

21.3.3 Access results

Return true if the results object has entries.

<Integration results: integration results: TBP>+≡

```
procedure :: exist => integration_results_exist
```

<Integration results: procedures>+≡


```

function integration_results_exist (results) result (flag)
  logical :: flag
  class(integration_results_t), intent(in) :: results
  flag = results%n_pass > 0
end function integration_results_exist

```

Retrieve information from the results record. If **last** is set and true, take the last iteration. If it is set instead, take this iteration. If **pass** is set, take this average. If none is set, take the final average.

If the result would be invalid, the entry is not assigned. Due to default initialization, this returns a null entry.

(Integration results: integration results: TBP)+≡

```

procedure :: get_entry => results_get_entry

```

(Integration results: procedures)+≡

```

function results_get_entry (results, last, it, pass) result (entry)
  class(integration_results_t), intent(in) :: results
  type(integration_entry_t) :: entry
  logical, intent(in), optional :: last
  integer, intent(in), optional :: it, pass
  if (present (last)) then
    if (allocated (results%entry) .and. results%n_it > 0) then
      entry = results%entry(results%n_it)
    else
      call error ()
    end if
  else if (present (it)) then
    if (allocated (results%entry) .and. it > 0 .and. it <= results%n_it) then
      entry = results%entry(it)
    else
      call error ()
    end if
  else if (present (pass)) then
    if (allocated (results%average) &
      .and. pass > 0 .and. pass <= results%n_pass) then
      entry = results%average (pass)
    else
      call error ()
    end if
  else
    if (allocated (results%average) .and. results%n_pass > 0) then
      entry = results%average (results%n_pass)
    else
      call error ()
    end if
  end if
contains
  subroutine error ()
    call msg_fatal ("Requested integration result is not available")
  end subroutine error
end function results_get_entry

```

The individual procedures. The **results** record should have the **target at-**

tribute, but only locally within the function.

(Integration results: integration results: TBP)+≡

```

procedure :: get_n_calls => integration_results_get_n_calls
procedure :: get_integral => integration_results_get_integral
procedure :: get_error => integration_results_get_error
procedure :: get_accuracy => integration_results_get_accuracy
procedure :: get_chi2 => integration_results_get_chi2
procedure :: get_efficiency => integration_results_get_efficiency

```

(Integration results: procedures)+≡

```

function integration_results_get_n_calls (results, last, it, pass) &
    result (n_calls)
    class(integration_results_t), intent(in), target :: results
    integer :: n_calls
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    n_calls = entry%get_n_calls ()
end function integration_results_get_n_calls

function integration_results_get_integral (results, last, it, pass) &
    result (integral)
    class(integration_results_t), intent(in), target :: results
    real(default) :: integral
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    integral = entry%get_integral ()
end function integration_results_get_integral

function integration_results_get_error (results, last, it, pass) &
    result (error)
    class(integration_results_t), intent(in), target :: results
    real(default) :: error
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    error = entry%get_error ()
end function integration_results_get_error

function integration_results_get_accuracy (results, last, it, pass) &
    result (accuracy)
    class(integration_results_t), intent(in), target :: results
    real(default) :: accuracy
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    accuracy = entry%get_accuracy ()
end function integration_results_get_accuracy

function integration_results_get_chi2 (results, last, it, pass) &

```

```

        result (chi2)
    class(integration_results_t), intent(in), target :: results
    real(default) :: chi2
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    chi2 = entry%get_chi2 ()
end function integration_results_get_chi2

function integration_results_get_efficiency (results, last, it, pass) &
    result (efficiency)
    class(integration_results_t), intent(in), target :: results
    real(default) :: efficiency
    logical, intent(in), optional :: last
    integer, intent(in), optional :: it, pass
    type(integration_entry_t) :: entry
    entry = results%get_entry (last, it, pass)
    efficiency = entry%get_efficiency ()
end function integration_results_get_efficiency

```

Return the last pass index and the index of the last iteration *within* the last pass. The third routine returns the absolute index of the last iteration.

(*Integration results: procedures*) +=

```

function integration_results_get_current_pass (results) result (pass)
    integer :: pass
    type(integration_results_t), intent(in) :: results
    pass = results%n_pass
end function integration_results_get_current_pass

function integration_results_get_current_it (results) result (it)
    integer :: it
    type(integration_results_t), intent(in) :: results
    it = 0
    if (allocated (results%entry)) then
        it = count (results%entry(1:results%n_it)%pass == results%n_pass)
    end if
end function integration_results_get_current_it

function integration_results_get_last_it (results) result (it)
    integer :: it
    type(integration_results_t), intent(in) :: results
    it = results%n_it
end function integration_results_get_last_it

```

Return the index of the best iteration (lowest accuracy value) within the current pass. If none qualifies, return zero.

(*Integration results: procedures*) +=

```

function integration_results_get_best_it (results) result (it)
    integer :: it
    type(integration_results_t), intent(in) :: results
    integer :: i
    real(default) :: acc, acc_best

```

```

acc_best = -1
it = 0
do i = 1, results%n_it
  if (results%entry(i)%pass == results%n_pass) then
    acc = integration_entry_get_accuracy (results%entry(i))
    if (acc_best < 0 .or. acc <= acc_best) then
      acc_best = acc
      it = i
    end if
  end if
end do
end function integration_results_get_best_it

```

Compute the MD5 sum by printing everything and checksumming the resulting file.

```

<Integration results: procedures>+≡
function integration_results_get_md5sum (results) result (md5sum_results)
  character(32) :: md5sum_results
  type(integration_results_t), intent(in) :: results
  integer :: u
  u = free_unit ()
  open (unit = u, status = "scratch", action = "readwrite")
  call results%write_verbose (u)
  rewind (u)
  md5sum_results = md5sum (u)
  close (u)
end function integration_results_get_md5sum

```

This is (ab)used to suppress numerical noise when integrating constant matrix elements.

```

<Integration results: integration results: TBP>+≡
  procedure :: pacify => integration_results_pacify

<Integration results: procedures>+≡
subroutine integration_results_pacify (results, efficiency_reset)
  class(integration_results_t), intent(inout) :: results
  logical, intent(in), optional :: efficiency_reset
  integer :: i
  logical :: reset
  reset = .false.
  if (present (efficiency_reset)) reset = efficiency_reset
  if (allocated (results%entry)) then
    do i = 1, size (results%entry)
      call pacify (results%entry(i)%error, &
        results%entry(i)%integral * 1.E-9_default)
      if (reset) results%entry(i)%efficiency = 1
    end do
  end if
  if (allocated (results%average)) then
    do i = 1, size (results%average)
      call pacify (results%average(i)%error, &
        results%average(i)%integral * 1.E-9_default)
      if (reset) results%average(i)%efficiency = 1
    end do
  end if
end subroutine integration_results_pacify

```

```

        end do
    end if
end subroutine integration_results_pacify

```

```

<Integration results: integration results: TBP>+≡
    procedure :: record_correction => integration_results_record_correction

<Integration results: procedures>+≡
    subroutine integration_results_record_correction (object, corr, err)
        class(integration_results_t), intent(inout) :: object
        real(default), intent(in) :: corr, err
        integer :: u
        u = given_output_unit ()
        if (object%screen) then
            call object%write_hline (u)
            call msg_message ("NLO Correction: [O(alpha_s+1)/O(alpha_s)]")
            write(msg_buffer,'(1X,A1,F7.2,A4,F6.2,1X,A3)') '( ', corr, ' +- ', err, ' ) %'
            call msg_message ()
        end if
    end subroutine integration_results_record_correction

```

21.3.4 Results display

Write a driver file for history visualization.

The ratio of y range over y value must not become too small, otherwise we run into an arithmetic overflow in GAMELAN. 2% appears to be safe.

```

<Integration results: parameters>+≡
    real, parameter, public :: GML_MIN_RANGE_RATIO = 0.02

<Integration results: public>+≡
    public :: integration_results_write_driver

<Integration results: procedures>+≡
    subroutine integration_results_write_driver (results, filename, eff_reset)
        type(integration_results_t), intent(inout) :: results
        type(string_t), intent(in) :: filename
        logical, intent(in), optional :: eff_reset
        type(string_t) :: file_tex
        integer :: unit
        integer :: n, i, n_pass, pass
        integer, dimension(:), allocatable :: ipass
        real(default) :: ymin, ymax, yavg, ydif, y0, y1
        real(default), dimension(results%n_it) :: ymin_arr, ymax_arr
        logical :: reset
        file_tex = filename // ".tex"
        unit = free_unit ()
        open (unit=unit, file=char(file_tex), action="write", status="replace")
        reset = .false.; if (present (eff_reset)) reset = eff_reset
        n = results%n_it
        n_pass = results%n_pass
        allocate (ipass (results%n_pass))
        ipass(1) = 0
        pass = 2

```

```

do i = 1, n-1
  if (integration_entry_get_pass (results%entry(i)) &
      /= integration_entry_get_pass (results%entry(i+1))) then
    ipass(pass) = i
    pass = pass + 1
  end if
end do
ymin_arr = integration_entry_get_integral (results%entry(:n)) &
           - integration_entry_get_error (results%entry(:n))
ymin = minval (ymin_arr)
ymax_arr = integration_entry_get_integral (results%entry(:n)) &
           + integration_entry_get_error (results%entry(:n))
ymax = maxval (ymax_arr)
yavg = (ymax + ymin) / 2
ydif = (ymax - ymin)
if (ydif * 1.5 > GML_MIN_RANGE_RATIO * yavg) then
  y0 = yavg - ydif * 0.75
  y1 = yavg + ydif * 0.75
else
  y0 = yavg * (1 - GML_MIN_RANGE_RATIO / 2)
  y1 = yavg * (1 + GML_MIN_RANGE_RATIO / 2)
end if
write (unit, "(A)") "\documentclass{article}"
write (unit, "(A)") "\usepackage{a4wide}"
write (unit, "(A)") "\usepackage{gamelan}"
write (unit, "(A)") "\usepackage{amsmath}"
write (unit, "(A)") ""
write (unit, "(A)") "\begin{document}"
write (unit, "(A)") "\begin{gmlfile}"
write (unit, "(A)") "\section*{Integration Results Display}"
write (unit, "(A)") ""
write (unit, "(A)") "Process: \verb|" // char (filename) // "|"
write (unit, "(A)") ""
write (unit, "(A)") "\vspace*{2\baselineskip}"
write (unit, "(A)") "\unitlength 1mm"
write (unit, "(A)") "\begin{gmlcode}"
write (unit, "(A)") "  picture sym; sym = fshape (circle scaled 1mm());"
write (unit, "(A)") "  color col.band; col.band = 0.9white;"
write (unit, "(A)") "  color col.eband; col.eband = 0.98white;"
write (unit, "(A)") "\end{gmlcode}"
write (unit, "(A)") "\begin{gmlgraph*}(130,180)[history]"
write (unit, "(A)") "  setup (linear, linear);"
write (unit, "(A,I0,A)") "  history.n_pass = ", n_pass, ";"
write (unit, "(A,I0,A)") "  history.n_it   = ", n, ";"
write (unit, "(A,A,A)") "  history.y0 = #""", char (mp_format (y0)), """";
write (unit, "(A,A,A)") "  history.y1 = #""", char (mp_format (y1)), """";
write (unit, "(A)") &
  "  graphrange (#0.5, history.y0), (#(n+0.5), history.y1);"
do pass = 1, n_pass
  write (unit, "(A,I0,A,I0,A)") &
    "  history.pass[", pass, "] = ", ipass(pass), ";"
  write (unit, "(A,I0,A,A,A)") &
    "  history.avg[", pass, "] = #""", &
    char (mp_format &

```

```

        (integration_entry_get_integral (results%average(pass)))), &
        """, "
write (unit, "(A,I0,A,A,A)") &
    " history.err[" , pass, "] = #""", &
    char (mp_format &
        (integration_entry_get_error (results%average(pass)))), &
        """, "
write (unit, "(A,I0,A,A,A)") &
    " history.chi[" , pass, "] = #""", &
    char (mp_format &
        (integration_entry_get_chi2 (results%average(pass)))), &
        """, "
end do
write (unit, "(A,I0,A,I0,A)") &
    " history.pass[" , n_pass + 1, "] = " , n, ";"
write (unit, "(A)") " for i = 1 upto history.n_pass:"
write (unit, "(A)") " if history.chi[i] greater one:"
write (unit, "(A)") " fill plot ("
write (unit, "(A)") &
    " (#(history.pass[i] +.5), " &
    // "history.avg[i] minus history.err[i] times history.chi[i]),"
write (unit, "(A)") &
    " (#(history.pass[i+1]+.5), " &
    // "history.avg[i] minus history.err[i] times history.chi[i]),"
write (unit, "(A)") &
    " (#(history.pass[i+1]+.5), " &
    // "history.avg[i] plus history.err[i] times history.chi[i]),"
write (unit, "(A)") &
    " (#(history.pass[i] +.5), " &
    // "history.avg[i] plus history.err[i] times history.chi[i])"
write (unit, "(A)") " ) withcolor col.eband fi;"
write (unit, "(A)") " fill plot ("
write (unit, "(A)") &
    " (#(history.pass[i] +.5), history.avg[i] minus history.err[i]),"
write (unit, "(A)") &
    " (#(history.pass[i+1]+.5), history.avg[i] minus history.err[i]),"
write (unit, "(A)") &
    " (#(history.pass[i+1]+.5), history.avg[i] plus history.err[i]),"
write (unit, "(A)") &
    " (#(history.pass[i] +.5), history.avg[i] plus history.err[i])"
write (unit, "(A)") " ) withcolor col.band;"
write (unit, "(A)") " draw plot ("
write (unit, "(A)") &
    " (#(history.pass[i] +.5), history.avg[i]),"
write (unit, "(A)") &
    " (#(history.pass[i+1]+.5), history.avg[i])"
write (unit, "(A)") " ) dashed evenly;"
write (unit, "(A)") " endfor"
write (unit, "(A)") " for i = 1 upto history.n_pass + 1:"
write (unit, "(A)") " draw plot ("
write (unit, "(A)") &
    " (#(history.pass[i]+.5), history.y0),"
write (unit, "(A)") &
    " (#(history.pass[i]+.5), history.y1)"

```

```

write (unit, "(A)" "      ) dashed withdots;"
write (unit, "(A)" "   endfor"
do i = 1, n
  write (unit, "(A,I0,A,A,A,A,A)" "   plot (history) (#", &
    i, ", #""", &
char (mp_format (integration_entry_get_integral (results%entry(i))),&
  """) vbar #""", &
  char (mp_format (integration_entry_get_error (results%entry(i))), &
    """);"
end do
write (unit, "(A)" "   draw piecewise from (history) " &
  // "withsymbol sym;"
write (unit, "(A)" "   fullgrid.lr (5,20);"
write (unit, "(A)" "   standardgrid.bt (n);"
write (unit, "(A)" "   begingmleps ""Whizard-Logo.eps"";"
write (unit, "(A)" "   base := (120*unitlength,170*unitlength);"
write (unit, "(A)" "   height := 9.6*unitlength;"
write (unit, "(A)" "   width := 11.2*unitlength;"
write (unit, "(A)" "   endgmleps;"
write (unit, "(A)" "\end{gmlgraph*}"
write (unit, "(A)" "\end{gmlfile}"
write (unit, "(A)" "\clearpage"
write (unit, "(A)" "\begin{verbatim}"
if (reset) then
  call results%pacify (reset)
end if
call integration_results_write (results, unit)
write (unit, "(A)" "\end{verbatim}"
write (unit, "(A)" "\end{document}"
close (unit)
end subroutine integration_results_write_driver

```

Call L^AT_EX and Metapost for the history driver file, and convert to PS and PDF.

```

<Integration results: public>+=
  public :: integration_results_compile_driver

<Integration results: procedures>+=
  subroutine integration_results_compile_driver (results, filename, os_data)
    type(integration_results_t), intent(in) :: results
    type(string_t), intent(in) :: filename
    type(os_data_t), intent(in) :: os_data
    integer :: unit_dev, status
    type(string_t) :: file_tex, file_dvi, file_ps, file_pdf, file_mp
    type(string_t) :: setenv_tex, setenv_mp, pipe, pipe_dvi
    if (.not. os_data%event_analysis) then
      call msg_warning ("Skipping integration history display " &
        // "because latex or mpost is not available")
      return
    end if
    file_tex = filename // ".tex"
    file_dvi = filename // ".dvi"
    file_ps = filename // ".ps"
    file_pdf = filename // ".pdf"
    file_mp = filename // ".mp"

```



```

call msg_message ("Creating integration history display "&
// char (file_ps) // " and " // char (file_pdf))
BLOCK: do
  unit_dev = free_unit ()
  open (file = "/dev/null", unit = unit_dev, &
    action = "write", iostat = status)
  if (status /= 0) then
    pipe = ""
    pipe_dvi = ""
  else
    pipe = " > /dev/null"
    pipe_dvi = " 2>/dev/null 1>/dev/null"
  end if
  close (unit_dev)
  if (os_data%whizard_texpath /= "") then
    setenv_tex = &
      "TEXINPUTS=" // os_data%whizard_texpath // ":$TEXINPUTS "
    setenv_mp = &
      "MPINPUTS=" // os_data%whizard_texpath // ":$MPINPUTS "
  else
    setenv_tex = ""
    setenv_mp = ""
  end if
  call os_system_call (setenv_tex // os_data%latex // " " // &
    file_tex // pipe, status)
  if (status /= 0) exit BLOCK
  if (os_data%gml /= "") then
    call os_system_call (setenv_mp // os_data%gml // " " // &
      file_mp // pipe, status)
  else
    call msg_error ("Could not use GAMELAN/MetaPOST.")
    exit BLOCK
  end if
  if (status /= 0) exit BLOCK
  call os_system_call (setenv_tex // os_data%latex // " " // &
    file_tex // pipe, status)
  if (status /= 0) exit BLOCK
  if (os_data%event_analysis_ps) then
    call os_system_call (os_data%dvips // " " // &
      file_dvi // pipe_dvi, status)
    if (status /= 0) exit BLOCK
  else
    call msg_warning ("Skipping PostScript generation because dvips " &
      // "is not available")
    exit BLOCK
  end if
  if (os_data%event_analysis_pdf) then
    call os_system_call (os_data%ps2pdf // " " // &
      file_ps, status)
    if (status /= 0) exit BLOCK
  else
    call msg_warning ("Skipping PDF generation because ps2pdf " &
      // "is not available")
    exit BLOCK
  end if

```

```

        end if
        exit BLOCK
    end do BLOCK
    if (status /= 0) then
        call msg_error ("Unable to compile integration history display")
    end if
end subroutine integration_results_compile_driver

```

21.3.5 Unit tests

Test module, followed by the corresponding implementation module.

<integration_results_ut.f90>≡
<File header>

```

module integration_results_ut
    use unit_tests
    use integration_results_ut

```

<Standard module head>

<integration results: public test>

contains

<integration results: test driver>

```

end module integration_results_ut

```

<integration_results_uti.f90>≡
<File header>

```

module integration_results_uti

```

<Use kinds>

```

    use integration_results

```

<Standard module head>

<integration results: test declarations>

contains

<integration results: tests>

```

end module integration_results_uti

```

API: driver for the unit tests below.

<integration results: public test>≡
 public :: integration_results_test

<integration results: test driver>≡
 subroutine integration_results_test (u, results)
 integer, intent(in) :: u

```

    type(test_results_t), intent(inout) :: results
    <integration results: execute tests>
end subroutine integration_results_test

```

Integration entry

```

<integration results: execute tests>≡
    call test (integration_results_1, "integration_results_1", &
        "record single line and write to log", &
        u, results)

<integration results: test declarations>≡
    public :: integration_results_1

<integration results: tests>≡
    subroutine integration_results_1 (u)
        integer, intent(in) :: u
        type(integration_entry_t) :: entry

        write (u, "(A)")  "* Test output: integration_results_1"
        write (u, "(A)")  "* Purpose: record single entry and write to log"
        write (u, "(A)")

        write (u, "(A)")  "* Write single line output"
        write (u, "(A)")

        entry = integration_entry_t ( &
            & process_type = 1, &
            & pass = 1, &
            & it = 1, &
            & n_it = 10, &
            & n_calls = 1000, &
            & n_calls_valid = 500, &
            & improved = .true., &
            & integral = 1.0_default, &
            & error = 0.5_default, &
            & efficiency = 0.25_default, &
            & efficiency_pos = 0.22_default, &
            & efficiency_neg = 0.03_default)
        call entry%write (u, 3)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: integration_results_1"

    end subroutine integration_results_1

<integration results: execute tests>+≡
    call test (integration_results_2, "integration_results_2", &
        "record single result and write to log", &
        u, results)

<integration results: test declarations>+≡
    public :: integration_results_2

```

```

<integration results: tests>+≡
  subroutine integration_results_2 (u)
    integer, intent(in) :: u
    type(integration_results_t) :: results

    write (u, "(A)")  "* Test output: integration_results_2"
    write (u, "(A)")  "*   Purpose: record single result and write to log"
    write (u, "(A)")

    write (u, "(A)")  "* Write single line output"
    write (u, "(A)")

    call results%init (PRC_DECAY)
    call results%append (1, 250, 0, 1.0_default, 0.5_default, 0.25_default,&
      & 0._default, 0._default)

    call results%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: integration_results_2"

  end subroutine integration_results_2

<integration results: execute tests>+≡
  call test (integration_results_3, "integration_results_3", &
    "initialize display and add/display each entry", &
    u, results)

<integration results: test declarations>+≡
  public :: integration_results_3

<integration results: tests>+≡
  subroutine integration_results_3 (u)
    integer, intent(in) :: u
    type(integration_results_t) :: results

    write (u, "(A)")  "* Test output: integration_results_2"
    write (u, "(A)")  "*   Purpose: intialize display, record three entries,&
      & display pass average and finalize display"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize display and add entry"
    write (u, "(A)")

    call results%init (PRC_DECAY)
    call results%set_verbosity (1)
    call results%display_init (screen = .false., unit = u)
    call results%new_pass ()

    call results%record (1, 250, 1.0_default, 0.5_default, 0.25_default)
    call results%record (1, 250, 1.1_default, 0.5_default, 0.25_default)
    call results%record (1, 250, 0.9_default, 0.5_default, 0.25_default)

    write (u, "(A)")
    write (u, "(A)")  "* Display pass"

```

```

write (u, "(A)")

call results%display_pass ()

write (u, "(A)")
write (u, "(A)")  "* Finalize displays"
write (u, "(A)")

call results%display_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integration_results_3"

end subroutine integration_results_3

<integration results: execute tests>+≡
call test (integration_results_4, "integration_results_4", &
  "record extended results and display", &
  u, results)

<integration results: test declarations>+≡
public :: integration_results_4

<integration results: tests>+≡
subroutine integration_results_4 (u)
  integer, intent(in) :: u
  type(integration_results_t) :: results

  write (u, "(A)")  "* Test output: integration_results_4"
  write (u, "(A)")  "* Purpose: record extended results and display with verbosity = 2"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize display and record extended result"
  write (u, "(A)")

  call results%init (PRC_DECAY)
  call results%set_verbosity (2)
  call results%display_init (screen = .false., unit = u)
  call results%new_pass ()

  call results%record (1, 250, 150, 1.0_default, 0.5_default, 0.25_default,&
    & 0.22_default, 0.03_default)
  call results%record (1, 250, 180, 1.1_default, 0.5_default, 0.25_default,&
    & 0.23_default, 0.02_default)
  call results%record (1, 250, 130, 0.9_default, 0.5_default, 0.25_default,&
    & 0.25_default, 0.00_default)

  write (u, "(A)")
  write (u, "(A)")  "* Display pass"
  write (u, "(A)")

  call results%display_pass ()

  write (u, "(A)")
  write (u, "(A)")  "* Finalize displays"

```

```

write (u, "(A)")

call results%display_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integration_results_4"

end subroutine integration_results_4

<integration results: execute tests>+≡
call test (integration_results_5, "integration_results_5", &
  "record extended results and display", &
  u, results)

<integration results: test declarations>+≡
public :: integration_results_5

<integration results: tests>+≡
subroutine integration_results_5 (u)
  integer, intent(in) :: u
  type(integration_results_t) :: results

  write (u, "(A)")  "* Test output: integration_results_5"
  write (u, "(A)")  "* Purpose: record extended results and display with verbosity = 3"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize display and record extended result"
  write (u, "(A)")

  call results%init (PRC_DECAY)
  call results%set_verbosity (3)
  call results%display_init (screen = .false., unit = u)
  call results%new_pass ()

  call results%record (1, 250, 150, 1.0_default, 0.5_default, 0.25_default,&
    & 0.22_default, 0.03_default)
  call results%record (1, 250, 180, 1.1_default, 0.5_default, 0.25_default,&
    & 0.23_default, 0.02_default)
  call results%record (1, 250, 130, 0.9_default, 0.5_default, 0.25_default,&
    & 0.25_default, 0.00_default)
  call results%display_pass ()
  call results%display_final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: integration_results_5"

end subroutine integration_results_5

```

21.4 Dummy integrator

This implementation acts as a placeholder for cases where no integration or event generation is required at all.

```
<mci_none.f90>≡  
<File header>  
  
module mci_none  
  
  <Use kinds>  
  use io_units, only: given_output_unit  
  use diagnostics, only: msg_message, msg_fatal  
  use phs_base, only: phs_channel_t  
  
  use mci_base  
  
  <Standard module head>  
  
  <MCI none: public>  
  
  <MCI none: types>  
  
contains  
  
  <MCI none: procedures>  
  
end module mci_none
```

21.4.1 Integrator

The object contains the methods for integration and event generation. For the actual work and data storage, it spawns an instance object.

After an integration pass, we update the `max` parameter to indicate the maximum absolute value of the integrand that the integrator encountered. This is required for event generation.

```
<MCI none: public>≡  
  public :: mci_none_t  
  
<MCI none: types>≡  
  type, extends (mci_t) :: mci_none_t  
  contains  
    <MCI none: mci none: TBP>  
  end type mci_none_t
```

Finalizer: no-op.

```
<MCI none: mci none: TBP>≡  
  procedure :: final => mci_none_final  
  
<MCI none: procedures>≡  
  subroutine mci_none_final (object)  
    class(mci_none_t), intent(inout) :: object  
  end subroutine mci_none_final
```

Output.

```
<MCI none: mci none: TBP>+≡
  procedure :: write => mci_none_write

<MCI none: procedures>+≡
  subroutine mci_none_write (object, unit, pacify, md5sum_version)
    class(mci_none_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    logical, intent(in), optional :: md5sum_version
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Integrator: non-functional dummy"
  end subroutine mci_none_write
```

Startup message: short version.

```
<MCI none: mci none: TBP>+≡
  procedure :: startup_message => mci_none_startup_message

<MCI none: procedures>+≡
  subroutine mci_none_startup_message (mci, unit, n_calls)
    class(mci_none_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
    call msg_message ("Integrator: none")
  end subroutine mci_none_startup_message
```

Log entry: just headline.

```
<MCI none: mci none: TBP>+≡
  procedure :: write_log_entry => mci_none_write_log_entry

<MCI none: procedures>+≡
  subroutine mci_none_write_log_entry (mci, u)
    class(mci_none_t), intent(in) :: mci
    integer, intent(in) :: u
    write (u, "(1x,A)") "MC Integrator is none (no-op)"
  end subroutine mci_none_write_log_entry
```

MD5 sum: nothing.

```
<MCI none: mci none: TBP>+≡
  procedure :: compute_md5sum => mci_none_compute_md5sum

<MCI none: procedures>+≡
  subroutine mci_none_compute_md5sum (mci, pacify)
    class(mci_none_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
  end subroutine mci_none_compute_md5sum
```

The number of channels must be one.

```
<CCC MCI none: mci none: TBP>≡
  procedure :: set_dimensions => mci_none_set_dimensions
```



```

<CCC MCI none: procedures>≡
subroutine mci_none_set_dimensions (mci, n_dim, n_channel)
  class(mci_none_t), intent(inout) :: mci
  integer, intent(in) :: n_dim
  integer, intent(in) :: n_channel
  if (n_channel == 1) then
    mci%n_channel = n_channel
    mci%n_dim = n_dim
    allocate (mci%dim_is_binned (mci%n_dim))
    mci%dim_is_binned = .true.
    mci%n_dim_binned = count (mci%dim_is_binned)
    allocate (mci%n_bin (mci%n_dim))
    mci%n_bin = 0
  else
    call msg_fatal ("Attempt to initialize single-channel integrator &
      &for multiple channels")
  end if
end subroutine mci_none_set_dimensions

```

Required by API.

```

<MCI none: mci none: TBP>+≡
  procedure :: declare_flat_dimensions => mci_none_ignore_flat_dimensions
<MCI none: procedures>+≡
subroutine mci_none_ignore_flat_dimensions (mci, dim_flat)
  class(mci_none_t), intent(inout) :: mci
  integer, dimension(:), intent(in) :: dim_flat
end subroutine mci_none_ignore_flat_dimensions

```

Required by API.

```

<MCI none: mci none: TBP>+≡
  procedure :: declare_equivalences => mci_none_ignore_equivalences
<MCI none: procedures>+≡
subroutine mci_none_ignore_equivalences (mci, channel, dim_offset)
  class(mci_none_t), intent(inout) :: mci
  type(phs_channel_t), dimension(:), intent(in) :: channel
  integer, intent(in) :: dim_offset
end subroutine mci_none_ignore_equivalences

```

Allocate instance with matching type.

```

<MCI none: mci none: TBP>+≡
  procedure :: allocate_instance => mci_none_allocate_instance
<MCI none: procedures>+≡
subroutine mci_none_allocate_instance (mci, mci_instance)
  class(mci_none_t), intent(in) :: mci
  class(mci_instance_t), intent(out), pointer :: mci_instance
  allocate (mci_none_instance_t :: mci_instance)
end subroutine mci_none_allocate_instance

```

Integrate. This must not be called at all.

```

<MCI none: mci none: TBP>+≡
  procedure :: integrate => mci_none_integrate

```

```

<MCI none: procedures>+≡
  subroutine mci_none_integrate (mci, instance, sampler, n_it, n_calls, &
    results, pacify)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: pacify
    class(mci_results_t), intent(inout), optional :: results
    call msg_fatal ("Integration: attempt to integrate with the 'mci_none' method")
  end subroutine mci_none_integrate

```

Simulation initializer and finalizer: nothing to do here.

```

<MCI none: mci none: TBP>+≡
  procedure :: prepare_simulation => mci_none_ignore_prepare_simulation

<MCI none: procedures>+≡
  subroutine mci_none_ignore_prepare_simulation (mci)
    class(mci_none_t), intent(inout) :: mci
  end subroutine mci_none_ignore_prepare_simulation

```

Generate events, must not be called.

```

<MCI none: mci none: TBP>+≡
  procedure :: generate_weighted_event => mci_none_generate_no_event
  procedure :: generate_unweighted_event => mci_none_generate_no_event

<MCI none: procedures>+≡
  subroutine mci_none_generate_no_event (mci, instance, sampler)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    call msg_fatal ("Integration: attempt to generate event with the 'mci_none' method")
  end subroutine mci_none_generate_no_event

```

Rebuild an event, no-op.

```

<MCI none: mci none: TBP>+≡
  procedure :: rebuild_event => mci_none_rebuild_event

<MCI none: procedures>+≡
  subroutine mci_none_rebuild_event (mci, instance, sampler, state)
    class(mci_none_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout) :: instance
    class(mci_sampler_t), intent(inout) :: sampler
    class(mci_state_t), intent(in) :: state
  end subroutine mci_none_rebuild_event

```

21.4.2 Integrator instance

Covering the case of flat dimensions, we store a complete x array. This is filled when generating events.

```

<MCI none: public>+≡
  public :: mci_none_instance_t

```

```

<MCI none: types>+≡
  type, extends (mci_instance_t) :: mci_none_instance_t
  contains
    <MCI none: mci none instance: TBP>
  end type mci_none_instance_t

```

Output.

```

<MCI none: mci none instance: TBP>≡
  procedure :: write => mci_none_instance_write

<MCI none: procedures>+≡
  subroutine mci_none_instance_write (object, unit, pacify)
    class(mci_none_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Integrator instance: non-functional dummy"
  end subroutine mci_none_instance_write

```

The finalizer is empty.

```

<MCI none: mci none instance: TBP>+≡
  procedure :: final => mci_none_instance_final

<MCI none: procedures>+≡
  subroutine mci_none_instance_final (object)
    class(mci_none_instance_t), intent(inout) :: object
  end subroutine mci_none_instance_final

```

Initializer, empty.

```

<MCI none: mci none instance: TBP>+≡
  procedure :: init => mci_none_instance_init

<MCI none: procedures>+≡
  subroutine mci_none_instance_init (mci_instance, mci)
    class(mci_none_instance_t), intent(out) :: mci_instance
    class(mci_t), intent(in), target :: mci
  end subroutine mci_none_instance_init

```

Copy the stored extrema of the integrand in the instance record.

```

<CCC MCI none: mci none instance: TBP>≡
  procedure :: get_max => mci_none_instance_get_max

<CCC MCI none: procedures>+≡
  subroutine mci_none_instance_get_max (instance)
    class(mci_none_instance_t), intent(inout) :: instance
    associate (mci => instance%mci)
      if (mci%max_known) then
        instance%max_known = .true.
        instance%max = mci%max
        instance%min = mci%min
        instance%max_abs = mci%max_abs
        instance%min_abs = mci%min_abs
      end if
    end associate
  end subroutine mci_none_instance_get_max

```

```

        end if
    end associate
end subroutine mci_none_instance_get_max

```

Reverse operations: recall the extrema, but only if they are wider than the extrema already stored in the configuration. Also recalculate the efficiency value.

```

<CCC MCI none: mci none instance: TBP>+≡
    procedure :: set_max => mci_none_instance_set_max

<CCC MCI none: procedures>+≡
    subroutine mci_none_instance_set_max (instance)
        class(mci_none_instance_t), intent(inout) :: instance
        associate (mci => instance%mci)
            if (instance%max_known) then
                if (mci%max_known) then
                    mci%max = max (mci%max, instance%max)
                    mci%min = min (mci%min, instance%min)
                    mci%max_abs = max (mci%max_abs, instance%max_abs)
                    mci%min_abs = min (mci%min_abs, instance%min_abs)
                else
                    mci%max = instance%max
                    mci%min = instance%min
                    mci%max_abs = instance%max_abs
                    mci%min_abs = instance%min_abs
                    mci%max_known = .true.
                end if
            end if
            if (mci%max_abs /= 0) then
                if (mci%integral_neg == 0) then
                    mci%efficiency = mci%integral / mci%max_abs
                    mci%efficiency_known = .true.
                else if (mci%n_calls /= 0) then
                    mci%efficiency = &
                        (mci%integral_pos - mci%integral_neg) / mci%max_abs
                    mci%efficiency_known = .true.
                end if
            end if
        end associate
    end subroutine mci_none_instance_set_max

```

The weight cannot be computed.

```

<MCI none: mci none instance: TBP>+≡
    procedure :: compute_weight => mci_none_instance_compute_weight

<MCI none: procedures>+≡
    subroutine mci_none_instance_compute_weight (mci, c)
        class(mci_none_instance_t), intent(inout) :: mci
        integer, intent(in) :: c
        call msg_fatal ("Integration: attempt to compute weight with the 'mci_none' method")
    end subroutine mci_none_instance_compute_weight

```

Record the integrand, no-op.

```
<MCI none: mci none instance: TBP>+≡
  procedure :: record_integrand => mci_none_instance_record_integrand

<MCI none: procedures>+≡
  subroutine mci_none_instance_record_integrand (mci, integrand)
    class(mci_none_instance_t), intent(inout) :: mci
    real(default), intent(in) :: integrand
  end subroutine mci_none_instance_record_integrand
```

No-op.

```
<MCI none: mci none instance: TBP>+≡
  procedure :: init_simulation => mci_none_instance_init_simulation
  procedure :: final_simulation => mci_none_instance_final_simulation

<MCI none: procedures>+≡
  subroutine mci_none_instance_init_simulation (instance, safety_factor)
    class(mci_none_instance_t), intent(inout) :: instance
    real(default), intent(in), optional :: safety_factor
  end subroutine mci_none_instance_init_simulation

  subroutine mci_none_instance_final_simulation (instance)
    class(mci_none_instance_t), intent(inout) :: instance
  end subroutine mci_none_instance_final_simulation
```

Return excess weight for the current event: return zero, just in case.

```
<MCI none: mci none instance: TBP>+≡
  procedure :: get_event_excess => mci_none_instance_get_event_excess

<MCI none: procedures>+≡
  function mci_none_instance_get_event_excess (mci) result (excess)
    class(mci_none_instance_t), intent(in) :: mci
    real(default) :: excess
    excess = 0
  end function mci_none_instance_get_event_excess
```

21.4.3 Unit tests

Test module, followed by the corresponding implementation module.

```
<mci_none.ut.f90>≡
  <File header>

  module mci_none_ut
    use unit_tests
    use mci_none_ut_i

    <Standard module head>

    <MCI none: public test>

    contains
```

```

    <MCI none: test driver>

    end module mci_none_ut

    <mci_none.uti.f90>≡
    <File header>

    module mci_none_uti

        use mci_base

        use mci_none

    <Standard module head>

    <MCI none: test declarations>

    <MCI none: test types>

    contains

    <MCI none: tests>

    end module mci_none_uti
API: driver for the unit tests below.
    <MCI none: public test>≡
        public :: mci_none_test
    <MCI none: test driver>≡
        subroutine mci_none_test (u, results)
            integer, intent(in) :: u
            type(test_results_t), intent(inout) :: results
        <MCI none: execute tests>
        end subroutine mci_none_test

```

Trivial sanity check

Construct an integrator and display it.

```

    <MCI none: execute tests>≡
        call test (mci_none_1, "mci_none_1", &
            "dummy integrator", &
            u, results)
    <MCI none: test declarations>≡
        public :: mci_none_1
    <MCI none: tests>≡
        subroutine mci_none_1 (u)
            integer, intent(in) :: u
            class(mci_t), allocatable, target :: mci
            class(mci_instance_t), pointer :: mci_instance => null ()
            class(mci_sampler_t), allocatable :: sampler

            write (u, "(A)")  "** Test output: mci_none_1"

```

```

write (u, "(A)")  "* Purpose: display mci configuration"
write (u, "(A)")

write (u, "(A)")  "* Allocate integrator"
write (u, "(A)")

allocate (mci_none_t :: mci)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

call mci_instance%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_none_1"

end subroutine mci_none_1

```

21.5 Simple midpoint integration

This is a most simple implementation of an integrator. The algorithm is the straightforward multi-dimensional midpoint rule, i.e., the integration hypercube is binned uniformly, the integrand is evaluated at the midpoints of each bin, and the result is the average. The binning is equivalent for all integration dimensions.

This rule is accurate to the order h^2 , where h is the bin width. Given that $h = N^{-1/d}$, where d is the integration dimension and N is the total number of sampling points, we get a relative error of order $N^{-2/d}$. This is superior to MC integration if $d < 4$, and equivalent if $d = 4$. It is not worse than higher-order formulas (such as Gauss integration) if the integrand is not smooth, e.g., if it contains cuts.

The integrator is specifically single-channel. However, we do not limit the dimension.

```
<mci_midpoint.f90>≡  
  <File header>  
  
  module mci_midpoint  
  
    <Use kinds>  
    use io_units  
    use diagnostics  
    use phs_base  
  
    use mci_base  
  
    <Standard module head>  
  
    <MCI midpoint: public>  
  
    <MCI midpoint: types>  
  
    contains  
  
    <MCI midpoint: procedures>  
  
  end module mci_midpoint
```

21.5.1 Integrator

The object contains the methods for integration and event generation. For the actual work and data storage, it spawns an instance object.

After an integration pass, we update the `max` parameter to indicate the maximum absolute value of the integrand that the integrator encountered. This is required for event generation.

```
<MCI midpoint: public>≡  
  public :: mci_midpoint_t  
  
<MCI midpoint: types>≡  
  type, extends (mci_t) :: mci_midpoint_t  
    integer :: n_dim_binned = 0  
    logical, dimension(:), allocatable :: dim_is_binned
```



```

        logical :: calls_known = .false.
        integer :: n_calls = 0
        integer :: n_calls_pos = 0
        integer :: n_calls_nul = 0
        integer :: n_calls_neg = 0
        real(default) :: integral_pos = 0
        real(default) :: integral_neg = 0
        integer, dimension(:), allocatable :: n_bin
        logical :: max_known = .false.
        real(default) :: max = 0
        real(default) :: min = 0
        real(default) :: max_abs = 0
        real(default) :: min_abs = 0
    contains
        <MCI midpoint: mci midpoint: TBP>
    end type mci_midpoint_t

```

Finalizer: base version is sufficient

```

<MCI midpoint: mci midpoint: TBP>≡
    procedure :: final => mci_midpoint_final

<MCI midpoint: procedures>≡
    subroutine mci_midpoint_final (object)
        class(mci_midpoint_t), intent(inout) :: object
        call object%base_final ()
    end subroutine mci_midpoint_final

```

Output.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: write => mci_midpoint_write

<MCI midpoint: procedures>+≡
    subroutine mci_midpoint_write (object, unit, pacify, md5sum_version)
        class(mci_midpoint_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
        logical, intent(in), optional :: md5sum_version
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Single-channel midpoint rule integrator:"
        call object%base_write (u, pacify, md5sum_version)
        if (object%n_dim_binned < object%n_dim) then
            write (u, "(3x,A,99(1x,I0))") "Flat dimensions      =", &
                pack ([(i, i = 1, object%n_dim)], mask = .not. object%dim_is_binned)
            write (u, "(3x,A,I0)") "Number of binned dim =", object%n_dim_binned
        end if
        if (object%calls_known) then
            write (u, "(3x,A,99(1x,I0))") "Number of bins      =", object%n_bin
            write (u, "(3x,A,I0)") "Number of calls      =", object%n_calls
            if (object%n_calls_pos /= object%n_calls) then
                write (u, "(3x,A,I0)") "  positive value      =", object%n_calls_pos
                write (u, "(3x,A,I0)") "  zero value          =", object%n_calls_nul
                write (u, "(3x,A,I0)") "  negative value       =", object%n_calls_neg
            end if
            write (u, "(3x,A,ES17.10)") &

```

```

        "Integral (pos. part) = ", object%integral_pos
        write (u, "(3x,A,ES17.10)") &
        "Integral (neg. part) = ", object%integral_neg
    end if
end if
if (object%max_known) then
    write (u, "(3x,A,ES17.10)") "Maximum of integrand = ", object%max
    write (u, "(3x,A,ES17.10)") "Minimum of integrand = ", object%min
    if (object%min /= object%min_abs) then
        write (u, "(3x,A,ES17.10)") "Maximum (abs. value) = ", object%max_abs
        write (u, "(3x,A,ES17.10)") "Minimum (abs. value) = ", object%min_abs
    end if
end if
if (allocated (object%rng)) call object%rng%write (u)
end subroutine mci_midpoint_write

```

Startup message: short version.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: startup_message => mci_midpoint_startup_message

<MCI midpoint: procedures>+≡
    subroutine mci_midpoint_startup_message (mci, unit, n_calls)
        class(mci_midpoint_t), intent(in) :: mci
        integer, intent(in), optional :: unit, n_calls
        call mci%base_startup_message (unit = unit, n_calls = n_calls)
        if (mci%n_dim_binned < mci%n_dim) then
            write (msg_buffer, "(A,2(1x,I0,1x,A))") &
                "Integrator: Midpoint rule:", &
                mci%n_dim_binned, "binned dimensions"
        else
            write (msg_buffer, "(A,2(1x,I0,1x,A))") &
                "Integrator: Midpoint rule"
        end if
        call msg_message (unit = unit)
    end subroutine mci_midpoint_startup_message

```

Log entry: just headline.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: write_log_entry => mci_midpoint_write_log_entry

<MCI midpoint: procedures>+≡
    subroutine mci_midpoint_write_log_entry (mci, u)
        class(mci_midpoint_t), intent(in) :: mci
        integer, intent(in) :: u
        write (u, "(1x,A)") "MC Integrator is Midpoint rule"
    end subroutine mci_midpoint_write_log_entry

```

MD5 sum: nothing.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: compute_md5sum => mci_midpoint_compute_md5sum

<MCI midpoint: procedures>+≡
    subroutine mci_midpoint_compute_md5sum (mci, pacify)
        class(mci_midpoint_t), intent(inout) :: mci

```

```

        logical, intent(in), optional :: pacify
    end subroutine mci_midpoint_compute_md5sum

```

The number of channels must be one.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: set_dimensions => mci_midpoint_set_dimensions

<MCI midpoint: procedures>+≡
    subroutine mci_midpoint_set_dimensions (mci, n_dim, n_channel)
        class(mci_midpoint_t), intent(inout) :: mci
        integer, intent(in) :: n_dim
        integer, intent(in) :: n_channel
        if (n_channel == 1) then
            mci%n_channel = n_channel
            mci%n_dim = n_dim
            allocate (mci%dim_is_binned (mci%n_dim))
            mci%dim_is_binned = .true.
            mci%n_dim_binned = count (mci%dim_is_binned)
            allocate (mci%n_bin (mci%n_dim))
            mci%n_bin = 0
        else
            call msg_fatal ("Attempt to initialize single-channel integrator &
                &for multiple channels")
        end if
    end subroutine mci_midpoint_set_dimensions

```

Declare particular dimensions as flat. These dimensions will not be binned.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: declare_flat_dimensions => mci_midpoint_declare_flat_dimensions

<MCI midpoint: procedures>+≡
    subroutine mci_midpoint_declare_flat_dimensions (mci, dim_flat)
        class(mci_midpoint_t), intent(inout) :: mci
        integer, dimension(:), intent(in) :: dim_flat
        integer :: d
        mci%n_dim_binned = mci%n_dim - size (dim_flat)
        do d = 1, size (dim_flat)
            mci%dim_is_binned(dim_flat(d)) = .false.
        end do
        mci%n_dim_binned = count (mci%dim_is_binned)
    end subroutine mci_midpoint_declare_flat_dimensions

```

Declare particular channels as equivalent. This has no effect.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: declare_equivalences => mci_midpoint_ignore_equivalences

<MCI midpoint: procedures>+≡
    subroutine mci_midpoint_ignore_equivalences (mci, channel, dim_offset)
        class(mci_midpoint_t), intent(inout) :: mci
        type(phs_channel_t), dimension(:), intent(in) :: channel
        integer, intent(in) :: dim_offset
    end subroutine mci_midpoint_ignore_equivalences

```

Allocate instance with matching type.

```

<MCI midpoint: mci midpoint: TBP>+≡
  procedure :: allocate_instance => mci_midpoint_allocate_instance

<MCI midpoint: procedures>+≡
  subroutine mci_midpoint_allocate_instance (mci, mci_instance)
    class(mci_midpoint_t), intent(in) :: mci
    class(mci_instance_t), intent(out), pointer :: mci_instance
    allocate (mci_midpoint_instance_t :: mci_instance)
  end subroutine mci_midpoint_allocate_instance

```

Integrate. The number of dimensions is arbitrary. We make sure that the number of calls is evenly distributed among the dimensions. The actual number of calls will typically be smaller than the requested number, but never smaller than 1.

The sampling over a variable number of dimensions implies a variable number of nested loops. We implement this by a recursive subroutine, one loop in each recursion level.

The number of iterations `n_it` is ignored. Also, the error is set to zero in the current implementation.

With this integrator, we allow the calculation to abort immediately when forced by a signal. There is no state that we can save, hence we do not catch an interrupt.

```

<MCI midpoint: mci midpoint: TBP>+≡
  procedure :: integrate => mci_midpoint_integrate

<MCI midpoint: procedures>+≡
  subroutine mci_midpoint_integrate (mci, instance, sampler, n_it, n_calls, &
    results, pacify)
    class(mci_midpoint_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: pacify
    class(mci_results_t), intent(inout), optional :: results
    real(default), dimension(:), allocatable :: x
    real(default) :: integral, integral_pos, integral_neg
    integer :: n_bin
    select type (instance)
    type is (mci_midpoint_instance_t)
      allocate (x (mci%n_dim))
      integral = 0
      integral_pos = 0
      integral_neg = 0
      select case (mci%n_dim_binned)
      case (1)
        n_bin = n_calls
      case (2:)
        n_bin = max (int (n_calls ** (1. / mci%n_dim_binned)), 1)
      end select
      where (mci%dim_is_binned)
        mci%n_bin = n_bin
    end select
  end subroutine mci_midpoint_integrate

```

```

elsewhere
    mci%n_bin = 1
end where
mci%n_calls = product (mci%n_bin)
mci%n_calls_pos = 0
mci%n_calls_nul = 0
mci%n_calls_neg = 0
mci%calls_known = .true.
call sample_dim (mci%n_dim)
mci%integral = integral / mci%n_calls
mci%integral_pos = integral_pos / mci%n_calls
mci%integral_neg = integral_neg / mci%n_calls
mci%integral_known = .true.
call instance%set_max ()
if (present (results)) then
    call results%record (1, mci%n_calls, &
        mci%integral, mci%error, mci%efficiency)
end if
end select
contains
recursive subroutine sample_dim (d)
    integer, intent(in) :: d
    integer :: i
    real(default) :: value
    do i = 1, mci%n_bin(d)
        x(d) = (i - 0.5_default) / mci%n_bin(d)
        if (d > 1) then
            call sample_dim (d - 1)
        else
            if (signal_is_pending ()) return
            call instance%evaluate (sampler, 1, x)
            value = instance%get_value ()
            if (value > 0) then
                mci%n_calls_pos = mci%n_calls_pos + 1
                integral = integral + value
                integral_pos = integral_pos + value
            else if (value == 0) then
                mci%n_calls_nul = mci%n_calls_nul + 1
            else
                mci%n_calls_neg = mci%n_calls_neg + 1
                integral = integral + value
                integral_neg = integral_neg + value
            end if
        end if
    end do
end subroutine sample_dim
end subroutine mci_midpoint_integrate

```

Simulation initializer and finalizer: nothing to do here.

(MCI midpoint: mci midpoint: TBP)+≡

procedure :: prepare_simulation => mci_midpoint_ignore_prepare_simulation

(MCI midpoint: procedures)+≡

subroutine mci_midpoint_ignore_prepare_simulation (mci)

```

class(mci_midpoint_t), intent(inout) :: mci
end subroutine mci_midpoint_ignore_prepare_simulation

```

Generate weighted event.

```

<MCI midpoint: mci midpoint: TBP>+≡
  procedure :: generate_weighted_event => mci_midpoint_generate_weighted_event

<MCI midpoint: procedures>+≡
  subroutine mci_midpoint_generate_weighted_event (mci, instance, sampler)
    class(mci_midpoint_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    real(default), dimension(mci%n_dim) :: x
    select type (instance)
    type is (mci_midpoint_instance_t)
      call mci%rng%generate (x)
      call instance%evaluate (sampler, 1, x)
      instance%excess_weight = 0
    end select
  end subroutine mci_midpoint_generate_weighted_event

```

For unweighted events, we generate weighted events and apply a simple rejection step to the relative event weight, until an event passes.

Note that we use the `max_abs` value stored in the configuration record, not the one stored in the instance. The latter may change during event generation. After an event generation pass is over, we may update the value for a subsequent pass.

```

<MCI midpoint: mci midpoint: TBP>+≡
  procedure :: generate_unweighted_event => &
    mci_midpoint_generate_unweighted_event

<MCI midpoint: procedures>+≡
  subroutine mci_midpoint_generate_unweighted_event (mci, instance, sampler)
    class(mci_midpoint_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    real(default) :: x, norm, int
    select type (instance)
    type is (mci_midpoint_instance_t)
      if (mci%max_known .and. mci%max_abs > 0) then
        norm = abs (mci%max_abs * instance%safety_factor)
        REJECTION: do
          call mci%generate_weighted_event (instance, sampler)
          if (sampler%is_valid ()) then
            call mci%rng%generate (x)
            int = abs (instance%integrand)
            if (x * norm <= int) then
              if (norm > 0 .and. norm < int) then
                instance%excess_weight = int / norm - 1
              end if
              exit REJECTION
            end if
          end if
        end if
      end if
    end select
  end subroutine mci_midpoint_generate_unweighted_event

```

```

        if (signal_is_pending ()) return
    end do REJECTION
else
    call msg_fatal ("Unweighted event generation: &
        &maximum of integrand is zero or unknown")
    end if
end select
end subroutine mci_midpoint_generate_unweighted_event

```

Rebuild an event, using the state input.

```

<MCI midpoint: mci midpoint: TBP>+≡
    procedure :: rebuild_event => mci_midpoint_rebuild_event

<MCI midpoint: procedures>+≡
    subroutine mci_midpoint_rebuild_event (mci, instance, sampler, state)
        class(mci_midpoint_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout) :: instance
        class(mci_sampler_t), intent(inout) :: sampler
        class(mci_state_t), intent(in) :: state
        select type (instance)
        type is (mci_midpoint_instance_t)
            call instance%recall (sampler, state)
        end select
    end subroutine mci_midpoint_rebuild_event

```

21.5.2 Integrator instance

Covering the case of flat dimensions, we store a complete x array. This is filled when generating events.

```

<MCI midpoint: public>+≡
    public :: mci_midpoint_instance_t

<MCI midpoint: types>+≡
    type, extends (mci_instance_t) :: mci_midpoint_instance_t
        type(mci_midpoint_t), pointer :: mci => null ()
        logical :: max_known = .false.
        real(default) :: max = 0
        real(default) :: min = 0
        real(default) :: max_abs = 0
        real(default) :: min_abs = 0
        real(default) :: safety_factor = 1
        real(default) :: excess_weight = 0
    contains
        <MCI midpoint: mci midpoint instance: TBP>
    end type mci_midpoint_instance_t

```

Output.

```

<MCI midpoint: mci midpoint instance: TBP>≡
    procedure :: write => mci_midpoint_instance_write

```

```

<MCI midpoint: procedures>+≡
subroutine mci_midpoint_instance_write (object, unit, pacify)
  class(mci_midpoint_instance_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A,9(1x,F12.10))") "x =", object%x(:,1)
  write (u, "(1x,A,ES19.12)") "Integrand = ", object%integrand
  write (u, "(1x,A,ES19.12)") "Weight    = ", object%mci_weight
  if (object%safety_factor /= 1) then
    write (u, "(1x,A,ES19.12)") "Safety f  = ", object%safety_factor
  end if
  if (object%excess_weight /= 0) then
    write (u, "(1x,A,ES19.12)") "Excess    = ", object%excess_weight
  end if
  if (object%max_known) then
    write (u, "(1x,A,ES19.12)") "Maximum   = ", object%max
    write (u, "(1x,A,ES19.12)") "Minimum   = ", object%min
    if (object%min /= object%min_abs) then
      write (u, "(1x,A,ES19.12)") "Max.(abs) = ", object%max_abs
      write (u, "(1x,A,ES19.12)") "Min.(abs) = ", object%min_abs
    end if
  end if
end subroutine mci_midpoint_instance_write

```

The finalizer is empty.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
procedure :: final => mci_midpoint_instance_final

<MCI midpoint: procedures>+≡
subroutine mci_midpoint_instance_final (object)
  class(mci_midpoint_instance_t), intent(inout) :: object
end subroutine mci_midpoint_instance_final

```

Initializer.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
procedure :: init => mci_midpoint_instance_init

<MCI midpoint: procedures>+≡
subroutine mci_midpoint_instance_init (mci_instance, mci)
  class(mci_midpoint_instance_t), intent(out) :: mci_instance
  class(mci_t), intent(in), target :: mci
  call mci_instance%base_init (mci)
  select type (mci)
  type is (mci_midpoint_t)
    mci_instance%mci => mci
    call mci_instance%get_max ()
    mci_instance%selected_channel = 1
  end select
end subroutine mci_midpoint_instance_init

```


Copy the stored extrema of the integrand in the instance record.

```

(MCI midpoint: mci midpoint instance: TBP)+≡
  procedure :: get_max => mci_midpoint_instance_get_max
(MCI midpoint: procedures)+≡
  subroutine mci_midpoint_instance_get_max (instance)
    class(mci_midpoint_instance_t), intent(inout) :: instance
    associate (mci => instance%mci)
      if (mci%max_known) then
        instance%max_known = .true.
        instance%max = mci%max
        instance%min = mci%min
        instance%max_abs = mci%max_abs
        instance%min_abs = mci%min_abs
      end if
    end associate
  end subroutine mci_midpoint_instance_get_max

```

Reverse operations: recall the extrema, but only if they are wider than the extrema already stored in the configuration. Also recalculate the efficiency value.

```

(MCI midpoint: mci midpoint instance: TBP)+≡
  procedure :: set_max => mci_midpoint_instance_set_max
(MCI midpoint: procedures)+≡
  subroutine mci_midpoint_instance_set_max (instance)
    class(mci_midpoint_instance_t), intent(inout) :: instance
    associate (mci => instance%mci)
      if (instance%max_known) then
        if (mci%max_known) then
          mci%max = max (mci%max, instance%max)
          mci%min = min (mci%min, instance%min)
          mci%max_abs = max (mci%max_abs, instance%max_abs)
          mci%min_abs = min (mci%min_abs, instance%min_abs)
        else
          mci%max = instance%max
          mci%min = instance%min
          mci%max_abs = instance%max_abs
          mci%min_abs = instance%min_abs
          mci%max_known = .true.
        end if
      end if
      if (mci%max_abs /= 0) then
        if (mci%integral_neg == 0) then
          mci%efficiency = mci%integral / mci%max_abs
          mci%efficiency_known = .true.
        else if (mci%n_calls /= 0) then
          mci%efficiency = &
            (mci%integral_pos - mci%integral_neg) / mci%max_abs
          mci%efficiency_known = .true.
        end if
      end if
    end associate
  end subroutine mci_midpoint_instance_set_max

```

The weight is the Jacobian of the mapping for the only channel.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
  procedure :: compute_weight => mci_midpoint_instance_compute_weight

<MCI midpoint: procedures>+≡
  subroutine mci_midpoint_instance_compute_weight (mci, c)
    class(mci_midpoint_instance_t), intent(inout) :: mci
    integer, intent(in) :: c
    select case (c)
    case (1)
      mci%mci_weight = mci%f(1)
    case default
      call msg_fatal ("MCI midpoint integrator: only single channel supported")
    end select
  end subroutine mci_midpoint_instance_compute_weight

```

Record the integrand. Update stored values for maximum and minimum.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
  procedure :: record_integrand => mci_midpoint_instance_record_integrand

<MCI midpoint: procedures>+≡
  subroutine mci_midpoint_instance_record_integrand (mci, integrand)
    class(mci_midpoint_instance_t), intent(inout) :: mci
    real(default), intent(in) :: integrand
    mci%integrand = integrand
    if (mci%max_known) then
      mci%max = max (mci%max, integrand)
      mci%min = min (mci%min, integrand)
      mci%max_abs = max (mci%max_abs, abs (integrand))
      mci%min_abs = min (mci%min_abs, abs (integrand))
    else
      mci%max = integrand
      mci%min = integrand
      mci%max_abs = abs (integrand)
      mci%min_abs = abs (integrand)
      mci%max_known = .true.
    end if
  end subroutine mci_midpoint_instance_record_integrand

```

We store the safety factor, otherwise nothing to do here.

```

<MCI midpoint: mci midpoint instance: TBP>+≡
  procedure :: init_simulation => mci_midpoint_instance_init_simulation
  procedure :: final_simulation => mci_midpoint_instance_final_simulation

<MCI midpoint: procedures>+≡
  subroutine mci_midpoint_instance_init_simulation (instance, safety_factor)
    class(mci_midpoint_instance_t), intent(inout) :: instance
    real(default), intent(in), optional :: safety_factor
    if (present (safety_factor)) instance%safety_factor = safety_factor
  end subroutine mci_midpoint_instance_init_simulation

  subroutine mci_midpoint_instance_final_simulation (instance)
    class(mci_midpoint_instance_t), intent(inout) :: instance
  end subroutine mci_midpoint_instance_final_simulation

```

Return excess weight for the current event.

```
<MCI midpoint: mci midpoint instance: TBP>+≡
    procedure :: get_event_excess => mci_midpoint_instance_get_event_excess

<MCI midpoint: procedures>+≡
    function mci_midpoint_instance_get_event_excess (mci) result (excess)
        class(mci_midpoint_instance_t), intent(in) :: mci
        real(default) :: excess
        excess = mci%excess_weight
    end function mci_midpoint_instance_get_event_excess
```

21.5.3 Unit tests

Test module, followed by the corresponding implementation module.

```
<mci_midpoint.ut.f90>≡
    <File header>

    module mci_midpoint_ut
        use unit_tests
        use mci_midpoint_uti

    <Standard module head>

    <MCI midpoint: public test>

    contains

    <MCI midpoint: test driver>

    end module mci_midpoint_ut

<mci_midpoint.uti.f90>≡
    <File header>

    module mci_midpoint_uti

    <Use kinds>
        use io_units
        use rng_base
        use mci_base

        use mci_midpoint

        use rng_base_ut, only: rng_test_t

    <Standard module head>

    <MCI midpoint: test declarations>

    <MCI midpoint: test types>

    contains
```

<MCI midpoint: tests>

end module mci_midpoint_util

API: driver for the unit tests below.

<MCI midpoint: public test>≡

public :: mci_midpoint_test

<MCI midpoint: test driver>≡

subroutine mci_midpoint_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<MCI midpoint: execute tests>

end subroutine mci_midpoint_test

Test sampler

A test sampler object should implement a function with known integral that we can use to check the integrator.

This is the function $f(x) = 3x^2$ with integral $\int_0^1 f(x) dx = 1$ and maximum $f(1) = 3$. If the integration dimension is greater than one, the function is extended as a constant in the other dimension(s).

Mimicking the behavior of a process object, we store the argument and result inside the sampler, so we can fetch results.

<MCI midpoint: test types>≡

type, extends (mci_sampler_t) :: test_sampler_1_t

real(default), dimension(:), allocatable :: x

real(default) :: val

contains

<MCI midpoint: test sampler 1: TBP>

end type test_sampler_1_t

Output: There is nothing stored inside, so just print an informative line.

<MCI midpoint: test sampler 1: TBP>≡

procedure :: write => test_sampler_1_write

<MCI midpoint: tests>≡

subroutine test_sampler_1_write (object, unit, testflag)

class(test_sampler_1_t), intent(in) :: object

integer, intent(in), optional :: unit

logical, intent(in), optional :: testflag

integer :: u

u = given_output_unit (unit)

write (u, "(1x,A)") "Test sampler: f(x) = 3 x^2"

end subroutine test_sampler_1_write

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

<MCI midpoint: test sampler 1: TBP>+≡

procedure :: evaluate => test_sampler_1_evaluate

```

<MCI midpoint: tests>+≡
  subroutine test_sampler_1_evaluate (sampler, c, x_in, val, x, f)
    class(test_sampler_1_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    if (allocated (sampler%x)) deallocate (sampler%x)
    allocate (sampler%x (size (x_in)))
    sampler%x = x_in
    sampler%val = 3 * x_in(1) ** 2
    call sampler%fetch (val, x, f)
  end subroutine test_sampler_1_evaluate

```

The point is always valid.

```

<MCI midpoint: test sampler 1: TBP>+≡
  procedure :: is_valid => test_sampler_1_is_valid

<MCI midpoint: tests>+≡
  function test_sampler_1_is_valid (sampler) result (valid)
    class(test_sampler_1_t), intent(in) :: sampler
    logical :: valid
    valid = .true.
  end function test_sampler_1_is_valid

```

Rebuild: compute all but the function value.

```

<MCI midpoint: test sampler 1: TBP>+≡
  procedure :: rebuild => test_sampler_1_rebuild

<MCI midpoint: tests>+≡
  subroutine test_sampler_1_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_1_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    if (allocated (sampler%x)) deallocate (sampler%x)
    allocate (sampler%x (size (x_in)))
    sampler%x = x_in
    sampler%val = val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_1_rebuild

```

Extract the results.

```

<MCI midpoint: test sampler 1: TBP>+≡
  procedure :: fetch => test_sampler_1_fetch

<MCI midpoint: tests>+≡
  subroutine test_sampler_1_fetch (sampler, val, x, f)
    class(test_sampler_1_t), intent(in) :: sampler
    real(default), intent(out) :: val

```

```

    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x(:,1) = sampler%x
    f = 1
end subroutine test_sampler_1_fetch

```

This is the function $f(x) = 3x^2 + 2y$ with integral $\int_0^1 f(x,y) dx dy = 2$ and maximum $f(1) = 5$.

```

⟨MCI midpoint: test types⟩+≡
  type, extends (mci_sampler_t) :: test_sampler_2_t
    real(default) :: val
    real(default), dimension(2) :: x
  contains
    ⟨MCI midpoint: test sampler 2: TBP⟩
  end type test_sampler_2_t

```

Output: There is nothing stored inside, so just print an informative line.

```

⟨MCI midpoint: test sampler 2: TBP⟩≡
  procedure :: write => test_sampler_2_write

⟨MCI midpoint: tests⟩+≡
  subroutine test_sampler_2_write (object, unit, testflag)
    class(test_sampler_2_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Test sampler: f(x) = 3 x^2 + 2 y"
  end subroutine test_sampler_2_write

```

Evaluate: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

⟨MCI midpoint: test sampler 2: TBP⟩+≡
  procedure :: evaluate => test_sampler_2_evaluate

⟨MCI midpoint: tests⟩+≡
  subroutine test_sampler_2_evaluate (sampler, c, x_in, val, x, f)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    sampler%x = x_in
    sampler%val = 3 * x_in(1) ** 2 + 2 * x_in(2)
    call sampler%fetch (val, x, f)
  end subroutine test_sampler_2_evaluate

```

The point is always valid.

```

⟨MCI midpoint: test sampler 2: TBP⟩+≡
  procedure :: is_valid => test_sampler_2_is_valid

```

```

⟨MCI midpoint: tests⟩+≡
  function test_sampler_2_is_valid (sampler) result (valid)
    class(test_sampler_2_t), intent(in) :: sampler
    logical :: valid
    valid = .true.
  end function test_sampler_2_is_valid

```

Rebuild: compute all but the function value.

```

⟨MCI midpoint: test sampler 2: TBP⟩+≡
  procedure :: rebuild => test_sampler_2_rebuild

⟨MCI midpoint: tests⟩+≡
  subroutine test_sampler_2_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    sampler%x = x_in
    sampler%val = val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_2_rebuild

```

```

⟨MCI midpoint: test sampler 2: TBP⟩+≡
  procedure :: fetch => test_sampler_2_fetch

```

```

⟨MCI midpoint: tests⟩+≡
  subroutine test_sampler_2_fetch (sampler, val, x, f)
    class(test_sampler_2_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_2_fetch

```

This is the function $f(x) = (1 - 3x^2)\theta(x - 1/2)$ with integral $\int_0^1 f(x) dx = -3/8$, minimum $f(1) = -2$ and maximum $f(1/2) = 1/4$. If the integration dimension is greater than one, the function is extended as a constant in the other dimension(s).

```

⟨MCI midpoint: test types⟩+≡
  type, extends (mci_sampler_t) :: test_sampler_4_t
    real(default) :: val
    real(default), dimension(:), allocatable :: x
  contains
    ⟨MCI midpoint: test sampler 4: TBP⟩
  end type test_sampler_4_t

```

Output: There is nothing stored inside, so just print an informative line.

```

<MCI midpoint: test sampler 4: TBP>≡
  procedure :: write => test_sampler_4_write

<MCI midpoint: tests>+≡
  subroutine test_sampler_4_write (object, unit, testflag)
    class(test_sampler_4_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Test sampler: f(x) = 1 - 3 x^2"
  end subroutine test_sampler_4_write

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

<MCI midpoint: test sampler 4: TBP>+≡
  procedure :: evaluate => test_sampler_4_evaluate

<MCI midpoint: tests>+≡
  subroutine test_sampler_4_evaluate (sampler, c, x_in, val, x, f)
    class(test_sampler_4_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    if (x_in(1) >= .5_default) then
      sampler%val = 1 - 3 * x_in(1) ** 2
    else
      sampler%val = 0
    end if
    if (.not. allocated (sampler%x)) allocate (sampler%x (size (x_in)))
    sampler%x = x_in
    call sampler%fetch (val, x, f)
  end subroutine test_sampler_4_evaluate

```

The point is always valid.

```

<MCI midpoint: test sampler 4: TBP>+≡
  procedure :: is_valid => test_sampler_4_is_valid

<MCI midpoint: tests>+≡
  function test_sampler_4_is_valid (sampler) result (valid)
    class(test_sampler_4_t), intent(in) :: sampler
    logical :: valid
    valid = .true.
  end function test_sampler_4_is_valid

```

Rebuild: compute all but the function value.

```

<MCI midpoint: test sampler 4: TBP>+≡
  procedure :: rebuild => test_sampler_4_rebuild

```



```

<MCI midpoint: tests>+≡
  subroutine test_sampler_4_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_4_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    sampler%x = x_in
    sampler%val = val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_4_rebuild

```

```

<MCI midpoint: test sampler 4: TBP>+≡
  procedure :: fetch => test_sampler_4_fetch

```

```

<MCI midpoint: tests>+≡
  subroutine test_sampler_4_fetch (sampler, val, x, f)
    class(test_sampler_4_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_4_fetch

```

One-dimensional integration

Construct an integrator and use it for a one-dimensional sampler.

```

<MCI midpoint: execute tests>≡
  call test (mci_midpoint_1, "mci_midpoint_1", &
    "one-dimensional integral", &
    u, results)

<MCI midpoint: test declarations>≡
  public :: mci_midpoint_1

<MCI midpoint: tests>+≡
  subroutine mci_midpoint_1 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

    write (u, "(A)")  "* Test output: mci_midpoint_1"
    write (u, "(A)")  "* Purpose: integrate function in one dimension"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_midpoint_t :: mci)

```

```

call mci%set_dimensions (1, 1)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_1_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.8"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.8_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.7"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.7_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.9"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.9_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_1"

end subroutine mci_midpoint_1

```

Two-dimensional integration

Construct an integrator and use it for a two-dimensional sampler.

```
<MCI midpoint: execute tests>+≡
    call test (mci_midpoint_2, "mci_midpoint_2", &
               "two-dimensional integral", &
               u, results)

<MCI midpoint: test declarations>+≡
    public :: mci_midpoint_2

<MCI midpoint: tests>+≡
    subroutine mci_midpoint_2 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler

        write (u, "(A)")  "* Test output: mci_midpoint_2"
        write (u, "(A)")  "* Purpose: integrate function in two dimensions"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator"
        write (u, "(A)")

        allocate (mci_midpoint_t :: mci)
        call mci%set_dimensions (2, 1)

        call mci%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Initialize instance"
        write (u, "(A)")

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        write (u, "(A)")  "* Initialize test sampler"
        write (u, "(A)")

        allocate (test_sampler_2_t :: sampler)
        call sampler%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Evaluate for x = 0.8, y = 0.2"
        write (u, "(A)")

        call mci_instance%evaluate (sampler, 1, [0.8_default, 0.2_default])
        call mci_instance%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Integrate with n_calls = 1000"
        write (u, "(A)")

        call mci%integrate (mci_instance, sampler, 1, 1000)
```

```

call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_2"

end subroutine mci_midpoint_2

```

Two-dimensional integration with flat dimension

Construct an integrator and use it for a two-dimensional sampler, where the function is constant in the second dimension.

```

<MCI midpoint: execute tests>+≡
call test (mci_midpoint_3, "mci_midpoint_3", &
  "two-dimensional integral with flat dimension", &
  u, results)

<MCI midpoint: test declarations>+≡
public :: mci_midpoint_3

<MCI midpoint: tests>+≡
subroutine mci_midpoint_3 (u)
  integer, intent(in) :: u
  class(mci_t), allocatable, target :: mci
  class(mci_instance_t), pointer :: mci_instance => null ()
  class(mci_sampler_t), allocatable :: sampler

  write (u, "(A)")  "* Test output: mci_midpoint_3"
  write (u, "(A)")  "* Purpose: integrate function with one flat dimension"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize integrator"
  write (u, "(A)")

  allocate (mci_midpoint_t :: mci)
  select type (mci)
  type is (mci_midpoint_t)
    call mci%set_dimensions (2, 1)
    call mci%declare_flat_dimensions ([2])
  end select

  call mci%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Initialize instance"
  write (u, "(A)")

  call mci%allocate_instance (mci_instance)
  call mci_instance%init (mci)

  write (u, "(A)")  "* Initialize test sampler"

```

```

write (u, "(A)")

allocate (test_sampler_1_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.8, y = 0.2"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.8_default, 0.2_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_3"

end subroutine mci_midpoint_3

```

Integrand with sign flip

Construct an integrator and use it for a one-dimensional sampler.

```

<MCI midpoint: execute tests>+≡
  call test (mci_midpoint_4, "mci_midpoint_4", &
    "integrand with sign flip", &
    u, results)

<MCI midpoint: test declarations>+≡
  public :: mci_midpoint_4

<MCI midpoint: tests>+≡
  subroutine mci_midpoint_4 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler

    write (u, "(A)")  "* Test output: mci_midpoint_4"
    write (u, "(A)")  "* Purpose: integrate function with sign flip &
      &in one dimension"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize integrator"
    write (u, "(A)")

    allocate (mci_midpoint_t :: mci)

```

```

call mci%set_dimensions (1, 1)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_4_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for x = 0.8"
write (u, "(A)")

call mci_instance%evaluate (sampler, 1, [0.8_default])
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")

call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_4"

end subroutine mci_midpoint_4

```

Weighted events

Generate weighted events. Without rejection, we do not need to know maxima and minima, so we can start generating events immediately. We have two dimensions.

```

<MCI midpoint: execute tests>+≡
  call test (mci_midpoint_5, "mci_midpoint_5", &
    "weighted events", &
    u, results)

<MCI midpoint: test declarations>+≡
  public :: mci_midpoint_5

```

```

<MCI midpoint: tests>+≡
subroutine mci_midpoint_5 (u)
  integer, intent(in) :: u
  class(mci_t), allocatable, target :: mci
  class(mci_instance_t), pointer :: mci_instance => null ()
  class(mci_sampler_t), allocatable :: sampler
  class(rng_t), allocatable :: rng
  class(mci_state_t), allocatable :: state

  write (u, "(A)")  "* Test output: mci_midpoint_5"
  write (u, "(A)")  "* Purpose: generate weighted events"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize integrator"
  write (u, "(A)")

  allocate (mci_midpoint_t :: mci)
  call mci%set_dimensions (2, 1)

  call mci%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Initialize instance"
  write (u, "(A)")

  call mci%allocate_instance (mci_instance)
  call mci_instance%init (mci)

  write (u, "(A)")  "* Initialize test sampler"
  write (u, "(A)")

  allocate (test_sampler_2_t :: sampler)

  write (u, "(A)")  "* Initialize random-number generator"
  write (u, "(A)")

  allocate (rng_test_t :: rng)
  call rng%init ()
  call mci%import_rng (rng)

  write (u, "(A)")  "* Generate weighted event"
  write (u, "(A)")

  call mci%generate_weighted_event (mci_instance, sampler)
  call mci_instance%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Generate weighted event"
  write (u, "(A)")

  call mci%generate_weighted_event (mci_instance, sampler)
  call mci_instance%write (u)

  write (u, "(A)")

```

```

write (u, "(A)")  "* Store data"
write (u, "(A)")

allocate (state)
call mci_instance%store (state)
call mci_instance%final ()
deallocate (mci_instance)

call state%write (u)

write (u, "(A)")
write (u, "(A)")  "* Recall data and rebuild event"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)
call mci%rebuild_event (mci_instance, sampler, state)

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
deallocate (mci_instance)
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_5"

end subroutine mci_midpoint_5

```

Unweighted events

Generate unweighted events. The integrand has a sign flip in it.

```

<MCI midpoint: execute tests>+≡
  call test (mci_midpoint_6, "mci_midpoint_6", &
    "unweighted events", &
    u, results)

<MCI midpoint: test declarations>+≡
  public :: mci_midpoint_6

<MCI midpoint: tests>+≡
  subroutine mci_midpoint_6 (u)
    integer, intent(in) :: u
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_midpoint_6"
    write (u, "(A)")  "* Purpose: generate unweighted events"
    write (u, "(A)")

```



```

write (u, "(A)")  "* Initialize integrator"
write (u, "(A)")

allocate (mci_midpoint_t :: mci)
call mci%set_dimensions (1, 1)

write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_4_t :: sampler)

write (u, "(A)")  "* Initialize random-number generator"
write (u, "(A)")

allocate (rng_test_t :: rng)
call rng%init ()
call mci%import_rng (rng)

write (u, "(A)")  "* Integrate (determine maximum of integrand"
write (u, "(A)")
call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate unweighted event"
write (u, "(A)")

call mci%generate_unweighted_event (mci_instance, sampler)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
deallocate (mci_instance)
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_6"

end subroutine mci_midpoint_6

```

Excess weight

Generate unweighted events. With only 2 points for integration, the maximum of the integrand is too low, and we produce excess weight.

```

<MCI midpoint: execute tests>+≡
    call test (mci_midpoint_7, "mci_midpoint_7", &
        "excess weight", &
        u, results)

<MCI midpoint: test declarations>+≡
    public :: mci_midpoint_7

<MCI midpoint: tests>+≡
    subroutine mci_midpoint_7 (u)
        integer, intent(in) :: u
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng

        write (u, "(A)")  "* Test output: mci_midpoint_7"
        write (u, "(A)")  "* Purpose: generate unweighted event &
            &with excess weight"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize integrator"
        write (u, "(A)")

        allocate (mci_midpoint_t :: mci)
        call mci%set_dimensions (1, 1)

        write (u, "(A)")  "* Initialize instance"
        write (u, "(A)")

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        write (u, "(A)")  "* Initialize test sampler"
        write (u, "(A)")

        allocate (test_sampler_4_t :: sampler)

        write (u, "(A)")  "* Initialize random-number generator"
        write (u, "(A)")

        allocate (rng_test_t :: rng)
        call rng%init ()
        call mci%import_rng (rng)

        write (u, "(A)")  "* Integrate (determine maximum of integrand"
        write (u, "(A)")
        call mci%integrate (mci_instance, sampler, 1, 2)
        call mci%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Generate unweighted event"
        write (u, "(A)")

        call mci_instance%init_simulation ()

```

```

call mci%generate_unweighted_event (mci_instance, sampler)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Use getter methods"
write (u, "(A)")

write (u, "(1x,A,1x,ES19.12)")  "weight =", mci_instance%get_event_weight ()
write (u, "(1x,A,1x,ES19.12)")  "excess =", mci_instance%get_event_excess ()

write (u, "(A)")
write (u, "(A)")  "* Apply safety factor"
write (u, "(A)")

call mci_instance%init_simulation (safety_factor = 2.1_default)

write (u, "(A)")  "* Generate unweighted event"
write (u, "(A)")

call mci%generate_unweighted_event (mci_instance, sampler)
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Use getter methods"
write (u, "(A)")

write (u, "(1x,A,1x,ES19.12)")  "weight =", mci_instance%get_event_weight ()
write (u, "(1x,A,1x,ES19.12)")  "excess =", mci_instance%get_event_excess ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
deallocate (mci_instance)
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_midpoint_7"

end subroutine mci_midpoint_7

```

21.6 VAMP interface

The standard method for integration is **VAMP**: the multi-channel version of the VEGAS algorithm. Each parameterization (channel) of the hypercube is binned in each dimension. The binning is equally equidistant, but an iteration of the integration procedure, the binning is updated for each dimension, according to the variance distribution of the integrand, summed over all other dimension. In the next iteration, the binning approximates (hopefully) follows the integrand more closely, and the accuracy of the result is increased. Furthermore, the relative weight of the individual channels is also updated after an iteration.

The bin distribution is denoted as the grid for a channel, which we can write to file and reuse later.

In our implementation we specify the generic **VAMP** algorithm more tightly: the number of bins is equal for all dimensions, the initial weights are all equal. The user controls whether to update bins and/or weights after each iteration. The integration is organized in passes, each one consisting of several iterations with a common number of calls to the integrand. The first passes are intended as warmup, so the results are displayed but otherwise discarded. In the final pass, the integration estimates for the individual iterations are averaged for the final result.

```
<mci_vamp.f90>≡  
  <File header>  
  
  module mci_vamp  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use constants, only: zero  
    use format_utils, only: pac_fmt  
    use format_utils, only: write_separator  
    use format_defs, only: FMT_12, FMT_14, FMT_17, FMT_19  
    use diagnostics  
    use md5  
    use phs_base  
    use rng_base  
    use rng_tao  
    use vamp !NODEP!  
    use exceptions !NODEP!  
  
    use mci_base  
  
    <Standard module head>  
  
    <MCI vamp: public>  
  
    <MCI vamp: types>  
  
    <MCI vamp: interfaces>  
  
  contains
```

```
⟨MCI vamp: procedures⟩
```

```
end module mci_vamp
```

21.6.1 Grid parameters

This is a transparent container. It holds the parameters that are stored in grid files, and are checked when grid files are read.

```
⟨MCI vamp: public⟩≡
```

```
public :: grid_parameters_t
```

```
⟨MCI vamp: types⟩≡
```

```
type :: grid_parameters_t
```

```
integer :: threshold_calls = 0
```

```
integer :: min_calls_per_channel = 10
```

```
integer :: min_calls_per_bin = 10
```

```
integer :: min_bins = 3
```

```
integer :: max_bins = 20
```

```
logical :: stratified = .true.
```

```
logical :: use_vamp_equivalences = .true.
```

```
real(default) :: channel_weights_power = 0.25_default
```

```
real(default) :: accuracy_goal = 0
```

```
real(default) :: error_goal = 0
```

```
real(default) :: rel_error_goal = 0
```

```
contains
```

```
⟨MCI vamp: grid parameters: TBP⟩
```

```
end type grid_parameters_t
```

I/O:

```
⟨MCI vamp: grid parameters: TBP⟩≡
```

```
procedure :: write => grid_parameters_write
```

```
⟨MCI vamp: procedures⟩≡
```

```
subroutine grid_parameters_write (object, unit)
```

```
class(grid_parameters_t), intent(in) :: object
```

```
integer, intent(in), optional :: unit
```

```
integer :: u
```

```
u = given_output_unit (unit)
```

```
write (u, "(3x,A,I0)") "threshold_calls      = ", &  
      object%threshold_calls
```

```
write (u, "(3x,A,I0)") "min_calls_per_channel = ", &  
      object%min_calls_per_channel
```

```
write (u, "(3x,A,I0)") "min_calls_per_bin      = ", &  
      object%min_calls_per_bin
```

```
write (u, "(3x,A,I0)") "min_bins              = ", &  
      object%min_bins
```

```
write (u, "(3x,A,I0)") "max_bins              = ", &  
      object%max_bins
```

```
write (u, "(3x,A,L1)") "stratified            = ", &  
      object%stratified
```

```
write (u, "(3x,A,L1)") "use_vamp_equivalences = ", &  
      object%use_vamp_equivalences
```

```
write (u, "(3x,A,F10.7)") "channel_weights_power = ", &  
      object%channel_weights_power
```

```

    if (object%accuracy_goal > 0) then
        write (u, "(3x,A,F10.7)" "accuracy_goal" = ", &
            object%accuracy_goal
    end if
    if (object%error_goal > 0) then
        write (u, "(3x,A,F10.7)" "error_goal" = ", &
            object%error_goal
    end if
    if (object%rel_error_goal > 0) then
        write (u, "(3x,A,F10.7)" "rel_error_goal" = ", &
            object%rel_error_goal
    end if
end subroutine grid_parameters_write

```

21.6.2 History parameters

The history parameters are also stored in a transparent container. This is not a part of the grid definition, and should not be included in the MD5 sum.

```

<MCI vamp: public>+≡
    public :: history_parameters_t

<MCI vamp: types>+≡
    type :: history_parameters_t
        logical :: global = .true.
        logical :: global_verbose = .false.
        logical :: channel = .false.
        logical :: channel_verbose = .false.
    contains
        <MCI vamp: history parameters: TBP>
    end type history_parameters_t

```

I/O:

```

<MCI vamp: history parameters: TBP>≡
    procedure :: write => history_parameters_write

<MCI vamp: procedures>+≡
    subroutine history_parameters_write (object, unit)
        class(history_parameters_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(3x,A,L1)" "history(global)" = ", object%global
        write (u, "(3x,A,L1)" "history(global) verb." = ", object%global_verbose
        write (u, "(3x,A,L1)" "history(channels)" = ", object%channel
        write (u, "(3x,A,L1)" "history(chann.) verb." = ", object%channel_verbose
    end subroutine history_parameters_write

```

21.6.3 Integration pass

We store the parameters for each integration pass in a linked list.

```

<MCI vamp: types>+≡

```

```

type :: pass_t
  integer :: i_pass = 0
  integer :: i_first_it = 0
  integer :: n_it = 0
  integer :: n_calls = 0
  integer :: n_bins = 0
  logical :: adapt_grids = .false.
  logical :: adapt_weights = .false.
  logical :: is_final_pass = .false.
  logical :: integral_defined = .false.
  integer, dimension(:), allocatable :: calls
  integer, dimension(:), allocatable :: calls_valid
  real(default), dimension(:), allocatable :: integral
  real(default), dimension(:), allocatable :: error
  real(default), dimension(:), allocatable :: efficiency
  type(vamp_history), dimension(:), allocatable :: v_history
  type(vamp_history), dimension(:, :), allocatable :: v_histories
  type(pass_t), pointer :: next => null ()
contains
  <MCI vamp: pass: TBP>
end type pass_t

```

Finalizer. The VAMP histories contain a pointer array.

```

<MCI vamp: pass: TBP>≡
  procedure :: final => pass_final

<MCI vamp: procedures>+≡
  subroutine pass_final (object)
    class(pass_t), intent(inout) :: object
    if (allocated (object%v_history)) then
      call vamp_delete_history (object%v_history)
    end if
    if (allocated (object%v_histories)) then
      call vamp_delete_history (object%v_histories)
    end if
  end subroutine pass_final

```

Output. Note that the precision of the numerical values should match the precision for comparing output from file with data.

```

<MCI vamp: pass: TBP>+≡
  procedure :: write => pass_write

<MCI vamp: procedures>+≡
  subroutine pass_write (object, unit, pacify)
    class(pass_t), intent(in) :: object
    integer, intent(in) :: unit
    logical, intent(in), optional :: pacify
    integer :: u, i
    character(len=7) :: fmt
    call pac_fmt (fmt, FMT_17, FMT_14, pacify)
    u = given_output_unit (unit)
    write (u, "(3x,A,I0)") "n_it" = ", object%n_it
    write (u, "(3x,A,I0)") "n_calls" = ", object%n_calls
    write (u, "(3x,A,I0)") "n_bins" = ", object%n_bins

```

```

write (u, "(3x,A,L1)") "adapt grids  = ", object%adapt_grids
write (u, "(3x,A,L1)") "adapt weights = ", object%adapt_weights
if (object%integral_defined) then
  write (u, "(3x,A)") "Results: [it, calls, valid, integral, error, efficiency]"
  do i = 1, object%n_it
    write (u, "(5x,I0,2(1x,I0),3(1x," // fmt // "))" &
      i, object%calls(i), object%calls_valid(i), object%integral(i), object%error(i), &
      object%efficiency(i)
  end do
else
  write (u, "(3x,A)") "Results: [undefined]"
end if
end subroutine pass_write

```

Read and reconstruct the pass.

(MCI vamp: pass: TBP)+≡

```

procedure :: read => pass_read

```

(MCI vamp: procedures)+≡

```

subroutine pass_read (object, u, n_pass, n_it)
  class(pass_t), intent(out) :: object
  integer, intent(in) :: u, n_pass, n_it
  integer :: i, j
  character(80) :: buffer
  object%i_pass = n_pass + 1
  object%i_first_it = n_it + 1
  call read_ival (u, object%n_it)
  call read_ival (u, object%n_calls)
  call read_ival (u, object%n_bins)
  call read_lval (u, object%adapt_grids)
  call read_lval (u, object%adapt_weights)
  allocate (object%calls (object%n_it), source = 0)
  allocate (object%calls_valid (object%n_it), source = 0)
  allocate (object%integral (object%n_it), source = 0._default)
  allocate (object%error (object%n_it), source = 0._default)
  allocate (object%efficiency (object%n_it), source = 0._default)
  read (u, "(A)") buffer
  select case (trim (adjustl (buffer)))
  case ("Results: [it, calls, valid, integral, error, efficiency]")
    do i = 1, object%n_it
      read (u, *) &
        j, object%calls(i), object%calls_valid(i), object%integral(i), object%error(i), &
        object%efficiency(i)
    end do
    object%integral_defined = .true.
  case ("Results: [undefined]")
    object%integral_defined = .false.
  case default
    call msg_fatal ("Reading integration pass: corrupted file")
  end select
end subroutine pass_read

```

Write the VAMP history for this pass. (The subroutine writes the whole array

at once.)

```

(MCI vamp: pass: TBP)+≡
  procedure :: write_history => pass_write_history

(MCI vamp: procedures)+≡
  subroutine pass_write_history (pass, unit)
    class(pass_t), intent(in) :: pass
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    if (allocated (pass%v_history)) then
      call vamp_write_history (u, pass%v_history)
    else
      write (u, "(1x,A)") "Global history: [undefined]"
    end if
    if (allocated (pass%v_histories)) then
      write (u, "(1x,A)") "Channel histories:"
      call vamp_write_history (u, pass%v_histories)
    else
      write (u, "(1x,A)") "Channel histories: [undefined]"
    end if
  end subroutine pass_write_history

```

Given a number of calls and iterations, compute remaining data.

```

(MCI vamp: pass: TBP)+≡
  procedure :: configure => pass_configure

(MCI vamp: procedures)+≡
  subroutine pass_configure (pass, n_it, n_calls, min_calls, &
    min_bins, max_bins, min_channel_calls)
    class(pass_t), intent(inout) :: pass
    integer, intent(in) :: n_it, n_calls, min_channel_calls
    integer, intent(in) :: min_calls, min_bins, max_bins
    pass%n_it = n_it
    if (min_calls /= 0) then
      pass%n_bins = max (min_bins, &
        min (n_calls / min_calls, max_bins))
    else
      pass%n_bins = max_bins
    end if
    pass%n_calls = max(n_calls, max (min_calls, min_channel_calls))
    if (pass%n_calls /= n_calls) then
      write (msg_buffer, "(A,I0)") "VAMP: too few calls, resetting " &
        // "n_calls to ", pass%n_calls
      call msg_warning ()
    end if
    allocate (pass%calls (n_it), source = 0)
    allocate (pass%calls_valid (n_it), source = 0)
    allocate (pass%integral (n_it), source = 0._default)
    allocate (pass%error (n_it), source = 0._default)
    allocate (pass%efficiency (n_it), source = 0._default)
  end subroutine pass_configure

```

Allocate the VAMP history and give options. We assume that the `configure` routine above has been executed, so the number of iterations is known.

```

(MCI vamp: pass: TBP)+≡
  procedure :: configure_history => pass_configure_history

(MCI vamp: procedures)+≡
  subroutine pass_configure_history (pass, n_channels, par)
    class(pass_t), intent(inout) :: pass
    integer, intent(in) :: n_channels
    type(history_parameters_t), intent(in) :: par
    if (par%global) then
      allocate (pass%v_history (pass%n_it))
      call vamp_create_history (pass%v_history, &
        verbose = par%global_verbose)
    end if
    if (par%channel) then
      allocate (pass%v_histories (pass%n_it, n_channels))
      call vamp_create_history (pass%v_histories, &
        verbose = par%channel_verbose)
    end if
  end subroutine pass_configure_history

```

Given two pass objects, compare them. All parameters must match. Where integrations are done in both (number of calls nonzero), the results must be equal (up to numerical noise).

The allocated array sizes might be different, but should match up to the common `n_it` value.

```

(MCI vamp: interfaces)≡
  interface operator (.matches.)
    module procedure pass_matches
  end interface operator (.matches.)

(MCI vamp: procedures)+≡
  function pass_matches (pass, ref) result (ok)
    type(pass_t), intent(in) :: pass, ref
    integer :: n
    logical :: ok
    ok = .true.
    if (ok) ok = pass%i_pass == ref%i_pass
    if (ok) ok = pass%i_first_it == ref%i_first_it
    if (ok) ok = pass%n_it == ref%n_it
    if (ok) ok = pass%n_calls == ref%n_calls
    if (ok) ok = pass%n_bins == ref%n_bins
    if (ok) ok = pass%adapt_grids .eqv. ref%adapt_grids
    if (ok) ok = pass%adapt_weights .eqv. ref%adapt_weights
    if (ok) ok = pass%integral_defined .eqv. ref%integral_defined
    if (pass%integral_defined) then
      n = pass%n_it
      if (ok) ok = all (pass%calls(:n) == ref%calls(:n))
      if (ok) ok = all (pass%calls_valid(:n) == ref%calls_valid(:n))
      if (ok) ok = all (pass%integral(:n) .matches. ref%integral(:n))
      if (ok) ok = all (pass%error(:n) .matches. ref%error(:n))
      if (ok) ok = all (pass%efficiency(:n) .matches. ref%efficiency(:n))
    end if
  end function pass_matches

```

```
end function pass_matches
```

Update a pass object, given a reference. The parameters must match, except for the `n_it` entry. The number of complete iterations must be less or equal to the reference, and the number of complete iterations in the reference must be no larger than `n_it`. Where results are present in both passes, they must match. Where results are present in the reference only, the pass is updated accordingly.

(MCI vamp: pass: TBP)+≡

```
procedure :: update => pass_update
```

(MCI vamp: procedures)+≡

```
subroutine pass_update (pass, ref, ok)
  class(pass_t), intent(inout) :: pass
  type(pass_t), intent(in) :: ref
  logical, intent(out) :: ok
  integer :: n, n_ref
  ok = .true.
  if (ok) ok = pass%i_pass == ref%i_pass
  if (ok) ok = pass%i_first_it == ref%i_first_it
  if (ok) ok = pass%n_calls == ref%n_calls
  if (ok) ok = pass%n_bins == ref%n_bins
  if (ok) ok = pass%adapt_grids .eqv. ref%adapt_grids
  if (ok) ok = pass%adapt_weights .eqv. ref%adapt_weights
  if (ok) then
    if (ref%integral_defined) then
      if (.not. allocated (pass%calls)) then
        allocate (pass%calls (pass%n_it), source = 0)
        allocate (pass%calls_valid (pass%n_it), source = 0)
        allocate (pass%integral (pass%n_it), source = 0._default)
        allocate (pass%error (pass%n_it), source = 0._default)
        allocate (pass%efficiency (pass%n_it), source = 0._default)
      end if
      n = count (pass%calls /= 0)
      n_ref = count (ref%calls /= 0)
      ok = n <= n_ref .and. n_ref <= pass%n_it
      if (ok) ok = all (pass%calls(:n) == ref%calls(:n))
      if (ok) ok = all (pass%calls_valid(:n) == ref%calls_valid(:n))
      if (ok) ok = all (pass%integral(:n) .matches. ref%integral(:n))
      if (ok) ok = all (pass%error(:n) .matches. ref%error(:n))
      if (ok) ok = all (pass%efficiency(:n) .matches. ref%efficiency(:n))
      if (ok) then
        pass%calls(n+1:n_ref) = ref%calls(n+1:n_ref)
        pass%calls_valid(n+1:n_ref) = ref%calls_valid(n+1:n_ref)
        pass%integral(n+1:n_ref) = ref%integral(n+1:n_ref)
        pass%error(n+1:n_ref) = ref%error(n+1:n_ref)
        pass%efficiency(n+1:n_ref) = ref%efficiency(n+1:n_ref)
        pass%integral_defined = any (pass%calls /= 0)
      end if
    end if
  end if
end subroutine pass_update
```

Match two real numbers: they are equal up to a tolerance, which is 10^{-8} ,

matching the number of digits that are output by `pass_write`. In particular, if one number is exactly zero, the other one must also be zero.

```

(MCI vamp: interfaces)+≡
  interface operator (.matches.)
    module procedure real_matches
  end interface operator (.matches.)

(MCI vamp: procedures)+≡
  elemental function real_matches (x, y) result (ok)
    real(default), intent(in) :: x, y
    logical :: ok
    real(default), parameter :: tolerance = 1.e-8_default
    ok = abs (x - y) <= tolerance * max (abs (x), abs (y))
  end function real_matches

```

Return the index of the most recent complete integration. If there is none, return zero.

```

(MCI vamp: pass: TBP)+≡
  procedure :: get_integration_index => pass_get_integration_index

(MCI vamp: procedures)+≡
  function pass_get_integration_index (pass) result (n)
    class (pass_t), intent(in) :: pass
    integer :: n
    integer :: i
    n = 0
    if (allocated (pass%calls)) then
      do i = 1, pass%n_it
        if (pass%calls(i) == 0) exit
        n = i
      end do
    end if
  end function pass_get_integration_index

```

Return the most recent integral and error, if available.

```

(MCI vamp: pass: TBP)+≡
  procedure :: get_calls => pass_get_calls
  procedure :: get_calls_valid => pass_get_calls_valid
  procedure :: get_integral => pass_get_integral
  procedure :: get_error => pass_get_error
  procedure :: get_efficiency => pass_get_efficiency

(MCI vamp: procedures)+≡
  function pass_get_calls (pass) result (calls)
    class (pass_t), intent(in) :: pass
    integer :: calls
    integer :: n
    n = pass%get_integration_index ()
    if (n /= 0) then
      calls = pass%calls(n)
    else
      calls = 0
    end if
  end function pass_get_calls

```

```

function pass_get_calls_valid (pass) result (calls_valid)
  class(pass_t), intent(in) :: pass
  integer :: calls_valid
  integer :: n
  n = pass%get_integration_index ()
  if (n /= 0) then
    calls_valid = pass%calls_valid(n)
  else
    calls_valid = 0
  end if
end function pass_get_calls_valid

function pass_get_integral (pass) result (integral)
  class(pass_t), intent(in) :: pass
  real(default) :: integral
  integer :: n
  n = pass%get_integration_index ()
  if (n /= 0) then
    integral = pass%integral(n)
  else
    integral = 0
  end if
end function pass_get_integral

function pass_get_error (pass) result (error)
  class(pass_t), intent(in) :: pass
  real(default) :: error
  integer :: n
  n = pass%get_integration_index ()
  if (n /= 0) then
    error = pass%error(n)
  else
    error = 0
  end if
end function pass_get_error

function pass_get_efficiency (pass) result (efficiency)
  class(pass_t), intent(in) :: pass
  real(default) :: efficiency
  integer :: n
  n = pass%get_integration_index ()
  if (n /= 0) then
    efficiency = pass%efficiency(n)
  else
    efficiency = 0
  end if
end function pass_get_efficiency

```

21.6.4 Integrator

```

<MCI vamp: public>+≡
public :: mci_vamp_t

```

```

<MCI vamp: types>+≡
  type, extends (mci_t) :: mci_vamp_t
    logical, dimension(:), allocatable :: dim_is_flat
    type(grid_parameters_t) :: grid_par
    type(history_parameters_t) :: history_par
    integer :: min_calls = 0
    type(pass_t), pointer :: first_pass => null ()
    type(pass_t), pointer :: current_pass => null ()
    type(vamp_equivalences_t) :: equivalences
    logical :: rebuild = .true.
    logical :: check_grid_file = .true.
    logical :: grid_filename_set = .false.
    logical :: negative_weights = .false.
    logical :: verbose = .false.
    type(string_t) :: grid_filename
    character(32) :: md5sum_adapted = ""
  contains
    <MCI vamp: mci vamp: TBP>
  end type mci_vamp_t

```

Reset: delete integration-pass entries.

```

<MCI vamp: mci vamp: TBP>≡
  procedure :: reset => mci_vamp_reset

<MCI vamp: procedures>+≡
  subroutine mci_vamp_reset (object)
    class(mci_vamp_t), intent(inout) :: object
    type(pass_t), pointer :: current_pass
    do while (associated (object%first_pass))
      current_pass => object%first_pass
      object%first_pass => current_pass%next
      call current_pass%final ()
      deallocate (current_pass)
    end do
    object%current_pass => null ()
  end subroutine mci_vamp_reset

```

Finalizer: reset and finalize the equivalences list.

```

<MCI vamp: mci vamp: TBP>+≡
  procedure :: final => mci_vamp_final

<MCI vamp: procedures>+≡
  subroutine mci_vamp_final (object)
    class(mci_vamp_t), intent(inout) :: object
    call object%reset ()
    call vamp_equivalences_final (object%equivalences)
    call object%base_final ()
  end subroutine mci_vamp_final

```

Output. Do not output the grids themselves, this may result in tons of data.

```

<MCI vamp: mci vamp: TBP>+≡
  procedure :: write => mci_vamp_write

```

```

<MCI vamp: procedures>+=
subroutine mci_vamp_write (object, unit, pacify, md5sum_version)
  class(mci_vamp_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  logical, intent(in), optional :: md5sum_version
  type(pass_t), pointer :: current_pass
  integer :: u, i
  u = given_output_unit (unit)
  write (u, "(1x,A)") "VAMP integrator:"
  call object%base_write (u, pacify, md5sum_version)
  if (allocated (object%dim_is_flat)) then
    write (u, "(3x,A,999(1x,I0))") "Flat dimensions      =", &
      pack ([i, i = 1, object%n_dim], object%dim_is_flat)
  end if
  write (u, "(1x,A)") "Grid parameters:"
  call object%grid_par%write (u)
  write (u, "(3x,A,I0)") "min_calls              = ", object%min_calls
  write (u, "(3x,A,L1)") "negative weights          = ", &
    object%negative_weights
  write (u, "(3x,A,L1)") "verbose                  = ", &
    object%verbose
  if (object%grid_par%use_vamp_equivalences) then
    call vamp_equivalences_write (object%equivalences, u)
  end if
  current_pass => object%first_pass
  do while (associated (current_pass))
    write (u, "(1x,A,I0,A)") "Integration pass:"
    call current_pass%write (u, pacify)
    current_pass => current_pass%next
  end do
  if (object%md5sum_adapted /= "") then
    write (u, "(1x,A,A,A)") "MD5 sum (including results) = '", &
      object%md5sum_adapted, "'"
  end if
end subroutine mci_vamp_write

```

Write the history parameters.

```

<MCI vamp: mci vamp: TBP>+=
procedure :: write_history_parameters => mci_vamp_write_history_parameters

<MCI vamp: procedures>+=
subroutine mci_vamp_write_history_parameters (mci, unit)
  class(mci_vamp_t), intent(in) :: mci
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "VAMP history parameters:"
  call mci%history_par%write (unit)
end subroutine mci_vamp_write_history_parameters

```

Write the history, iterating over passes. We keep this separate from the generic write routine.

```

<MCI vamp: mci vamp: TBP>+=

```

```

        procedure :: write_history => mci_vamp_write_history
<MCI vamp: procedures>+=
subroutine mci_vamp_write_history (mci, unit)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in), optional :: unit
    type(pass_t), pointer :: current_pass
    integer :: i_pass
    integer :: u
    u = given_output_unit (unit)
    if (associated (mci%first_pass)) then
        write (u, "(1x,A)") "VAMP history (global):"
        i_pass = 0
        current_pass => mci%first_pass
        do while (associated (current_pass))
            i_pass = i_pass + 1
            write (u, "(1x,A,I0,':')") "Pass #", i_pass
            call current_pass%write_history (u)
            current_pass => current_pass%next
        end do
    end if
end subroutine mci_vamp_write_history

```

Compute the MD5 sum, including the configuration MD5 sum and the printout, which incorporates the current results.

```

<MCI vamp: mci vamp: TBP>+=
        procedure :: compute_md5sum => mci_vamp_compute_md5sum
<MCI vamp: procedures>+=
subroutine mci_vamp_compute_md5sum (mci, pacify)
    class(mci_vamp_t), intent(inout) :: mci
    logical, intent(in), optional :: pacify
    integer :: u
    mci%md5sum_adapted = ""
    u = free_unit ()
    open (u, status = "scratch", action = "readwrite")
    write (u, "(A)") mci%md5sum
    call mci%write (u, pacify, md5sum_version = .true.)
    rewind (u)
    mci%md5sum_adapted = md5sum (u)
    close (u)
end subroutine mci_vamp_compute_md5sum

```

Return the MD5 sum: If available, return the adapted one.

```

<MCI vamp: mci vamp: TBP>+=
        procedure :: get_md5sum => mci_vamp_get_md5sum
<MCI vamp: procedures>+=
pure function mci_vamp_get_md5sum (mci) result (md5sum)
    class(mci_vamp_t), intent(in) :: mci
    character(32) :: md5sum
    if (mci%md5sum_adapted /= "") then
        md5sum = mci%md5sum_adapted
    else

```



```

        md5sum = mci%md5sum
    end if
end function mci_vamp_get_md5sum

```

Startup message: short version.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: startup_message => mci_vamp_startup_message

<MCI vamp: procedures>+≡
    subroutine mci_vamp_startup_message (mci, unit, n_calls)
        class(mci_vamp_t), intent(in) :: mci
        integer, intent(in), optional :: unit, n_calls
        integer :: num_calls, n_bins
        if (present (n_calls)) then
            num_calls = n_calls
        else
            num_calls = 0
        end if
        if (mci%min_calls /= 0) then
            n_bins = max (mci%grid_par%min_bins, &
                min (num_calls / mci%min_calls, &
                    mci%grid_par%max_bins))
        else
            n_bins = mci%grid_par%max_bins
        end if
        call mci%base_startup_message (unit = unit, n_calls = n_calls)
        if (mci%grid_par%use_vamp_equivalences) then
            write (msg_buffer, "(A,2(1x,I0,1x,A))") &
                "Integrator: Using VAMP channel equivalences"
            call msg_message (unit = unit)
        end if
        write (msg_buffer, "(A,2(1x,I0,1x,A),L1)") &
            "Integrator:", num_calls, &
            "initial calls,", n_bins, &
            "bins, stratified = ", &
            mci%grid_par%stratified
        call msg_message (unit = unit)
        write (msg_buffer, "(A,2(1x,I0,1x,A))") &
            "Integrator: VAMP"
        call msg_message (unit = unit)
    end subroutine mci_vamp_startup_message

```

Log entry: just headline.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: write_log_entry => mci_vamp_write_log_entry

<MCI vamp: procedures>+≡
    subroutine mci_vamp_write_log_entry (mci, u)
        class(mci_vamp_t), intent(in) :: mci
        integer, intent(in) :: u
        write (u, "(1x,A)") "MC Integrator is VAMP"
        call write_separator (u)
        call mci%write_history (u)
        call write_separator (u)
    end subroutine mci_vamp_write_log_entry

```

```

    if (mci%grid_par%use_vamp_equivalences) then
        call vamp_equivalences_write (mci%equivalences, u)
    else
        write (u, "(3x,A)") "No VAMP equivalences have been used"
    end if
    call write_separator (u)
    call mci%write_chain_weights (u)
end subroutine mci_vamp_write_log_entry

```

Set the MCI index (necessary for processes with multiple components). We append the index to the grid filename, just before the final dotted suffix.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: record_index => mci_vamp_record_index

<MCI vamp: procedures>+≡
    subroutine mci_vamp_record_index (mci, i_mci)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: i_mci
        type(string_t) :: basename, suffix
        character(32) :: buffer
        if (mci%grid_filename_set) then
            basename = mci%grid_filename
            call split (basename, suffix, ".", back=.true.)
            write (buffer, "(I0)") i_mci
            if (basename /= "") then
                mci%grid_filename = basename // ".m" // trim (buffer) // "." // suffix
            else
                mci%grid_filename = suffix // ".m" // trim (buffer) // ".vg"
            end if
        end if
    end subroutine mci_vamp_record_index

```

Set the grid parameters.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: set_grid_parameters => mci_vamp_set_grid_parameters

<MCI vamp: procedures>+≡
    subroutine mci_vamp_set_grid_parameters (mci, grid_par)
        class(mci_vamp_t), intent(inout) :: mci
        type(grid_parameters_t), intent(in) :: grid_par
        mci%grid_par = grid_par
        mci%min_calls = grid_par%min_calls_per_bin * mci%n_channel
    end subroutine mci_vamp_set_grid_parameters

```

Set the history parameters.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: set_history_parameters => mci_vamp_set_history_parameters

<MCI vamp: procedures>+≡
    subroutine mci_vamp_set_history_parameters (mci, history_par)
        class(mci_vamp_t), intent(inout) :: mci
        type(history_parameters_t), intent(in) :: history_par
        mci%history_par = history_par

```

```
end subroutine mci_vamp_set_history_parameters
```

Set the rebuild flag, also the flag for checking the grid file.

```
<MCI vamp: mci vamp: TBP>+=
  procedure :: set_rebuild_flag => mci_vamp_set_rebuild_flag

<MCI vamp: procedures>+=
  subroutine mci_vamp_set_rebuild_flag (mci, rebuild, check_grid_file)
    class(mci_vamp_t), intent(inout) :: mci
    logical, intent(in) :: rebuild
    logical, intent(in) :: check_grid_file
    mci%rebuild = rebuild
    mci%check_grid_file = check_grid_file
  end subroutine mci_vamp_set_rebuild_flag
```

Set the filename.

```
<MCI vamp: mci vamp: TBP>+=
  procedure :: set_grid_filename => mci_vamp_set_grid_filename

<MCI vamp: procedures>+=
  subroutine mci_vamp_set_grid_filename (mci, name, run_id)
    class(mci_vamp_t), intent(inout) :: mci
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: run_id
    if (present (run_id)) then
      mci%grid_filename = name // "." // run_id // ".vg"
    else
      mci%grid_filename = name // ".vg"
    end if
    mci%grid_filename_set = .true.
  end subroutine mci_vamp_set_grid_filename
```

To simplify the interface, we prepend a grid path in a separate subroutine.

```
<MCI vamp: mci vamp: TBP>+=
  procedure :: prepend_grid_path => mci_vamp_prepend_grid_path

<MCI vamp: procedures>+=
  subroutine mci_vamp_prepend_grid_path (mci, prefix)
    class(mci_vamp_t), intent(inout) :: mci
    type(string_t), intent(in) :: prefix
    if (mci%grid_filename_set) then
      mci%grid_filename = prefix // "/" // mci%grid_filename
    else
      call msg_warning ("Cannot add prefix to invalid grid filename!")
    end if
  end subroutine mci_vamp_prepend_grid_path
```

Declare particular dimensions as flat.

```
<MCI vamp: mci vamp: TBP>+=
  procedure :: declare_flat_dimensions => mci_vamp_declare_flat_dimensions
```

```

(MCI vamp: procedures)+≡
subroutine mci_vamp_declare_flat_dimensions (mci, dim_flat)
  class(mci_vamp_t), intent(inout) :: mci
  integer, dimension(:), intent(in) :: dim_flat
  integer :: d
  allocate (mci%dim_is_flat (mci%n_dim), source = .false.)
  do d = 1, size (dim_flat)
    mci%dim_is_flat(dim_flat(d)) = .true.
  end do
end subroutine mci_vamp_declare_flat_dimensions

```

Declare equivalences. We have an array of channel equivalences, provided by the phase-space module. Here, we translate this into the `vamp.equivalences` array.

```

(MCI vamp: mci vamp: TBP)+≡
  procedure :: declare_equivalences => mci_vamp_declare_equivalences

(MCI vamp: procedures)+≡
subroutine mci_vamp_declare_equivalences (mci, channel, dim_offset)
  class(mci_vamp_t), intent(inout) :: mci
  type(phas_channel_t), dimension(:), intent(in) :: channel
  integer, intent(in) :: dim_offset
  integer, dimension(:), allocatable :: perm, mode
  integer :: n_channels, n_dim, n_equivalences
  integer :: c, i, j, left, right
  integer :: n_dim_perm
  n_channels = mci%n_channel
  n_dim = mci%n_dim
  n_equivalences = 0
  do c = 1, n_channels
    n_equivalences = n_equivalences + size (channel(c)%eq)
  end do
  call vamp_equivalences_init (mci%equivalences, &
    n_equivalences, n_channels, n_dim)
  allocate (perm (n_dim))
  allocate (mode (n_dim))
  perm = [(i, i = 1, n_dim)]
  mode = VEQ_IDENTITY
  c = 1
  j = 0
  do i = 1, n_equivalences
    if (j < size (channel(c)%eq)) then
      j = j + 1
    else
      c = c + 1
      j = 1
    end if
    associate (eq => channel(c)%eq(j))
      left = c
      right = eq%c
      n_dim_perm = size (eq%perm)
      perm(dim_offset + 1:dim_offset + n_dim_perm) = eq%perm + dim_offset
      mode(dim_offset + 1:dim_offset + n_dim_perm) = eq%mode
      call vamp_equivalence_set (mci%equivalences, &

```

```

        i, left, right, perm, mode)
    end associate
end do
    call vamp_equivalences_complete (mci%equivalences)
end subroutine mci_vamp_declare_equivalences

```

Allocate instance with matching type.

```

<MCI vamp: mci vamp: TBP>+=
    procedure :: allocate_instance => mci_vamp_allocate_instance

<MCI vamp: procedures>+=
    subroutine mci_vamp_allocate_instance (mci, mci_instance)
        class(mci_vamp_t), intent(in) :: mci
        class(mci_instance_t), intent(out), pointer :: mci_instance
        allocate (mci_vamp_instance_t :: mci_instance)
    end subroutine mci_vamp_allocate_instance

```

Allocate a new integration pass. We can preset everything that does not depend on the number of iterations and calls. This is postponed to the `integrate` method.

In the final pass, we do not check accuracy goal etc., since we can assume that the user wants to perform and average all iterations in this pass.

```

<MCI vamp: mci vamp: TBP>+=
    procedure :: add_pass => mci_vamp_add_pass

<MCI vamp: procedures>+=
    subroutine mci_vamp_add_pass (mci, adapt_grids, adapt_weights, final_pass)
        class(mci_vamp_t), intent(inout) :: mci
        logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
        integer :: i_pass, i_it
        type(pass_t), pointer :: new
        allocate (new)
        if (associated (mci%current_pass)) then
            i_pass = mci%current_pass%i_pass + 1
            i_it = mci%current_pass%i_first_it + mci%current_pass%n_it
            mci%current_pass%next => new
        else
            i_pass = 1
            i_it = 1
            mci%first_pass => new
        end if
        mci%current_pass => new
        new%i_pass = i_pass
        new%i_first_it = i_it
        if (present (adapt_grids)) then
            new%adapt_grids = adapt_grids
        else
            new%adapt_grids = .false.
        end if
        if (present (adapt_weights)) then
            new%adapt_weights = adapt_weights
        else
            new%adapt_weights = .false.
        end if
    end subroutine mci_vamp_add_pass

```

```

end if
if (present (final_pass)) then
    new%is_final_pass = final_pass
else
    new%is_final_pass = .false.
end if
end subroutine mci_vamp_add_pass

```

Update the list of integration passes. All passes except for the last one must match exactly. For the last one, integration results are updated. The reference output may contain extra passes, these are ignored.

```

<MCI vamp: mci vamp: TBP>+=
    procedure :: update_from_ref => mci_vamp_update_from_ref

<MCI vamp: procedures>+=
    subroutine mci_vamp_update_from_ref (mci, mci_ref, success)
        class(mci_vamp_t), intent(inout) :: mci
        class(mci_t), intent(in) :: mci_ref
        logical, intent(out) :: success
        type(pass_t), pointer :: current_pass, ref_pass
        select type (mci_ref)
        type is (mci_vamp_t)
            current_pass => mci%first_pass
            ref_pass => mci_ref%first_pass
            success = .true.
            do while (success .and. associated (current_pass))
                if (associated (ref_pass)) then
                    if (associated (current_pass%next)) then
                        success = current_pass .matches. ref_pass
                    else
                        call current_pass%update (ref_pass, success)
                        if (current_pass%integral_defined) then
                            mci%integral = current_pass%get_integral ()
                            mci%error = current_pass%get_error ()
                            mci%efficiency = current_pass%get_efficiency ()
                            mci%integral_known = .true.
                            mci%error_known = .true.
                            mci%efficiency_known = .true.
                        end if
                    end if
                    current_pass => current_pass%next
                    ref_pass => ref_pass%next
                else
                    success = .false.
                end if
            end do
        end select
    end subroutine mci_vamp_update_from_ref

```

Update the MCI record (i.e., the integration passes) by reading from input stream. The stream should contain a `write` output from a previous run. We first check the MD5 sum of the configuration parameters. If that matches, we proceed directly to the stored integration passes. If successful, we may continue

to read the file; the position will be after a blank line that must follow the MCI record.

```

(MCI vamp: mci vamp: TBP)+≡
    procedure :: update => mci_vamp_update
(MCI vamp: procedures)+≡
    subroutine mci_vamp_update (mci, u, success)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: u
        logical, intent(out) :: success
        character(80) :: buffer
        character(32) :: md5sum_file
        type(mci_vamp_t) :: mci_file
        integer :: n_pass, n_it
        call read_sval (u, md5sum_file)
        if (mci%check_grid_file) then
            success = md5sum_file == mci%md5sum
        else
            success = .true.
        end if
        if (success) then
            read (u, *)
            read (u, "(A)") buffer
            if (trim (adjustl (buffer))) == "VAMP integrator:") then
                n_pass = 0
                n_it = 0
                do
                    read (u, "(A)") buffer
                    select case (trim (adjustl (buffer)))
                        case ("")
                            exit
                        case ("Integration pass:")
                            call mci_file%add_pass ()
                            call mci_file%current_pass%read (u, n_pass, n_it)
                            n_pass = n_pass + 1
                            n_it = n_it + mci_file%current_pass%n_it
                        end select
                    end do
                    call mci%update_from_ref (mci_file, success)
                    call mci_file%final ()
                else
                    call msg_fatal ("VAMP: reading grid file: corrupted data")
                end if
            end if
        end subroutine mci_vamp_update

```

Read / write grids from / to file.

Bug fix for 2.2.5: after reading grids from file, channel weights must be copied back to the mci_instance record.

```

(MCI vamp: mci vamp: TBP)+≡
    procedure :: write_grids => mci_vamp_write_grids
    procedure :: read_grids_header => mci_vamp_read_grids_header
    procedure :: read_grids_data => mci_vamp_read_grids_data
    procedure :: read_grids => mci_vamp_read_grids

```

```

<MCI vamp: procedures>+=
subroutine mci_vamp_write_grids (mci, instance)
  class(mci_vamp_t), intent(in) :: mci
  class(mci_instance_t), intent(inout) :: instance
  integer :: u
  select type (instance)
  type is (mci_vamp_instance_t)
    if (mci%grid_filename_set) then
      if (instance%grids_defined) then
        u = free_unit ()
        open (u, file = char (mci%grid_filename), &
              action = "write", status = "replace")
        write (u, "(1x,A,A,A)") "MD5sum = '", mci%md5sum, "'"
        write (u, *)
        call mci%write (u)
        write (u, *)
        write (u, "(1x,A)") "VAMP grids:"
        call vamp_write_grids (instance%grids, u, &
                               write_integrals = .true.)
        close (u)
      else
        call msg_bug ("VAMP: write grids: grids undefined")
      end if
    else
      call msg_bug ("VAMP: write grids: filename undefined")
    end if
  end select
end subroutine mci_vamp_write_grids

subroutine mci_vamp_read_grids_header (mci, success)
  class(mci_vamp_t), intent(inout) :: mci
  logical, intent(out) :: success
  logical :: exist
  integer :: u
  success = .false.
  if (mci%grid_filename_set) then
    inquire (file = char (mci%grid_filename), exist = exist)
    if (exist) then
      u = free_unit ()
      open (u, file = char (mci%grid_filename), &
            action = "read", status = "old")
      call mci%update (u, success)
      close (u)
      if (.not. success) then
        write (msg_buffer, "(A,A,A)") &
              "VAMP: parameter mismatch, discarding grid file '", &
              char (mci%grid_filename), "'"
        call msg_message ()
      end if
    end if
  else
    call msg_bug ("VAMP: read grids: filename undefined")
  end if
end subroutine mci_vamp_read_grids_header

```



```

subroutine mci_vamp_read_grids_data (mci, instance, read_integrals)
  class(mci_vamp_t), intent(in) :: mci
  class(mci_instance_t), intent(inout) :: instance
  logical, intent(in), optional :: read_integrals
  integer :: u
  character(80) :: buffer
  select type (instance)
  type is (mci_vamp_instance_t)
    if (.not. instance%grids_defined) then
      u = free_unit ()
      open (u, file = char (mci%grid_filename), &
        action = "read", status = "old")
      do
        read (u, "(A)") buffer
        if (trim (adjustl (buffer)) == "VAMP grids:") exit
      end do
      call vamp_read_grids (instance%grids, u, read_integrals)
      close (u)
      call instance%set_channel_weights (instance%grids%weights)
      instance%grids_defined = .true.
    else
      call msg_bug ("VAMP: read grids: grids already defined")
    end if
  end select
end subroutine mci_vamp_read_grids_data

subroutine mci_vamp_read_grids (mci, instance, success)
  class(mci_vamp_t), intent(inout) :: mci
  class(mci_instance_t), intent(inout) :: instance
  logical, intent(out) :: success
  logical :: exist
  integer :: u
  character(80) :: buffer
  select type (instance)
  type is (mci_vamp_instance_t)
    success = .false.
    if (mci%grid_filename_set) then
      if (.not. instance%grids_defined) then
        inquire (file = char (mci%grid_filename), exist = exist)
        if (exist) then
          u = free_unit ()
          open (u, file = char (mci%grid_filename), &
            action = "read", status = "old")
          call mci%update (u, success)
          if (success) then
            read (u, "(A)") buffer
            if (trim (adjustl (buffer)) == "VAMP grids:") then
              call vamp_read_grids (instance%grids, u)
            else
              call msg_fatal ("VAMP: reading grid file: &
                &corrupted grid data")
            end if
          end if
        else
          call msg_fatal ("VAMP: reading grid file: &
            &corrupted grid data")
        end if
      end if
    else
      call msg_fatal ("VAMP: reading grid file: &
        &corrupted grid data")
    end if
  end select
end subroutine mci_vamp_read_grids

```

```

        write (msg_buffer, "(A,A,A)") &
            "VAMP: parameter mismatch, discarding grid file '", &
            char (mci%grid_filename), "'"
        call msg_message ()
    end if
    close (u)
    instance%grids_defined = success
end if
else
    call msg_bug ("VAMP: read grids: grids already defined")
end if
else
    call msg_bug ("VAMP: read grids: filename undefined")
end if
end select
end subroutine mci_vamp_read_grids

```

Auxiliary: Read real, integer, string value. We search for an equals sign, the value must follow.

```

<MCI vamp: procedures>+≡
subroutine read_rval (u, rval)
    integer, intent(in) :: u
    real(default), intent(out) :: rval
    character(80) :: buffer
    read (u, "(A)") buffer
    buffer = adjustl (buffer(scan (buffer, "=") + 1:))
    read (buffer, *) rval
end subroutine read_rval

subroutine read_ival (u, ival)
    integer, intent(in) :: u
    integer, intent(out) :: ival
    character(80) :: buffer
    read (u, "(A)") buffer
    buffer = adjustl (buffer(scan (buffer, "=") + 1:))
    read (buffer, *) ival
end subroutine read_ival

subroutine read_sval (u, sval)
    integer, intent(in) :: u
    character(*), intent(out) :: sval
    character(80) :: buffer
    read (u, "(A)") buffer
    buffer = adjustl (buffer(scan (buffer, "=") + 1:))
    read (buffer, *) sval
end subroutine read_sval

subroutine read_lval (u, lval)
    integer, intent(in) :: u
    logical, intent(out) :: lval
    character(80) :: buffer
    read (u, "(A)") buffer
    buffer = adjustl (buffer(scan (buffer, "=") + 1:))

```

```

        read (buffer, *) lval
    end subroutine read_lval

```

Integrate. Perform a new integration pass (possibly reusing previous results), which may consist of several iterations.

Note: we record the integral once per iteration. The integral stored in the `mci` record itself is the last integral of the current iteration, no averaging done. The `results` record may average results.

In case we read the integration from file and we added new iterations to the pass preserving number of calls, we need to reshape the grids in order to incorporate the correct number of calls. Else the grids would be sampled with the number of calls from the grids file, which does not need to coincide with the number of calls from the pass.

Note: recording the efficiency is not supported yet.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: integrate => mci_vamp_integrate

<MCI vamp: procedures>+≡
    subroutine mci_vamp_integrate (mci, instance, sampler, &
        n_it, n_calls, results, pacify)
        class(mci_vamp_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
        class(mci_results_t), intent(inout), optional :: results
        logical, intent(in), optional :: pacify
        integer :: it
        logical :: reshape, from_file, success
        select type (instance)
        type is (mci_vamp_instance_t)
            if (associated (mci%current_pass)) then
                mci%current_pass%integral_defined = .false.
                call mci%current_pass%configure (n_it, n_calls, &
                    mci%min_calls, mci%grid_par%min_bins, &
                    mci%grid_par%max_bins, &
                    mci%grid_par%min_calls_per_channel * mci%n_channel)
                call mci%current_pass%configure_history &
                    (mci%n_channel, mci%history_par)
                instance%pass_complete = .false.
                instance%it_complete = .false.
                call instance%new_pass (reshape)
                if (.not. instance%grids_defined .or. instance%grids_from_file) then
                    if (mci%grid_filename_set .and. .not. mci%rebuild) then
                        call mci%read_grids_header (success)
                        from_file = success
                        if (.not. instance%grids_defined .and. success) then
                            call mci%read_grids_data (instance)
                        end if
                    else
                        from_file = .false.
                    end if
                else

```

```

        from_file = .false.
    end if
    if (from_file) then
        if (.not. mci%check_grid_file) &
            call msg_warning ("Reading grid file: MD5 sum check disabled")
        call msg_message ("VAMP: " &
            // "using grids and results from file '" &
            // char (mci%grid_filename) // "'")
    else if (.not. instance%grids_defined) then
        call instance%create_grids ()
    end if
    do it = 1, instance%n_it
        if (signal_is_pending ()) return
        reshape = reshape .or. &
            (instance%grids_from_file .and. n_it > mci%current_pass%get_integration_index ())
        instance%grids_from_file = from_file .and. &
            it <= mci%current_pass%get_integration_index ()
        if (.not. instance%grids_from_file) then
            instance%it_complete = .false.
            call instance%adapt_grids ()
            if (signal_is_pending ()) return
            call instance%adapt_weights ()
            if (signal_is_pending ()) return
            call instance%discard_integrals (reshape)
            if (mci%grid_par%use_vamp_equivalences) then
                call instance%sample_grids (mci%rng, sampler, &
                    mci%equivalences)
            else
                call instance%sample_grids (mci%rng, sampler)
            end if
            if (signal_is_pending ()) return
            instance%it_complete = .true.
            if (instance%integral /= 0) then
                mci%current_pass%calls(it) = instance%calls
                mci%current_pass%calls_valid(it) = instance%calls_valid
                mci%current_pass%integral(it) = instance%integral
                if (abs (instance%error / instance%integral) &
                    > epsilon (1._default)) then
                    mci%current_pass%error(it) = instance%error
                end if
                mci%current_pass%efficiency(it) = instance%efficiency
            end if
            mci%current_pass%integral_defined = .true.
        end if
        if (present (results)) then
            if (mci%has_chains ()) then
                call mci%collect_chain_weights (instance%w)
                call results%record (1, &
                    n_calls      = mci%current_pass%calls(it), &
                    n_calls_valid = mci%current_pass%calls_valid(it), &
                    integral      = mci%current_pass%integral(it), &
                    error         = mci%current_pass%error(it), &
                    efficiency    = mci%current_pass%efficiency(it), &
                    ! TODO Insert pos. and neg. Efficiency from VAMP.
                )
            end if
        end if
    end do
end function

```

```

        efficiency_pos = 0._default, &
        efficiency_neg = 0._default, &
        chain_weights = mci%chain_weights, &
        suppress = pacify)
    else
        call results%record (1, &
            n_calls      = mci%current_pass%calls(it), &
            n_calls_valid = mci%current_pass%calls_valid(it), &
            integral     = mci%current_pass%integral(it), &
            error        = mci%current_pass%error(it), &
            efficiency    = mci%current_pass%efficiency(it), &
            ! TODO Insert pos. and neg. Efficiency from VAMP.
            efficiency_pos = 0._default, &
            efficiency_neg = 0._default, &
            suppress = pacify)
    end if
end if
if (.not. instance%grids_from_file &
    .and. mci%grid_filename_set) then
    call mci%write_grids (instance)
end if
call instance%allow_adaptation ()
reshape = .false.
if (.not. mci%current_pass%is_final_pass) then
    call mci%check_goals (it, success)
    if (success) exit
end if
end do
if (signal_is_pending ()) return
instance%pass_complete = .true.
mci%integral = mci%current_pass%get_integral()
mci%error = mci%current_pass%get_error()
mci%efficiency = mci%current_pass%get_efficiency()
mci%integral_known = .true.
mci%error_known = .true.
mci%efficiency_known = .true.
call mci%compute_md5sum (pacify)
else
    call msg_bug ("MCI integrate: current_pass object not allocated")
end if
end select
end subroutine mci_vamp_integrate

```

Check whether we are already finished with this pass.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: check_goals => mci_vamp_check_goals

<MCI vamp: procedures>+≡
    subroutine mci_vamp_check_goals (mci, it, success)
        class(mci_vamp_t), intent(inout) :: mci
        integer, intent(in) :: it
        logical, intent(out) :: success
        success = .false.
        if (mci%error_reached (it)) then

```

```

        mci%current_pass%n_it = it
        call msg_message ("VAMP: error goal reached; &
            &skipping iterations")
        success = .true.
        return
    end if
    if (mci%rel_error_reached (it)) then
        mci%current_pass%n_it = it
        call msg_message ("VAMP: relative error goal reached; &
            &skipping iterations")
        success = .true.
        return
    end if
    if (mci%accuracy_reached (it)) then
        mci%current_pass%n_it = it
        call msg_message ("VAMP: accuracy goal reached; &
            &skipping iterations")
        success = .true.
        return
    end if
end subroutine mci_vamp_check_goals

```

Return true if the error, relative error, or accuracy goal has been reached, if any.

(MCI vamp: mci vamp: TBP)+≡

```

procedure :: error_reached => mci_vamp_error_reached
procedure :: rel_error_reached => mci_vamp_rel_error_reached
procedure :: accuracy_reached => mci_vamp_accuracy_reached

```

(MCI vamp: procedures)+≡

```

function mci_vamp_error_reached (mci, it) result (flag)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in) :: it
    logical :: flag
    real(default) :: error_goal, error
    error_goal = mci%grid_par%error_goal
    if (error_goal > 0) then
        associate (pass => mci%current_pass)
            if (pass%integral_defined) then
                error = abs (pass%error(it))
                flag = error < error_goal
            else
                flag = .false.
            end if
        end associate
    else
        flag = .false.
    end if
end function mci_vamp_error_reached

function mci_vamp_rel_error_reached (mci, it) result (flag)
    class(mci_vamp_t), intent(in) :: mci
    integer, intent(in) :: it
    logical :: flag

```

```

real(default) :: rel_error_goal, rel_error
rel_error_goal = mci%grid_par%rel_error_goal
if (rel_error_goal > 0) then
  associate (pass => mci%current_pass)
    if (pass%integral_defined) then
      if (pass%integral(it) /= 0) then
        rel_error = abs (pass%error(it) / pass%integral(it))
        flag = rel_error < rel_error_goal
      else
        flag = .true.
      end if
    else
      flag = .false.
    end if
  end associate
else
  flag = .false.
end if
end function mci_vamp_rel_error_reached

function mci_vamp_accuracy_reached (mci, it) result (flag)
class(mci_vamp_t), intent(in) :: mci
integer, intent(in) :: it
logical :: flag
real(default) :: accuracy_goal, accuracy
accuracy_goal = mci%grid_par%accuracy_goal
if (accuracy_goal > 0) then
  associate (pass => mci%current_pass)
    if (pass%integral_defined) then
      if (pass%integral(it) /= 0) then
        accuracy = abs (pass%error(it) / pass%integral(it)) &
          * sqrt (real (pass%calls(it), default))
        flag = accuracy < accuracy_goal
      else
        flag = .true.
      end if
    else
      flag = .false.
    end if
  end associate
else
  flag = .false.
end if
end function mci_vamp_accuracy_reached

```

Prepare an event generation pass. Should be called before a sequence of events is generated, then we should call the corresponding finalizer.

The pass-specific data of the previous integration pass are retained, but we reset the number of iterations and calls to zero. The latter now counts the number of events (calls to the sampling function, actually).

(MCI vamp: mci vamp: TBP) +=

```
procedure :: prepare_simulation => mci_vamp_prepare_simulation
```

(MCI vamp: procedures) +=

```

subroutine mci_vamp_prepare_simulation (mci)
  class(mci_vamp_t), intent(inout) :: mci
  logical :: success
  if (mci%grid_filename_set) then
    call mci%read_grids_header (success)
    call mci%compute_md5sum ()
    if (.not. success) then
      call msg_fatal ("Simulate: " &
        // "reading integration grids from file '" &
        // char (mci%grid_filename) // "' failed")
    end if
  else
    call msg_bug ("VAMP: simulation: no grids, no grid filename")
  end if
end subroutine mci_vamp_prepare_simulation

```

Generate weighted event. Note that the event weight (`vamp_weight`) is not just the MCI weight. `vamp_next_event` selects a channel based on the channel weights multiplied by the (previously recorded) maximum integrand value of the channel. The MCI weight is renormalized accordingly, to cancel this effect on the result.

```

<MCI vamp: mci vamp: TBP> +=
  procedure :: generate_weighted_event => mci_vamp_generate_weighted_event
<MCI vamp: procedures> +=
  subroutine mci_vamp_generate_weighted_event (mci, instance, sampler)
    class(mci_vamp_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    class(vamp_data_t), allocatable :: data
    type(exception) :: vamp_exception
    select type (instance)
    type is (mci_vamp_instance_t)
      instance%vamp_weight_set = .false.
      allocate (mci_workspace_t :: data)
      select type (data)
      type is (mci_workspace_t)
        data%sampler => sampler
        data%instance => instance
      end select
    select type (rng => mci%rng)
    type is (rng_tao_t)
      if (instance%grids_defined) then
        call vamp_next_event ( &
          instance%vamp_x, &
          rng%state, &
          instance%grids, &
          vamp_sampling_function, &
          data, &
          phi = phi_trivial, &
          weight = instance%vamp_weight, &
          exc = vamp_exception)
        call handle_vamp_exception (vamp_exception, mci%verbose)
        instance%vamp_excess = 0
      end if
    end select
  end subroutine

```



```

        instance%vamp_weight_set = .true.
    else
        call msg_bug ("VAMP: generate event: grids undefined")
    end if
class default
    call msg_fatal ("VAMP event generation: &
        &random-number generator must be TAO")
end select
end select
end subroutine mci_vamp_generate_weighted_event

```

Generate unweighted event.

(MCI vamp: mci vamp: TBP)+≡

```

    procedure :: generate_unweighted_event => &
        mci_vamp_generate_unweighted_event

```

(MCI vamp: procedures)+≡

```

subroutine mci_vamp_generate_unweighted_event (mci, instance, sampler)
    class(mci_vamp_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    class(vamp_data_t), allocatable :: data
    logical :: positive
    type(exception) :: vamp_exception
    select type (instance)
    type is (mci_vamp_instance_t)
        instance%vamp_weight_set = .false.
        allocate (mci_workspace_t :: data)
        select type (data)
        type is (mci_workspace_t)
            data%sampler => sampler
            data%instance => instance
        end select
        select type (rng => mci%rng)
        type is (rng_tao_t)
            if (instance%grids_defined) then
                REJECTION: do
                    call vamp_next_event ( &
                        instance%vamp_x, &
                        rng%state, &
                        instance%grids, &
                        vamp_sampling_function, &
                        data, &
                        phi = phi_trivial, &
                        excess = instance%vamp_excess, &
                        positive = positive, &
                        exc = vamp_exception)
                    if (signal_is_pending ()) return
                    if (sampler%is_valid ()) exit REJECTION
                end do REJECTION
            call handle_vamp_exception (vamp_exception, mci%verbose)
            if (positive) then
                instance%vamp_weight = 1
            else if (instance%negative_weights) then

```

```

        instance%vamp_weight = -1
    else
        call msg_fatal ("VAMP: event with negative weight generated")
        instance%vamp_weight = 0
    end if
    instance%vamp_weight_set = .true.
else
    call msg_bug ("VAMP: generate event: grids undefined")
end if
class default
    call msg_fatal ("VAMP event generation: &
        &random-number generator must be TAO")
end select
end select
end subroutine mci_vamp_generate_unweighted_event

```

Rebuild an event, using the state input.

Note: This feature is currently unused.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: rebuild_event => mci_vamp_rebuild_event

<MCI vamp: procedures>+≡
    subroutine mci_vamp_rebuild_event (mci, instance, sampler, state)
        class(mci_vamp_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout) :: instance
        class(mci_sampler_t), intent(inout) :: sampler
        class(mci_state_t), intent(in) :: state
        call msg_bug ("MCI vamp rebuild event not implemented yet")
    end subroutine mci_vamp_rebuild_event

```

Pacify: override the default no-op, since VAMP numerics might need some massage.

```

<MCI vamp: mci vamp: TBP>+≡
    procedure :: pacify => mci_vamp_pacify

<MCI vamp: procedures>+≡
    subroutine mci_vamp_pacify (object, efficiency_reset, error_reset)
        class(mci_vamp_t), intent(inout) :: object
        logical, intent(in), optional :: efficiency_reset, error_reset
        logical :: err_reset
        type(pass_t), pointer :: current_pass
        err_reset = .false.
        if (present (error_reset)) err_reset = error_reset
        current_pass => object%first_pass
        do while (associated (current_pass))
            if (allocated (current_pass%error) .and. err_reset) then
                current_pass%error = 0
            end if
            if (allocated (current_pass%efficiency) .and. err_reset) then
                current_pass%efficiency = 1
            end if
            current_pass => current_pass%next
        end do
    end subroutine mci_vamp_pacify

```

21.6.5 Sampler as Workspace

In the full setup, the sampling function requires the process instance object as workspace. We implement this by (i) implementing the process instance as a type extension of the abstract `sampler_t` object used by the MCI implementation and (ii) providing such an object as an extra argument to the sampling function that VAMP can call. To minimize cross-package dependencies, we use an abstract type `vamp_workspace` that VAMP declares and extend this by including a pointer to the `sampler` and `instance` objects. In the body of the sampling function, we dereference this pointer and can then work with the contents.

```
<MCI vamp: types>+≡
  type, extends (vamp_data_t) :: mci_workspace_t
    class(mci_sampler_t), pointer :: sampler => null ()
    class(mci_vamp_instance_t), pointer :: instance => null ()
  end type mci_workspace_t
```

21.6.6 Integrator instance

The history entries should point to the corresponding history entry in the `pass_t` object. If there is none, we may allocate a local history, which is then just transient.

```
<MCI vamp: public>+≡
  public :: mci_vamp_instance_t

<MCI vamp: types>+≡
  type, extends (mci_instance_t) :: mci_vamp_instance_t
    type(mci_vamp_t), pointer :: mci => null ()
    logical :: grids_defined = .false.
    logical :: grids_from_file = .false.
    integer :: n_it = 0
    integer :: it = 0
    logical :: pass_complete = .false.
    integer :: n_calls = 0
    integer :: calls = 0
    integer :: calls_valid = 0
    logical :: it_complete = .false.
    logical :: enable_adapt_grids = .false.
    logical :: enable_adapt_weights = .false.
    logical :: allow_adapt_grids = .false.
    logical :: allow_adapt_weights = .false.
    integer :: n_adapt_grids = 0
    integer :: n_adapt_weights = 0
    logical :: generating_events = .false.
    real(default) :: safety_factor = 1
    type(vamp_grids) :: grids
    real(default) :: g = 0
    real(default), dimension(:), allocatable :: gi
    real(default) :: integral = 0
```

```

real(default) :: error = 0
real(default) :: efficiency = 0
real(default), dimension(:), allocatable :: vamp_x
logical :: vamp_weight_set = .false.
real(default) :: vamp_weight = 0
real(default) :: vamp_excess = 0
logical :: allocate_global_history = .false.
type(vamp_history), dimension(:), pointer :: v_history => null ()
logical :: allocate_channel_history = .false.
type(vamp_history), dimension(:,,:), pointer :: v_histories => null ()
contains
  <MCI vamp: mci vamp instance: TBP>
end type mci_vamp_instance_t

```

Output.

```

<MCI vamp: mci vamp instance: TBP>≡
  procedure :: write => mci_vamp_instance_write
<MCI vamp: procedures>+≡
  subroutine mci_vamp_instance_write (object, unit, pacify)
    class(mci_vamp_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    integer :: u, i
    character(len=7) :: fmt
    call pac_fmt (fmt, FMT_17, FMT_14, pacify)
    u = given_output_unit (unit)
    write (u, "(3x,A," // FMT_19 // ")") "Integrand = ", object%integrand
    write (u, "(3x,A," // FMT_19 // ")") "Weight      = ", object%vamp_weight
    if (object%vamp_weight_set) then
      write (u, "(3x,A," // FMT_19 // ")") "VAMP wgt  = ", object%vamp_weight
      if (object%vamp_excess /= 0) then
        write (u, "(3x,A," // FMT_19 // ")") "VAMP exc  = ", &
          object%vamp_excess
      end if
    end if
    write (u, "(3x,A,L1)") "adapt grids  = ", object%enable_adapt_grids
    write (u, "(3x,A,L1)") "adapt weights = ", object%enable_adapt_weights
    if (object%grids_defined) then
      if (object%grids_from_file) then
        write (u, "(3x,A)") "VAMP grids: read from file"
      else
        write (u, "(3x,A)") "VAMP grids: defined"
      end if
    else
      write (u, "(3x,A)") "VAMP grids: [undefined]"
    end if
    write (u, "(3x,A,I0)") "n_it      = ", object%n_it
    write (u, "(3x,A,I0)") "it        = ", object%it
    write (u, "(3x,A,L1)") "pass complete = ", object%it_complete
    write (u, "(3x,A,I0)") "n_calls   = ", object%n_calls
    write (u, "(3x,A,I0)") "calls     = ", object%calls
    write (u, "(3x,A,I0)") "calls_valid = ", object%calls_valid
    write (u, "(3x,A,L1)") "it complete = ", object%it_complete
  end subroutine mci_vamp_instance_write

```

```

write (u, "(3x,A,I0)") "n adapt.(g)  = ", object%n_adapt_grids
write (u, "(3x,A,I0)") "n adapt.(w)  = ", object%n_adapt_weights
write (u, "(3x,A,L1)") "gen. events = ", object%generating_events
write (u, "(3x,A,L1)") "neg. weights = ", object%negative_weights
if (object%safety_factor /= 1) write &
    (u, "(3x,A," // fmt // ")") "safety f = ", object%safety_factor
write (u, "(3x,A," // fmt // ")") "integral = ", object%integral
write (u, "(3x,A," // fmt // ")") "error    = ", object%error
write (u, "(3x,A," // fmt // ")") "eff.     = ", object%efficiency
write (u, "(3x,A)") "weights:"
do i = 1, size (object%w)
    write (u, "(5x,I0,1x," // FMT_12 // ")") i, object%w(i)
end do
end subroutine mci_vamp_instance_write

```

Write the grids to the specified unit.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: write_grids => mci_vamp_instance_write_grids

<MCI vamp: procedures>+≡
    subroutine mci_vamp_instance_write_grids (object, unit)
        class(mci_vamp_instance_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (object%grids_defined) then
            call vamp_write_grids (object%grids, u, write_integrals = .true.)
        end if
    end subroutine mci_vamp_instance_write_grids

```

Finalizer: the history arrays are pointer arrays and need finalization.

```

<MCI vamp: mci vamp instance: TBP>+≡
    procedure :: final => mci_vamp_instance_final

<MCI vamp: procedures>+≡
    subroutine mci_vamp_instance_final (object)
        class(mci_vamp_instance_t), intent(inout) :: object
        if (object%allocate_global_history) then
            if (associated (object%v_history)) then
                call vamp_delete_history (object%v_history)
                deallocate (object%v_history)
            end if
        end if
        if (object%allocate_channel_history) then
            if (associated (object%v_histories)) then
                call vamp_delete_history (object%v_histories)
                deallocate (object%v_histories)
            end if
        end if
        if (object%grids_defined) then
            call vamp_delete_grids (object%grids)
            object%grids_defined = .false.
        end if
    end subroutine mci_vamp_instance_final

```

Initializer.

```

<MCI vamp: mci vamp instance: TBP>+≡
  procedure :: init => mci_vamp_instance_init

<MCI vamp: procedures>+≡
  subroutine mci_vamp_instance_init (mci_instance, mci)
    class(mci_vamp_instance_t), intent(out) :: mci_instance
    class(mci_t), intent(in), target :: mci
    call mci_instance%base_init (mci)
    select type (mci)
    type is (mci_vamp_t)
      mci_instance%mci => mci
      allocate (mci_instance%gi (mci%n_channel))
      mci_instance%allocate_global_history = .not. mci%history_par%global
      mci_instance%allocate_channel_history = .not. mci%history_par%channel
      mci_instance%negative_weights = mci%negative_weights
    end select
  end subroutine mci_vamp_instance_init

```

Prepare a new integration pass: write the pass-specific settings to the **instance** object. This should be called initially, together with the **create_grids** procedure, and whenever we start a new integration pass.

Set **reshape** if the number of calls is different than previously (unless it was zero, indicating the first pass).

We link VAMP histories to the allocated histories in the current pass object, so the recorded results are persistent. However, if there are no histories present there, we allocate them locally. In that case, the histories will disappear together with the MCI instance object.

```

<MCI vamp: mci vamp instance: TBP>+≡
  procedure :: new_pass => mci_vamp_instance_new_pass

<MCI vamp: procedures>+≡
  subroutine mci_vamp_instance_new_pass (instance, reshape)
    class(mci_vamp_instance_t), intent(inout) :: instance
    logical, intent(out) :: reshape
    type(pass_t), pointer :: current
    associate (mci => instance%mci)
      current => mci%current_pass
      instance%n_it = current%n_it
      if (instance%n_calls == 0) then
        reshape = .false.
        instance%n_calls = current%n_calls
      else if (instance%n_calls == current%n_calls) then
        reshape = .false.
      else
        reshape = .true.
        instance%n_calls = current%n_calls
      end if
      instance%it = 0
      instance%calls = 0
      instance%calls_valid = 0
      instance%enable_adapt_grids = current%adapt_grids
    end associate
  end subroutine mci_vamp_instance_new_pass

```

```

instance%enable_adapt_weights = current%adapt_weights
instance%generating_events = .false.
if (instance%allocate_global_history) then
  if (associated (instance%v_history)) then
    call vamp_delete_history (instance%v_history)
    deallocate (instance%v_history)
  end if
  allocate (instance%v_history (instance%n_it))
  call vamp_create_history (instance%v_history, verbose = .false.)
else
  instance%v_history => current%v_history
end if
if (instance%allocate_channel_history) then
  if (associated (instance%v_histories)) then
    call vamp_delete_history (instance%v_histories)
    deallocate (instance%v_histories)
  end if
  allocate (instance%v_histories (instance%n_it, mci%n_channel))
  call vamp_create_history (instance%v_histories, verbose = .false.)
else
  instance%v_histories => current%v_histories
end if
end associate
end subroutine mci_vamp_instance_new_pass

```

Create a grid set within the instance object, using the data of the current integration pass. Also reset counters that track this grid set.

```

(MCI vamp: mci vamp instance: TBP)+≡
  procedure :: create_grids => mci_vamp_instance_create_grids

(MCI vamp: procedures)+≡
  subroutine mci_vamp_instance_create_grids (instance)
    class(mci_vamp_instance_t), intent(inout) :: instance
    type (pass_t), pointer :: current
    integer, dimension(:), allocatable :: num_div
    real(default), dimension(:, :), allocatable :: region
    associate (mci => instance%mci)
      current => mci%current_pass
      allocate (num_div (mci%n_dim))
      allocate (region (2, mci%n_dim))
      region(1,:) = 0
      region(2,:) = 1
      num_div = current%n_bins
      instance%n_adapt_grids = 0
      instance%n_adapt_weights = 0
      if (.not. instance%grids_defined) then
        call vamp_create_grids (instance%grids, &
          region, &
          current%n_calls, &
          weights = instance%w, &
          num_div = num_div, &
          stratified = mci%grid_par%stratified)
        instance%grids_defined = .true.
      else

```

```

        call msg_bug ("VAMP: create grids: grids already defined")
    end if
end associate
end subroutine mci_vamp_instance_create_grids

```

Reset a grid set, so we can start a fresh integration pass. In effect, we delete results of previous integrations, but keep the grid shapes, weights, and variance arrays, so adaptation is still possible. The grids are prepared for a specific number of calls (per iteration) and sampling mode (stratified/importance).

The `vamp_discard_integrals` implementation will reshape the grids only if the argument `num_calls` is present.

```

<MCI vamp: mci vamp instance: TBP>+=
    procedure :: discard_integrals => mci_vamp_instance_discard_integrals

<MCI vamp: procedures>+=
    subroutine mci_vamp_instance_discard_integrals (instance, reshape)
        class(mci_vamp_instance_t), intent(inout) :: instance
        logical, intent(in) :: reshape
        instance%calls = 0
        instance%calls_valid = 0
        instance%integral = 0
        instance%error = 0
        instance%efficiency = 0
        associate (mci => instance%mci)
            if (instance%grids_defined) then
                if (mci%grid_par%use_vamp_equivalences) then
                    if (reshape) then
                        call vamp_discard_integrals (instance%grids, &
                            num_calls = instance%n_calls, &
                            stratified = mci%grid_par%stratified, &
                            eq = mci%equivalences)
                    else
                        call vamp_discard_integrals (instance%grids, &
                            stratified = mci%grid_par%stratified, &
                            eq = mci%equivalences)
                    end if
                else if
                else
                    if (reshape) then
                        call vamp_discard_integrals (instance%grids, &
                            num_calls = instance%n_calls, &
                            stratified = mci%grid_par%stratified)
                    else
                        call vamp_discard_integrals (instance%grids, &
                            stratified = mci%grid_par%stratified)
                    end if
                end if
            else
                call msg_bug ("VAMP: discard integrals: grids undefined")
            end if
        end associate
    end subroutine mci_vamp_instance_discard_integrals

```

After grids are created (with equidistant binning and equal weight), adaptation

is redundant. Therefore, we should allow it only after a complete integration step has been performed, calling this.

```

(MCI vamp: mci vamp instance: TBP)+≡
  procedure :: allow_adaptation => mci_vamp_instance_allow_adaptation

(MCI vamp: procedures)+≡
  subroutine mci_vamp_instance_allow_adaptation (instance)
    class(mci_vamp_instance_t), intent(inout) :: instance
    instance%allow_adapt_grids = .true.
    instance%allow_adapt_weights = .true.
  end subroutine mci_vamp_instance_allow_adaptation

```

Adapt grids.

```

(MCI vamp: mci vamp instance: TBP)+≡
  procedure :: adapt_grids => mci_vamp_instance_adapt_grids

(MCI vamp: procedures)+≡
  subroutine mci_vamp_instance_adapt_grids (instance)
    class(mci_vamp_instance_t), intent(inout) :: instance
    if (instance%enable_adapt_grids .and. instance%allow_adapt_grids) then
      if (instance%grids_defined) then
        call vamp_refine_grids (instance%grids)
        instance%n_adapt_grids = instance%n_adapt_grids + 1
      else
        call msg_bug ("VAMP: adapt grids: grids undefined")
      end if
    end if
  end subroutine mci_vamp_instance_adapt_grids

```

Adapt weights. Use the variance array returned by VAMP for recalculating the weight array. The parameter `channel_weights_power` dampens fluctuations.

If the number of calls in a given channel falls below a user-defined threshold, the weight is not lowered further but kept at this threshold. The other channel weights are reduced accordingly.

```

(MCI vamp: mci vamp instance: TBP)+≡
  procedure :: adapt_weights => mci_vamp_instance_adapt_weights

(MCI vamp: procedures)+≡
  subroutine mci_vamp_instance_adapt_weights (instance)
    class(mci_vamp_instance_t), intent(inout) :: instance
    real(default) :: w_sum, w_avg_ch, sum_w_underflow, w_min
    real(default), dimension(:), allocatable :: weights
    integer :: n_ch, ch, n_underflow
    logical, dimension(:), allocatable :: mask, underflow
    type(exception) :: vamp_exception
    logical :: wsum_non_zero
    if (instance%enable_adapt_weights .and. instance%allow_adapt_weights) then
      associate (mci => instance%mci)
        if (instance%grids_defined) then
          allocate (weights (size (instance%grids%weights)))
          weights = instance%grids%weights &
            * vamp_get_variance (instance%grids%grids) &
            ** mci%grid_par%channel_weights_power
          w_sum = sum (weights)

```

```

if (w_sum /= 0) then
  weights = weights / w_sum
  if (mci%n_chain /= 0) then
    allocate (mask (mci%n_channel))
    do ch = 1, mci%n_chain
      mask = mci%chain == ch
      n_ch = count (mask)
      if (n_ch /= 0) then
        w_avg_ch = sum (weights, mask) / n_ch
        where (mask) weights = w_avg_ch
      end if
    end do
  end if
  if (mci%grid_par%threshold_calls /= 0) then
    w_min = &
      real (mci%grid_par%threshold_calls, default) &
      / instance%n_calls
    allocate (underflow (mci%n_channel))
    underflow = weights /= 0 .and. abs (weights) < w_min
    n_underflow = count (underflow)
    sum_w_underflow = sum (weights, mask=underflow)
    if (sum_w_underflow /= 1) then
      where (underflow)
        weights = w_min
      elsewhere
        weights = weights &
          * (1 - n_underflow * w_min) / (1 - sum_w_underflow)
      end where
    end if
  end if
  call instance%set_channel_weights (weights, wsum_non_zero)
  if (wsum_non_zero) call vamp_update_weights &
    (instance%grids, weights, exc = vamp_exception)
  call handle_vamp_exception (vamp_exception, mci%verbose)
else
  call msg_bug ("VAMP: adapt weights: grids undefined")
end if
end associate
instance%n_adapt_weights = instance%n_adapt_weights + 1
end if
end subroutine mci_vamp_instance_adapt_weights

```

Integration: sample the VAMP grids. The number of calls etc. are already stored inside the grids. We provide the random-number generator, the sampling function, and a link to the workspace object, which happens to contain a pointer to the sampler object. The sampler object thus becomes the workspace of the sampling function.

Note: in the current implementation, the random-number generator must be the TAO generator. This explicit dependence should be removed from the VAMP implementation.

(MCI vamp: mci vamp instance: TBP)+≡
 procedure :: sample_grids => mci_vamp_instance_sample_grids

```

(MCI vamp: procedures)+≡
subroutine mci_vamp_instance_sample_grids (instance, rng, sampler, eq)
  class(mci_vamp_instance_t), intent(inout), target :: instance
  class(rng_t), intent(inout) :: rng
  class(mci_sampler_t), intent(inout), target :: sampler
  type(vamp_equivalences_t), intent(in), optional :: eq
  class(vamp_data_t), allocatable :: data
  type(exception) :: vamp_exception
  allocate (mci_workspace_t :: data)
  select type (data)
  type is (mci_workspace_t)
    data%ampler => sampler
    data%instance => instance
  end select
  select type (rng)
  type is (rng_tao_t)
    instance%it = instance%it + 1
    instance%calls = 0
    if (instance%grids_defined) then
      call vamp_sample_grids ( &
        rng%state, &
        instance%grids, &
        vamp_sampling_function, &
        data, &
        1, &
        eq = eq, &
        history = instance%v_history(instance%it:), &
        histories = instance%v_histories(instance%it,:), &
        integral = instance%integral, &
        std_dev = instance%error, &
        exc = vamp_exception, &
        negative_weights = instance%negative_weights)
      call handle_vamp_exception (vamp_exception, instance%mci%verbose)
      instance%efficiency = instance%get_efficiency ()
    else
      call msg_bug ("VAMP: sample grids: grids undefined")
    end if
  class default
    call msg_fatal ("VAMP integration: random-number generator must be TAO")
  end select
end subroutine mci_vamp_instance_sample_grids

```

Compute the reweighting efficiency for the current grids, suitable averaged over all active channels.

```

(MCI vamp: mci_vamp_instance: TBP)+≡
  procedure :: get_efficiency_array => mci_vamp_instance_get_efficiency_array
  procedure :: get_efficiency => mci_vamp_instance_get_efficiency

(MCI vamp: procedures)+≡
function mci_vamp_instance_get_efficiency_array (mci) result (efficiency)
  class(mci_vamp_instance_t), intent(in) :: mci
  real(default), dimension(:), allocatable :: efficiency
  allocate (efficiency (mci%mci%n_channel))
  if (.not. mci%negative_weights) then

```

```

      where (mci%grids%grids%f_max /= 0)
        efficiency = mci%grids%grids%mu(1) / abs (mci%grids%grids%f_max)
      elsewhere
        efficiency = 0
      end where
    else
      where (mci%grids%grids%f_max /= 0)
        efficiency = &
          (mci%grids%grids%mu_plus(1) - mci%grids%grids%mu_minus(1)) &
          / abs (mci%grids%grids%f_max)
      elsewhere
        efficiency = 0
      end where
    end if
  end function mci_vamp_instance_get_efficiency_array

function mci_vamp_instance_get_efficiency (mci) result (efficiency)
  class(mci_vamp_instance_t), intent(in) :: mci
  real(default) :: efficiency
  real(default), dimension(:), allocatable :: weight
  real(default) :: norm
  allocate (weight (mci%mci%n_channel))
  weight = mci%grids%weights * abs (mci%grids%grids%f_max)
  norm = sum (weight)
  if (norm /= 0) then
    efficiency = dot_product (mci%get_efficiency_array (), weight) / norm
  else
    efficiency = 1
  end if
end function mci_vamp_instance_get_efficiency

```

Prepare an event generation pass. Should be called before a sequence of events is generated, then we should call the corresponding finalizer.

The pass-specific data of the previous integration pass are retained, but we reset the number of iterations and calls to zero. The latter now counts the number of events (calls to the sampling function, actually).

```

<MCI vamp: mci vamp instance: TBP>+=
  procedure :: init_simulation => mci_vamp_instance_init_simulation

<MCI vamp: procedures>+=
  subroutine mci_vamp_instance_init_simulation (instance, safety_factor)
    class(mci_vamp_instance_t), intent(inout) :: instance
    real(default), intent(in), optional :: safety_factor
    associate (mci => instance%mci)
      allocate (instance%vamp_x (mci%n_dim))
      instance%it = 0
      instance%calls = 0
      instance%generating_events = .true.
      if (present (safety_factor)) instance%safety_factor = safety_factor
      if (.not. instance%grids_defined) then
        if (mci%grid_filename_set) then
          if (.not. mci%check_grid_file) &
            call msg_warning ("Reading grid file: MD5 sum check disabled")
          call msg_message ("Simulate: " &

```

```

        // "using integration grids from file '" &
        // char (mci%grid_filename) // """)
    call mci%read_grids_data (instance)
    if (instance%safety_factor /= 1) then
        write (msg_buffer, "(A,ES10.3,A)") "Simulate: &
            &applying safety factor", instance%safety_factor, &
            " to event rejection"
        call msg_message ()
        instance%grids%grids%f_max = &
            instance%grids%grids%f_max * instance%safety_factor
    end if
else
    call msg_bug ("VAMP: simulation: no grids, no grid filename")
end if
end if
end associate
end subroutine mci_vamp_instance_init_simulation

```

Finalize an event generation pass. Should be called before a sequence of events is generated, then we should call the corresponding finalizer.

```

<MCI vamp: mci vamp instance: TBP>+=
    procedure :: final_simulation => mci_vamp_instance_final_simulation

<MCI vamp: procedures>+=
    subroutine mci_vamp_instance_final_simulation (instance)
        class(mci_vamp_instance_t), intent(inout) :: instance
        if (allocated (instance%vamp_x)) deallocate (instance%vamp_x)
    end subroutine mci_vamp_instance_final_simulation

```

21.6.7 Sampling function

The VAMP sampling function has a well-defined interface which we have to implement. The `data` argument allows us to pass pointers to the `sampler` and `instance` objects, so we can access configuration data and fill point-dependent contents within these objects.

The `weights` and `channel` argument must be present in the call.

Note: this is the place where we must look for external signals, i.e., interrupt from the OS. We would like to raise a VAMP exception which is then caught by `vamp_sample_grids` as the caller, so it dumps its current state and returns (with the signal still pending). WHIZARD will then terminate gracefully. Of course, VAMP should be able to resume from the dump.

In the current implementation, we handle the exception in place and terminate immediately. The incomplete current integration pass is lost.

```

<MCI vamp: procedures>+=
    function vamp_sampling_function &
        (xi, data, weights, channel, grids) result (f)
        real(default) :: f
        real(default), dimension(:), intent(in) :: xi
        class(vamp_data_t), intent(in) :: data
        real(default), dimension(:), intent(in), optional :: weights
        integer, intent(in), optional :: channel
    end function vamp_sampling_function

```

```

type(vamp_grid), dimension(:), intent(in), optional :: grids
type(exception) :: exc
logical :: verbose
character(*), parameter :: FN = "WHIZARD sampling function"
class(mci_instance_t), pointer :: instance
select type (data)
type is (mci_workspace_t)
  instance => data%instance
  select type (instance)
  class is (mci_vamp_instance_t)
    verbose = instance%mci%verbose
    call instance%evaluate (data%sampler, channel, xi)
    if (signal_is_pending ()) then
      call raise_exception (exc, EXC_FATAL, FN, "signal received")
      call handle_vamp_exception (exc, verbose)
      call terminate_now_if_signal ()
    end if
    instance%calls = instance%calls + 1
    if (data%sampler%is_valid ()) &
      & instance%calls_valid = instance%calls_valid + 1
    f = instance%get_value ()
    call terminate_now_if_single_event ()
  class default
    call msg_bug("VAMP: " // FN // ": unknown MCI instance type")
  end select
end select
end function vamp_sampling_function

```

This is supposed to be the mapping between integration channels. The VAMP event generating procedures technically require it, but it is meaningless in our setup where all transformations happen inside the sampler object. So, this implementation is trivial:

```

⟨MCI vamp: procedures⟩+≡
pure function phi_trivial (xi, channel_dummy) result (x)
  real(default), dimension(:), intent(in) :: xi
  integer, intent(in) :: channel_dummy
  real(default), dimension(size(xi)) :: x
  x = xi
end function phi_trivial

```

21.6.8 Integrator instance: evaluation

Here, we compute the multi-channel reweighting factor for the current channel, that accounts for the Jacobians of the transformations from/to all other channels.

The computation of the VAMP probabilities may consume considerable time, therefore we enable parallel evaluation. (Collecting the contributions to `mci%g` is a reduction, which we should also implement via OpenMP.)

```

⟨MCI vamp: mci vamp instance: TBP⟩+≡
procedure :: compute_weight => mci_vamp_instance_compute_weight

```

```

<MCI vamp: procedures>+=
subroutine mci_vamp_instance_compute_weight (mci, c)
  class(mci_vamp_instance_t), intent(inout) :: mci
  integer, intent(in) :: c
  integer :: i
  mci%selected_channel = c
  !$OMP PARALLEL PRIVATE(i) SHARED(mci)
  !$OMP DO
  do i = 1, mci%nc
    if (mci%w(i) /= 0) then
      mci%gi(i) = vamp_probability (mci%gids%gids(i), mci%x(:,i))
    else
      mci%gi(i) = 0
    end if
  end do
  !$OMP END DO
  !$OMP END PARALLEL
  mci%g = 0
  if (mci%gi(c) /= 0) then
    do i = 1, mci%nc
      if (mci%w(i) /= 0 .and. mci%f(i) /= 0) then
        mci%g = mci%g + mci%w(i) * mci%gi(i) / mci%f(i)
      end if
    end do
  end if
  if (mci%g /= 0) then
    mci%weight = mci%gi(c) / mci%g
  else
    mci%weight = 0
  end if
end subroutine mci_vamp_instance_compute_weight

```

Record the integrand.

```

<MCI vamp: mci vamp instance: TBP>+=
procedure :: record_integrand => mci_vamp_instance_record_integrand

<MCI vamp: procedures>+=
subroutine mci_vamp_instance_record_integrand (mci, integrand)
  class(mci_vamp_instance_t), intent(inout) :: mci
  real(default), intent(in) :: integrand
  mci%integrand = integrand
end subroutine mci_vamp_instance_record_integrand

```

Get the event weight. The default routine returns the same value that we would use for integration. This is correct if we select the integration channel according to the channel weight. `vamp_next_event` does differently, so we should rather rely on the weight that VAMP returns. This is the value stored in `vamp_weight`. We override the default TBP accordingly.

```

<MCI vamp: mci vamp instance: TBP>+=
procedure :: get_event_weight => mci_vamp_instance_get_event_weight
procedure :: get_event_excess => mci_vamp_instance_get_event_excess

<MCI vamp: procedures>+=

```

```

function mci_vamp_instance_get_event_weight (mci) result (value)
  class(mci_vamp_instance_t), intent(in) :: mci
  real(default) :: value
  if (mci%vamp_weight_set) then
    value = mci%vamp_weight
  else
    call msg_bug ("VAMP: attempt to read undefined event weight")
  end if
end function mci_vamp_instance_get_event_weight

function mci_vamp_instance_get_event_excess (mci) result (value)
  class(mci_vamp_instance_t), intent(in) :: mci
  real(default) :: value
  if (mci%vamp_weight_set) then
    value = mci%vamp_excess
  else
    call msg_bug ("VAMP: attempt to read undefined event excess weight")
  end if
end function mci_vamp_instance_get_event_excess

```

21.6.9 VAMP exceptions

A VAMP routine may have raised an exception. Turn this into a WHIZARD error message.

An external signal could raise a fatal exception, but this should be delayed and handled by the correct termination routine.

(MCI vamp: procedures)+≡

```

subroutine handle_vamp_exception (exc, verbose)
  type(exception), intent(in) :: exc
  logical, intent(in) :: verbose
  integer :: exc_level
  if (verbose) then
    exc_level = EXC_INFO
  else
    exc_level = EXC_ERROR
  end if
  if (exc%level >= exc_level) then
    write (msg_buffer, "(A,':',1x,A)") trim (exc%origin), trim (exc%message)
    select case (exc%level)
      case (EXC_INFO); call msg_message ()
      case (EXC_WARN); call msg_warning ()
      case (EXC_ERROR); call msg_error ()
      case (EXC_FATAL)
        if (signal_is_pending ()) then
          call msg_message ()
        else
          call msg_fatal ()
        end if
      end select
  end if
end subroutine handle_vamp_exception

```


21.6.10 Unit tests

Test module, followed by the corresponding implementation module.

```
<mci_vamp.ut.f90>≡  
  <File header>  
  
  module mci_vamp_ut  
    use unit_tests  
    use mci_vamp_util  
  
    <Standard module head>  
  
    <MCI vamp: public test>  
  
    contains  
  
    <MCI vamp: test driver>  
  
  end module mci_vamp_ut  
  
<mci_vamp.uti.f90>≡  
  <File header>  
  
  module mci_vamp_util  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use constants, only: PI, TWOPI  
    use rng_base  
    use rng_tao  
    use phs_base  
    use mci_base  
    use vamp, only: vamp_write_grids !NODEP!  
  
    use mci_vamp  
  
    <Standard module head>  
  
    <MCI vamp: test declarations>  
  
    <MCI vamp: test types>  
  
    contains  
  
    <MCI vamp: tests>  
  
  end module mci_vamp_util  
API: driver for the unit tests below.  
<MCI vamp: public test>≡  
  public :: mci_vamp_test  
<MCI vamp: test driver>≡  
  subroutine mci_vamp_test (u, results)  
    integer, intent(in) :: u
```

```

    type(test_results_t), intent(inout) :: results
    <MCI vamp: execute tests>
end subroutine mci_vamp_test

```

Test sampler

A test sampler object should implement a function with known integral that we can use to check the integrator.

In mode 1, the function is $f(x) = 3x^2$ with integral $\int_0^1 f(x) dx = 1$ and maximum $f(1) = 3$. If the integration dimension is greater than one, the function is extended as a constant in the other dimension(s).

In mode 2, the function is $11x^{10}$, also with integral 1.

Mode 4 includes ranges of zero and negative function value, the integral is negative. The results should be identical to the results of `mci_midpoint_4`, where the same function is evaluated. The function is $f(x) = (1 - 3x^2)\theta(x - 1/2)$ with integral $\int_0^1 f(x) dx = -3/8$, minimum $f(1) = -2$ and maximum $f(1/2) = 1/4$.

```

<MCI vamp: test types>≡
type, extends (mci_sampler_t) :: test_sampler_1_t
    real(default), dimension(:), allocatable :: x
    real(default) :: val
    integer :: mode = 1
contains
    <MCI vamp: test sampler 1: TBP>
end type test_sampler_1_t

```

Output: There is nothing stored inside, so just print an informative line.

```

<MCI vamp: test sampler 1: TBP>≡
    procedure :: write => test_sampler_1_write

<MCI vamp: tests>≡
    subroutine test_sampler_1_write (object, unit, testflag)
        class(test_sampler_1_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u
        u = given_output_unit (unit)
        select case (object%mode)
        case (1)
            write (u, "(1x,A)") "Test sampler: f(x) = 3 x^2"
        case (2)
            write (u, "(1x,A)") "Test sampler: f(x) = 11 x^10"
        case (3)
            write (u, "(1x,A)") "Test sampler: f(x) = 11 x^10 * 2 * cos^2 (2 pi y)"
        case (4)
            write (u, "(1x,A)") "Test sampler: f(x) = (1 - 3 x^2) theta(x - 1/2)"
        end select
    end subroutine test_sampler_1_write

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

<MCI vamp: test sampler 1: TBP>+≡

```

```

    procedure :: evaluate => test_sampler_1_evaluate
<MCI vamp: tests>+=
    subroutine test_sampler_1_evaluate (sampler, c, x_in, val, x, f)
        class(test_sampler_1_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        if (allocated (sampler%x)) deallocate (sampler%x)
        allocate (sampler%x (size (x_in)))
        sampler%x = x_in
        select case (sampler%mode)
        case (1)
            sampler%val = 3 * x_in(1) ** 2
        case (2)
            sampler%val = 11 * x_in(1) ** 10
        case (3)
            sampler%val = 11 * x_in(1) ** 10 * 2 * cos (twopi * x_in(2)) ** 2
        case (4)
            if (x_in(1) >= .5_default) then
                sampler%val = 1 - 3 * x_in(1) ** 2
            else
                sampler%val = 0
            end if
        end select
        call sampler%fetch (val, x, f)
    end subroutine test_sampler_1_evaluate

```

The point is always valid.

```

<MCI vamp: test sampler 1: TBP>+=
    procedure :: is_valid => test_sampler_1_is_valid
<MCI vamp: tests>+=
    function test_sampler_1_is_valid (sampler) result (valid)
        class(test_sampler_1_t), intent(in) :: sampler
        logical :: valid
        valid = .true.
    end function test_sampler_1_is_valid

```

Rebuild: compute all but the function value.

```

<MCI vamp: test sampler 1: TBP>+=
    procedure :: rebuild => test_sampler_1_rebuild
<MCI vamp: tests>+=
    subroutine test_sampler_1_rebuild (sampler, c, x_in, val, x, f)
        class(test_sampler_1_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(in) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        if (allocated (sampler%x)) deallocate (sampler%x)

```

```

allocate (sampler%x (size (x_in)))
sampler%x = x_in
sampler%val = val
x(:,1) = sampler%x
f = 1
end subroutine test_sampler_1_rebuild

```

Extract the results.

```

⟨MCI vamp: test sampler 1: TBP⟩+=
  procedure :: fetch => test_sampler_1_fetch
⟨MCI vamp: tests⟩+=
  subroutine test_sampler_1_fetch (sampler, val, x, f)
    class(test_sampler_1_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_1_fetch

```

Two-channel, two dimension test sampler

This sampler implements the function

$$f(x, y) = 4 \sin^2(\pi x) \sin^2(\pi y) + 2 \sin^2(\pi v) \quad (21.11)$$

where

$$x = u^v \quad u = xy \quad (21.12)$$

$$y = u^{(1-v)} \quad v = \frac{1}{2} \left(1 + \frac{\log(x/y)}{\log xy} \right) \quad (21.13)$$

Each term contributes 1 to the integral. The first term in the function is peaked along a cross aligned to the coordinates x and y , while the second term is peaked along the diagonal $x = y$.

The Jacobian is

$$\frac{\partial(x, y)}{\partial(u, v)} = |\log u| \quad (21.14)$$

```

⟨MCI vamp: test types⟩+=
  type, extends (mci_sampler_t) :: test_sampler_2_t
    real(default), dimension(:,:), allocatable :: x
    real(default), dimension(:), allocatable :: f
    real(default) :: val
  contains
    ⟨MCI vamp: test sampler 2: TBP⟩
  end type test_sampler_2_t

```

Output: There is nothing stored inside, so just print an informative line.

```

⟨MCI vamp: test sampler 2: TBP⟩=
  procedure :: write => test_sampler_2_write

```

```

<MCI vamp: tests>+≡
  subroutine test_sampler_2_write (object, unit, testflag)
    class(test_sampler_2_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Two-channel test sampler 2"
  end subroutine test_sampler_2_write

```

Kinematics: compute x and Jacobians, given the input parameter array.

```

<MCI vamp: test sampler 2: TBP>+≡
  procedure :: compute => test_sampler_2_compute

<MCI vamp: tests>+≡
  subroutine test_sampler_2_compute (sampler, c, x_in)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default) :: xx, yy, uu, vv
    if (.not. allocated (sampler%x)) &
      allocate (sampler%x (size (x_in), 2))
    if (.not. allocated (sampler%f)) &
      allocate (sampler%f (2))
    select case (c)
    case (1)
      xx = x_in(1)
      yy = x_in(2)
      uu = xx * yy
      vv = (1 + log (xx/yy) / log (xx*yy)) / 2
    case (2)
      uu = x_in(1)
      vv = x_in(2)
      xx = uu ** vv
      yy = uu ** (1 - vv)
    end select
    sampler%val = (2 * sin (pi * xx) * sin (pi * yy)) ** 2 &
      + 2 * sin (pi * vv) ** 2
    sampler%f(1) = 1
    sampler%f(2) = abs (log (uu))
    sampler%x(:,1) = [xx, yy]
    sampler%x(:,2) = [uu, vv]
  end subroutine test_sampler_2_compute

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

<MCI vamp: test sampler 2: TBP>+≡
  procedure :: evaluate => test_sampler_2_evaluate

<MCI vamp: tests>+≡
  subroutine test_sampler_2_evaluate (sampler, c, x_in, val, x, f)
    class(test_sampler_2_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in

```

```

    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    call sampler%compute (c, x_in)
    call sampler%fetch (val, x, f)
end subroutine test_sampler_2_evaluate

```

The point is always valid.

```

⟨MCI vamp: test sampler 2: TBP⟩+≡
    procedure :: is_valid => test_sampler_2_is_valid

⟨MCI vamp: tests⟩+≡
    function test_sampler_2_is_valid (sampler) result (valid)
        class(test_sampler_2_t), intent(in) :: sampler
        logical :: valid
        valid = .true.
    end function test_sampler_2_is_valid

```

Rebuild: compute all but the function value.

```

⟨MCI vamp: test sampler 2: TBP⟩+≡
    procedure :: rebuild => test_sampler_2_rebuild

⟨MCI vamp: tests⟩+≡
    subroutine test_sampler_2_rebuild (sampler, c, x_in, val, x, f)
        class(test_sampler_2_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(in) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        call sampler%compute (c, x_in)
        x = sampler%x
        f = sampler%f
    end subroutine test_sampler_2_rebuild

```

Extract the results.

```

⟨MCI vamp: test sampler 2: TBP⟩+≡
    procedure :: fetch => test_sampler_2_fetch

⟨MCI vamp: tests⟩+≡
    subroutine test_sampler_2_fetch (sampler, val, x, f)
        class(test_sampler_2_t), intent(in) :: sampler
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        val = sampler%val
        x = sampler%x
        f = sampler%f
    end subroutine test_sampler_2_fetch

```

Two-channel, one dimension test sampler

This sampler implements the function

$$f(x, y) = a * 5x^4 + b * 5(1 - x)^4 \quad (21.15)$$

Each term contributes 1 to the integral, multiplied by a or b , respectively. The first term is peaked at $x = 1$, the second one at $x = 0$.

We implement the two mappings

$$x = u^{1/5} \quad \text{and} \quad x = 1 - v^{1/5}, \quad (21.16)$$

with Jacobians

$$\frac{\partial(x)}{\partial(u)} = u^{-4/5}/5 \quad \text{and} \quad v^{-4/5}/5, \quad (21.17)$$

respectively. The first mapping concentrates points near $x = 1$, the second one near $x = 0$.

```

<MCI vamp: test types>+≡
  type, extends (mci_sampler_t) :: test_sampler_3_t
    real(default), dimension(:,:), allocatable :: x
    real(default), dimension(:), allocatable :: f
    real(default) :: val
    real(default) :: a = 1
    real(default) :: b = 1
  contains
    <MCI vamp: test sampler 3: TBP>
  end type test_sampler_3_t

```

Output: display a and b

```

<MCI vamp: test sampler 3: TBP>≡
  procedure :: write => test_sampler_3_write

<MCI vamp: tests>+≡
  subroutine test_sampler_3_write (object, unit, testflag)
    class(test_sampler_3_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Two-channel test sampler 3"
    write (u, "(3x,A,F5.2)") "a = ", object%a
    write (u, "(3x,A,F5.2)") "b = ", object%b
  end subroutine test_sampler_3_write

```

Kinematics: compute x and Jacobians, given the input parameter array.

```

<MCI vamp: test sampler 3: TBP>+≡
  procedure :: compute => test_sampler_3_compute

<MCI vamp: tests>+≡
  subroutine test_sampler_3_compute (sampler, c, x_in)
    class(test_sampler_3_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in

```

```

real(default) :: u, v, xx
if (.not. allocated (sampler%x)) &
    allocate (sampler%x (size (x_in), 2))
if (.not. allocated (sampler%f)) &
    allocate (sampler%f (2))
select case (c)
case (1)
    u = x_in(1)
    xx = u ** 0.2_default
    v = (1 - xx) ** 5._default
case (2)
    v = x_in(1)
    xx = 1 - v ** 0.2_default
    u = xx ** 5._default
end select
sampler%val = sampler%a * 5 * xx ** 4 + sampler%b * 5 * (1 - xx) ** 4
sampler%f(1) = 0.2_default * u ** (-0.8_default)
sampler%f(2) = 0.2_default * v ** (-0.8_default)
sampler%x(:,1) = [u]
sampler%x(:,2) = [v]
end subroutine test_sampler_3_compute

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

<MCI vamp: test sampler 3: TBP>+=
    procedure :: evaluate => test_sampler_3_evaluate

<MCI vamp: tests>+=
    subroutine test_sampler_3_evaluate (sampler, c, x_in, val, x, f)
        class(test_sampler_3_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        call sampler%compute (c, x_in)
        call sampler%fetch (val, x, f)
    end subroutine test_sampler_3_evaluate

```

The point is always valid.

```

<MCI vamp: test sampler 3: TBP>+=
    procedure :: is_valid => test_sampler_3_is_valid

<MCI vamp: tests>+=
    function test_sampler_3_is_valid (sampler) result (valid)
        class(test_sampler_3_t), intent(in) :: sampler
        logical :: valid
        valid = .true.
    end function test_sampler_3_is_valid

```

Rebuild: compute all but the function value.

```

<MCI vamp: test sampler 3: TBP>+=
    procedure :: rebuild => test_sampler_3_rebuild

```



```

<MCI vamp: tests>+≡
  subroutine test_sampler_3_rebuild (sampler, c, x_in, val, x, f)
    class(test_sampler_3_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(in) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    call sampler%compute (c, x_in)
    x = sampler%x
    f = sampler%f
  end subroutine test_sampler_3_rebuild

```

Extract the results.

```

<MCI vamp: test sampler 3: TBP>+≡
  procedure :: fetch => test_sampler_3_fetch

<MCI vamp: tests>+≡
  subroutine test_sampler_3_fetch (sampler, val, x, f)
    class(test_sampler_3_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x = sampler%x
    f = sampler%f
  end subroutine test_sampler_3_fetch

```

One-dimensional integration

Construct an integrator and use it for a one-dimensional sampler.

Note: We would like to check the precise contents of the grid allocated during integration, but the output format for reals is very long (for good reasons), so the last digits in the grid content display are numerical noise. So, we just check the integration results.

```

<MCI vamp: execute tests>≡
  call test (mci_vamp_1, "mci_vamp_1", &
    "one-dimensional integral", &
    u, results)

<MCI vamp: test declarations>≡
  public :: mci_vamp_1

<MCI vamp: tests>+≡
  subroutine mci_vamp_1 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_1"

```

```

write (u, "(A)")  "* Purpose: integrate function in one dimension &
                    &(single channel)"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 1)
select type (mci)
type is (mci_vamp_t)
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize instance"
write (u, "(A)")

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Initialize test sampler"
write (u, "(A)")

allocate (test_sampler_1_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")  "    (lower precision to avoid"
write (u, "(A)")  "        numerical noise)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass ()
end select
call mci%integrate (mci_instance, sampler, 1, 1000, pacify = .true.)
call mci%write (u, .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u, .true.)

write (u, "(A)")

```

```

write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_1"

end subroutine mci_vamp_1

```

Multiple iterations

Construct an integrator and use it for a one-dimensional sampler. Integrate with five iterations without grid adaptation.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_2, "mci_vamp_2", &
    "multiple iterations", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_2

<MCI vamp: tests>+≡
  subroutine mci_vamp_2 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_2"
    write (u, "(A)")  "* Purpose: integrate function in one dimension &
      &(single channel)"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (1, 1)
    select type (mci)
      type is (mci_vamp_t)
        grid_par%use_vamp_equivalences = .false.
        call mci%set_grid_parameters (grid_par)
      end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

```

```

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 2
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 100"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .false.)
end select
call mci%integrate (mci_instance, sampler, 3, 100)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_2"

end subroutine mci_vamp_2

```

Grid adaptation

Construct an integrator and use it for a one-dimensional sampler. Integrate with three iterations and in-between grid adaptations.

```

<MCI vamp: execute tests>+≡
    call test (mci_vamp_3, "mci_vamp_3", &
        "grid adaptation", &
        u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_3

<MCI vamp: tests>+≡
    subroutine mci_vamp_3 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par
        class(mci_t), allocatable, target :: mci

```

```

class(mci_instance_t), pointer :: mci_instance => null ()
class(mci_sampler_t), allocatable :: sampler
class(rng_t), allocatable :: rng

write (u, "(A)")  "* Test output: mci_vamp_3"
write (u, "(A)")  "* Purpose: integrate function in one dimension &
                    &(single channel)"
write (u, "(A)")  "*               and adapt grid"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 1)
select type (mci)
type is (mci_vamp_t)
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 2
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 100"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 100)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_3"

end subroutine mci_vamp_3

```

Two-dimensional integral

Construct an integrator and use it for a two-dimensional sampler. Integrate with three iterations and in-between grid adaptations.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_4, "mci_vamp_4", &
    "two-dimensional integration", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_4

<MCI vamp: tests>+≡
  subroutine mci_vamp_4 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_4"
    write (u, "(A)")  "* Purpose: integrate function in two dimensions &
      &(single channel)"
    write (u, "(A)")  "*               and adapt grid"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (2, 1)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

```

```

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 3
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_4"

end subroutine mci_vamp_4

```

Two-channel integral

Construct an integrator and use it for a two-dimensional sampler with two channels.

Integrate with three iterations and in-between grid adaptations.

```

<MCI vamp: execute tests>+≡
    call test (mci_vamp_5, "mci_vamp_5", &
        "two-dimensional integration", &
        u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_5

<MCI vamp: tests>+≡
    subroutine mci_vamp_5 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par

```

```

class(mci_t), allocatable, target :: mci
class(mci_instance_t), pointer :: mci_instance => null ()
class(mci_sampler_t), allocatable :: sampler
class(rng_t), allocatable :: rng

write (u, "(A)")  "* Test output: mci_vamp_5"
write (u, "(A)")  "* Purpose: integrate function in two dimensions &
                    &(two channels)"
write (u, "(A)")  "*           and adapt grid"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_2_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()

```



```

call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_5"

end subroutine mci_vamp_5

```

Weight adaptation

Construct an integrator and use it for a one-dimensional sampler with two channels.

Integrate with three iterations and in-between weight adaptations.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_6, "mci_vamp_6", &
    "weight adaptation", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_6

<MCI vamp: tests>+≡
  subroutine mci_vamp_6 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_6"
    write (u, "(A)")  "* Purpose: integrate function in one dimension &
      &(two channels)"
    write (u, "(A)")  "*           and adapt weights"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (1, 2)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%stratified = .false.
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()
    call mci%import_rng (rng)

    call mci%allocate_instance (mci_instance)
    call mci_instance%init (mci)

```

```

allocate (test_sampler_3_t :: sampler)
select type (sampler)
type is (test_sampler_3_t)
    sampler%a = 0.9_default
    sampler%b = 0.1_default
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_weights = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()
deallocate (mci_instance)
deallocate (mci)

write (u, "(A)")
write (u, "(A)")  "* Re-initialize with chained channels"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 2)
call mci%declare_chains ([1,1])
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

```

```

write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass (adapt_weights = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_6"

end subroutine mci_vamp_6

```

Equivalences

Construct an integrator and use it for a one-dimensional sampler with two channels.

Integrate with three iterations and in-between grid adaptations. Apply an equivalence between the two channels, so the binning of the two channels is forced to coincide. Compare this with the behavior without equivalences.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_7, "mci_vamp_7", &
    "use channel equivalences", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_7

<MCI vamp: tests>+≡
  subroutine mci_vamp_7 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    type(phs_channel_t), dimension(:), allocatable :: channel
    class(rng_t), allocatable :: rng
    real(default), dimension(:,:), allocatable :: x

```

```

integer :: u_grid, iostat, i, div, ch
character(16) :: buffer

write (u, "(A)")  "* Test output: mci_vamp_7"
write (u, "(A)")  "* Purpose: check effect of channel equivalences"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_3_t :: sampler)
select type (sampler)
type is (test_sampler_3_t)
    sampler%a = 0.7_default
    sampler%b = 0.3_default
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 2 and n_calls = 1000, &
    &adapt grids"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 2, 1000)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write grids and extract binning"
write (u, "(A)")

u_grid = free_unit ()
open (u_grid, status = "scratch", action = "readwrite")
select type (mci_instance)

```

```

type is (mci_vamp_instance_t)
    call vamp_write_grids (mci_instance%grids, u_grid)
end select
rewind (u_grid)
allocate (x (0:20, 2))
do div = 1, 2
    FIND_BINS1: do
        read (u_grid, "(A)") buffer
        if (trim (adjustl (buffer)) == "begin d%x") then
            do
                read (u_grid, *, iostat = iostat) i, x(i,div)
                if (iostat /= 0) exit FIND_BINS1
            end do
        end if
    end do FIND_BINS1
end do
close (u_grid)

write (u, "(1x,A,L1)") "Equal binning in both channels = ", &
    all (x(:,1) == x(:,2))
deallocate (x)

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mci_instance%final ()
call mci%final ()
deallocate (mci_instance)
deallocate (mci)

write (u, "(A)")
write (u, "(A)") "* Re-initialize integrator, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .true.
    call mci%set_grid_parameters (grid_par)
end select

write (u, "(A)") "* Define equivalences"
write (u, "(A)")

allocate (channel (2))
do ch = 1, 2
    allocate (channel(ch)%eq (2))
    do i = 1, 2
        associate (eq => channel(ch)%eq(i))
            call eq%init (1)
            eq%c = i
            eq%perm = [1]
        end associate
    end do
end do

```

```

        eq%mode = [0]
    end associate
end do
write (u, "(1x,I0,':')", advance = "no")  ch
call channel(ch)%write (u)
end do
call mci%declare_equivalences (channel, dim_offset = 0)

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 2 and n_calls = 1000, &
&adapt grids"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 2, 1000)

call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write grids and extract binning"
write (u, "(A)")

u_grid = free_unit ()
open (u_grid, status = "scratch", action = "readwrite")
select type (mci_instance)
type is (mci_vamp_instance_t)
    call vamp_write_grids (mci_instance%grids, u_grid)
end select
rewind (u_grid)
allocate (x (0:20, 2))
do div = 1, 2
    FIND_BINS2: do
        read (u_grid, "(A)")  buffer
        if (trim (adjustl (buffer)) == "begin d%x") then
            do
                read (u_grid, *, iostat = iostat)  i, x(i,div)
                if (iostat /= 0)  exit FIND_BINS2
            end do
        end if
    end do FIND_BINS2
end do
close (u_grid)

write (u, "(1x,A,L1)")  "Equal binning in both channels = ", &

```

```

        all (x(:,1) == x(:,2))
deallocate (x)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_7"

end subroutine mci_vamp_7

```

Multiple passes

Integrate with three passes and different settings for weight and grid adaptation.

```

<MCI vamp: execute tests>+≡
    call test (mci_vamp_8, "mci_vamp_8", &
        "integration passes", &
        u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_8

<MCI vamp: tests>+≡
    subroutine mci_vamp_8 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng

        write (u, "(A)")  "* Test output: mci_vamp_8"
        write (u, "(A)")  "*   Purpose: integrate function in one dimension &
            &(two channels)"
        write (u, "(A)")  "*               in three passes"

        write (u, "(A)")
        write (u, "(A)")  "* Initialize integrator, sampler, instance"
        write (u, "(A)")

        allocate (mci_vamp_t :: mci)
        call mci%set_dimensions (1, 2)
        select type (mci)
        type is (mci_vamp_t)
            grid_par%stratified = .false.
            grid_par%use_vamp_equivalences = .false.
            call mci%set_grid_parameters (grid_par)
        end select

        allocate (rng_tao_t :: rng)

```

```

call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_3_t :: sampler)
select type (sampler)
type is (test_sampler_3_t)
    sampler%a = 0.9_default
    sampler%b = 0.1_default
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with grid and weight adaptation"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true., adapt_weights = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with grid adaptation"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate without adaptation"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)

```



```

        call mci%add_pass ()
    end select
    call mci%integrate (mci_instance, sampler, 3, 1000)
    call mci%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Contents of mci_instance:"
    write (u, "(A)")

    call mci_instance%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call mci_instance%final ()
    call mci%final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: mci_vamp_8"

end subroutine mci_vamp_8

```

Weighted events

Construct an integrator and use it for a two-dimensional sampler with two channels. Integrate and generate a weighted event.

```

<MCI vamp: execute tests>+≡
    call test (mci_vamp_9, "mci_vamp_9", &
        "weighted event", &
        u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_9

<MCI vamp: tests>+≡
    subroutine mci_vamp_9 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng

        write (u, "(A)")  "* Test output: mci_vamp_9"
        write (u, "(A)")  "*   Purpose: integrate function in two dimensions &
            &(two channels)"
        write (u, "(A)")  "*               and generate a weighted event"

        write (u, "(A)")
        write (u, "(A)")  "* Initialize integrator, sampler, instance"
        write (u, "(A)")

        allocate (mci_vamp_t :: mci)

```

```

call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_2_t :: sampler)
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

call mci%add_pass ()
call mci%integrate (mci_instance, sampler, 1, 1000)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate a weighted event"
write (u, "(A)")

call mci_instance%init_simulation ()
call mci%generate_weighted_event (mci_instance, sampler)

write (u, "(1x,A)")  "MCI instance:"
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final_simulation ()
call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_9"

end subroutine mci_vamp_9

```

Grids I/O

Construct an integrator and allocate grids. Write grids to file, read them in again and compare.

```

<MCI vamp: execute tests>+≡
    call test (mci_vamp_10, "mci_vamp_10", &
               "grids I/O", &
               u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_10

<MCI vamp: tests>+≡
    subroutine mci_vamp_10 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng
        type(string_t) :: file1, file2
        character(80) :: buffer1, buffer2
        integer :: u1, u2, iostat1, iostat2
        logical :: equal, success

        write (u, "(A)")  "* Test output: mci_vamp_10"
        write (u, "(A)")  "* Purpose: write and read VAMP grids"

        write (u, "(A)")
        write (u, "(A)")  "* Initialize integrator, sampler, instance"
        write (u, "(A)")

        allocate (mci_vamp_t :: mci)
        call mci%set_dimensions (2, 2)
        select type (mci)
        type is (mci_vamp_t)
            grid_par%stratified = .false.
            grid_par%use_vamp_equivalences = .false.
            call mci%set_grid_parameters (grid_par)
        end select

        allocate (rng_tao_t :: rng)
        call rng%init ()
        call mci%import_rng (rng)

        mci%md5sum = "1234567890abcdef1234567890abcdef"

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        allocate (test_sampler_2_t :: sampler)
        call sampler%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
        write (u, "(A)")

        call mci%add_pass ()
        call mci%integrate (mci_instance, sampler, 1, 1000)

```

```

write (u, "(A)")  "* Write grids to file"
write (u, "(A)")

file1 = "mci_vamp_10.1"
select type (mci)
type is (mci_vamp_t)
    call mci%set_grid_filename (file1)
    call mci%write_grids (mci_instance)
end select

call mci_instance%final ()
call mci%final ()
deallocate (mci)

write (u, "(A)")  "* Read grids from file"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_vamp_t)
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

mci%md5sum = "1234567890abcdef1234567890abcdef"

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

select type (mci)
type is (mci_vamp_t)
    call mci%set_grid_filename (file1)
    call mci%add_pass ()
    call mci%current_pass%configure (1, 1000, &
        mci%min_calls, &
        mci%grid_par%min_bins, mci%grid_par%max_bins, &
        mci%grid_par%min_calls_per_channel * mci%n_channel)
    call mci%read_grids_header (success)
    call mci%compute_md5sum ()
    call mci%read_grids_data (mci_instance, read_integrals = .true.)
end select
write (u, "(1x,A,L1)")  "success = ", success

write (u, "(A)")
write (u, "(A)")  "* Write grids again"
write (u, "(A)")

file2 = "mci_vamp_10.2"
select type (mci)

```

```

type is (mci_vamp_t)
  call mci%set_grid_filename (file2)
  call mci%write_grids (mci_instance)
end select

u1 = free_unit ()
open (u1, file = char (file1) // ".vg", action = "read", status = "old")
u2 = free_unit ()
open (u2, file = char (file2) // ".vg", action = "read", status = "old")

equal = .true.
iostat1 = 0
iostat2 = 0
do while (equal .and. iostat1 == 0 .and. iostat2 == 0)
  read (u1, "(A)", iostat = iostat1) buffer1
  read (u2, "(A)", iostat = iostat2) buffer2
  equal = buffer1 == buffer2 .and. iostat1 == iostat2
end do
close (u1)
close (u2)

if (equal) then
  write (u, "(1x,A)") "Success: grid files are identical"
else
  write (u, "(1x,A)") "Failure: grid files differ"
end if

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: mci_vamp_10"

end subroutine mci_vamp_10

```

Weighted events with grid I/O

Construct an integrator and use it for a two-dimensional sampler with two channels. Integrate, write grids, and generate a weighted event using the grids from file.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_11, "mci_vamp_11", &
    "weighted events with grid I/O", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_11

<MCI vamp: tests>+≡
  subroutine mci_vamp_11 (u)

```

```

integer, intent(in) :: u
type(grid_parameters_t) :: grid_par
class(mci_t), allocatable, target :: mci
class(mci_instance_t), pointer :: mci_instance => null ()
class(mci_sampler_t), allocatable :: sampler
class(rng_t), allocatable :: rng

write (u, "(A)")  "* Test output: mci_vamp_11"
write (u, "(A)")  "*   Purpose: integrate function in two dimensions &
                    &(two channels)"
write (u, "(A)")  "*               and generate a weighted event"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
    call mci%set_grid_filename (var_str ("mci_vamp_11"))
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_2_t :: sampler)

write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

call mci%add_pass ()
call mci%integrate (mci_instance, sampler, 1, 1000)

write (u, "(A)")  "* Reset instance"
write (u, "(A)")

call mci_instance%final ()
call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Generate a weighted event"
write (u, "(A)")

call mci_instance%init_simulation ()
call mci%generate_weighted_event (mci_instance, sampler)

```

```

write (u, "(A)")  "* Cleanup"

call mci_instance%final_simulation ()
call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_11"

end subroutine mci_vamp_11

```

Unweighted events with grid I/O

Construct an integrator and use it for a two-dimensional sampler with two channels.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_12, "mci_vamp_12", &
    "unweighted events with grid I/O", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_12

<MCI vamp: tests>+≡
  subroutine mci_vamp_12 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_12"
    write (u, "(A)")  "*   Purpose: integrate function in two dimensions &
      &(two channels)"
    write (u, "(A)")  "*               and generate an unweighted event"

    write (u, "(A)")
    write (u, "(A)")  "* Initialize integrator, sampler, instance"
    write (u, "(A)")

    allocate (mci_vamp_t :: mci)
    call mci%set_dimensions (2, 2)
    select type (mci)
    type is (mci_vamp_t)
      grid_par%stratified = .false.
      grid_par%use_vamp_equivalences = .false.
      call mci%set_grid_parameters (grid_par)
      call mci%set_grid_filename (var_str ("mci_vamp_12"))
    end select

    allocate (rng_tao_t :: rng)
    call rng%init ()

```

```

call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_2_t :: sampler)

write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 1000"
write (u, "(A)")

call mci%add_pass ()
call mci%integrate (mci_instance, sampler, 1, 1000)

write (u, "(A)")  "* Reset instance"
write (u, "(A)")

call mci_instance%final ()
call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

write (u, "(A)")  "* Generate an unweighted event"
write (u, "(A)")

call mci_instance%init_simulation ()
call mci%generate_unweighted_event (mci_instance, sampler)

write (u, "(1x,A)")  "MCI instance:"
call mci_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final_simulation ()
call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_12"

end subroutine mci_vamp_12

```

Update integration results

Compare two mci objects; match the two and update the first if successful.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_13, "mci_vamp_13", &
    "updating integration results", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_13

<MCI vamp: tests>+≡
  subroutine mci_vamp_13 (u)

```



```

integer, intent(in) :: u
type(grid_parameters_t) :: grid_par
class(mci_t), allocatable, target :: mci, mci_ref
logical :: success

write (u, "(A)")  "* Test output: mci_vamp_13"
write (u, "(A)")  "* Purpose: match and update integrators"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator with no passes"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (2, 2)
select type (mci)
type is (mci_vamp_t)
    grid_par%stratified = .false.
    grid_par%use_vamp_equivalences = .false.
    call mci%set_grid_parameters (grid_par)
end select
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize reference"
write (u, "(A)")

allocate (mci_vamp_t :: mci_ref)
call mci_ref%set_dimensions (2, 2)
select type (mci_ref)
type is (mci_vamp_t)
    call mci_ref%set_grid_parameters (grid_par)
end select

select type (mci_ref)
type is (mci_vamp_t)
    call mci_ref%add_pass (adapt_grids = .true.)
    call mci_ref%current_pass%configure (2, 1000, 0, 1, 5, 0)
    mci_ref%current_pass%calls = [77, 77]
    mci_ref%current_pass%integral = [1.23_default, 3.45_default]
    mci_ref%current_pass%error = [0.23_default, 0.45_default]
    mci_ref%current_pass%efficiency = [0.1_default, 0.6_default]
    mci_ref%current_pass%integral_defined = .true.

    call mci_ref%add_pass ()
    call mci_ref%current_pass%configure (2, 2000, 0, 1, 7, 0)
    mci_ref%current_pass%calls = [99, 0]
    mci_ref%current_pass%integral = [7.89_default, 0._default]
    mci_ref%current_pass%error = [0.89_default, 0._default]
    mci_ref%current_pass%efficiency = [0.86_default, 0._default]
    mci_ref%current_pass%integral_defined = .true.
end select

call mci_ref%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Update integrator (no-op, should succeed)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)")  "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Add pass to integrator"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass (adapt_grids = .true.)
  call mci%current_pass%configure (2, 1000, 0, 1, 5, 0)
  mci%current_pass%calls = [77, 77]
  mci%current_pass%integral = [1.23_default, 3.45_default]
  mci%current_pass%error = [0.23_default, 0.45_default]
  mci%current_pass%efficiency = [0.1_default, 0.6_default]
  mci%current_pass%integral_defined = .true.
end select

write (u, "(A)")  "* Update integrator (no-op, should succeed)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)")  "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Add pass to integrator, wrong parameters"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass ()
  call mci%current_pass%configure (2, 1000, 0, 1, 7, 0)
end select

write (u, "(A)")  "* Update integrator (should fail)"
write (u, "(A)")

select type (mci)

```

```

type is (mci_vamp_t)
    call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)") "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Reset and add passes to integrator"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%reset ()
    call mci%add_pass (adapt_grids = .true.)
    call mci%current_pass%configure (2, 1000, 0, 1, 5, 0)
    mci%current_pass%calls = [77, 77]
    mci%current_pass%integral = [1.23_default, 3.45_default]
    mci%current_pass%error = [0.23_default, 0.45_default]
    mci%current_pass%efficiency = [0.1_default, 0.6_default]
    mci%current_pass%integral_defined = .true.

    call mci%add_pass ()
    call mci%current_pass%configure (2, 2000, 0, 1, 7, 0)
end select

write (u, "(A)")  "* Update integrator (should succeed)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)") "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Update again (no-op, should succeed)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)") "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Add extra result to integrator"

```

```

write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  mci%current_pass%calls(2) = 1234
end select

write (u, "(A)")  "* Update integrator (should fail)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%update_from_ref (mci_ref, success)
end select

write (u, "(1x,A,L1)")  "success = ", success
write (u, "(A)")
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci%final ()
call mci_ref%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_13"

end subroutine mci_vamp_13

```

Accuracy Goal

Integrate with multiple iterations. Skip iterations once an accuracy goal has been reached.

```

<MCI vamp: execute tests>+≡
  call test (mci_vamp_14, "mci_vamp_14", &
    "accuracy goal", &
    u, results)

<MCI vamp: test declarations>+≡
  public :: mci_vamp_14

<MCI vamp: tests>+≡
  subroutine mci_vamp_14 (u)
    integer, intent(in) :: u
    type(grid_parameters_t) :: grid_par
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng

    write (u, "(A)")  "* Test output: mci_vamp_14"
    write (u, "(A)")  "* Purpose: integrate function in one dimension &

```

```

        &(single channel)"
write (u, "(A)")  "*"                and check accuracy goal"

write (u, "(A)")
write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp_t :: mci)
call mci%set_dimensions (1, 1)
select type (mci)
type is (mci_vamp_t)
    grid_par%use_vamp_equivalences = .false.
    grid_par%accuracy_goal = 5E-2_default
    call mci%set_grid_parameters (grid_par)
end select

allocate (rng_tao_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 2
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 5 and n_calls = 100"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 5, 100)
call mci%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_14"

end subroutine mci_vamp_14

```

VAMP history

Integrate with three passes and different settings for weight and grid adaptation.
Then show the VAMP history.

```
<MCI vamp: execute tests>+≡
    call test (mci_vamp_15, "mci_vamp_15", &
               "VAMP history", &
               u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_15

<MCI vamp: tests>+≡
    subroutine mci_vamp_15 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par
        type(history_parameters_t) :: history_par
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng

        write (u, "(A)")  "*" Test output: mci_vamp_15"
        write (u, "(A)")  "*" Purpose: integrate function in one dimension &
                           &(two channels)"
        write (u, "(A)")  "*"           in three passes, show history"

        write (u, "(A)")
        write (u, "(A)")  "*" Initialize integrator, sampler, instance"
        write (u, "(A)")

        history_par%channel = .true.

        allocate (mci_vamp_t :: mci)
        call mci%set_dimensions (1, 2)
        select type (mci)
        type is (mci_vamp_t)
            grid_par%stratified = .false.
            grid_par%use_vamp_equivalences = .false.
            call mci%set_grid_parameters (grid_par)
            call mci%set_history_parameters (history_par)
        end select

        allocate (rng_tao_t :: rng)
        call rng%init ()
        call mci%import_rng (rng)

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        allocate (test_sampler_3_t :: sampler)
        select type (sampler)
        type is (test_sampler_3_t)
            sampler%a = 0.9_default
            sampler%b = 0.1_default
```

```

end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Pass 1: grid and weight adaptation"

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true., adapt_weights = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)

write (u, "(A)")
write (u, "(A)")  "* Pass 2: grid adaptation"

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000)

write (u, "(A)")
write (u, "(A)")  "* Pass 3: without adaptation"

select type (mci)
type is (mci_vamp_t)
    call mci%add_pass ()
end select
call mci%integrate (mci_instance, sampler, 3, 1000)

write (u, "(A)")
write (u, "(A)")  "* Contents of MCI record, with history"
write (u, "(A)")

call mci%write (u)
select type (mci)
type is (mci_vamp_t)
    call mci%write_history (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_15"

end subroutine mci_vamp_15

```

One-dimensional integration with sign change

Construct an integrator and use it for a one-dimensional sampler.

```
<MCI vamp: execute tests>+≡
    call test (mci_vamp_16, "mci_vamp_16", &
               "1-D integral with sign change", &
               u, results)

<MCI vamp: test declarations>+≡
    public :: mci_vamp_16

<MCI vamp: tests>+≡
    subroutine mci_vamp_16 (u)
        integer, intent(in) :: u
        type(grid_parameters_t) :: grid_par
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable :: sampler
        class(rng_t), allocatable :: rng

        write (u, "(A)")  "* Test output: mci_vamp_16"
        write (u, "(A)")  "* Purpose: integrate function in one dimension &
                           &(single channel)"

        write (u, "(A)")
        write (u, "(A)")  "* Initialize integrator"
        write (u, "(A)")

        allocate (mci_vamp_t :: mci)
        call mci%set_dimensions (1, 1)
        select type (mci)
            type is (mci_vamp_t)
                grid_par%use_vamp_equivalences = .false.
                call mci%set_grid_parameters (grid_par)
                mci%negative_weights = .true.
            end select

        allocate (rng_tao_t :: rng)
        call rng%init ()
        call mci%import_rng (rng)

        call mci%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Initialize instance"
        write (u, "(A)")

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        write (u, "(A)")  "* Initialize test sampler"
        write (u, "(A)")

        allocate (test_sampler_1_t :: sampler)
        select type (sampler)
```



```

type is (test_sampler_1_t)
  sampler%mode = 4
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")  "  (lower precision to avoid"
write (u, "(A)")  "    numerical noise)"
write (u, "(A)")

select type (mci)
type is (mci_vamp_t)
  call mci%add_pass ()
end select
call mci%integrate (mci_instance, sampler, 1, 1000, pacify = .true.)
call mci%write (u, .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u, .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp_16"

end subroutine mci_vamp_16

```

21.7 Multi-channel integration with VAMP2

The multi-channel integration uses VEGAS as backbone integrator. The base interface for the multi-channel integration is given by `mci_base` module.

We interface the VAMP2 interface given by `vamp2` module.

```

⟨mci_vamp2.f90⟩≡
  ⟨File header⟩

```

```

module mci_vamp2

```

```

  ⟨Use kinds⟩

```

```

  ⟨Use strings⟩

```

```

  use io_units

```

```

  use format_utils, only: pac_fmt

```

```

  use format_utils, only: write_separator, write_indent

```

```

  use format_defs, only: FMT_12, FMT_14, FMT_17, FMT_19

```

```

    use constants, only: tiny_13
    use diagnostics
    use md5
    use phs_base
    use rng_base
    use os_interface, only: mpi_get_comm_id
    use rng_stream, only: rng_stream_t

    use mci_base

    use vegas, only: VEGAS_MODE_IMPORTANCE, VEGAS_MODE_IMPORTANCE_ONLY
    use vamp2

    <MCI vamp2: modules>

    <Standard module head>

    <MCI vamp2: public>

    <MCI vamp2: types>

    <MCI vamp2: interfaces>

    contains

    <MCI vamp2: procedures>

    end module mci_vamp2
    <MCI vamp2: modules>≡
    <MPI: MCI vamp2: modules>≡
        use mpi_f08 !NODEP!

```

21.7.1 Type: mci_vamp2_func_t

```

    <MCI vamp2: types>≡
    type, extends (vamp2_func_t) :: mci_vamp2_func_t
    private
    real(default) :: integrand = 0.
    class(mci_sampler_t), pointer :: sampler => null ()
    class(mci_vamp2_instance_t), pointer :: instance => null ()
    contains
    <MCI vamp2: mci vamp2 func: TBP>
    end type mci_vamp2_func_t

```

Set instance and sampler aka workspace. Also, reset number of `n_calls`.

```

    <MCI vamp2: mci vamp2 func: TBP>≡
    procedure, public :: set_workspace => mci_vamp2_func_set_workspace

    <MCI vamp2: procedures>≡
    subroutine mci_vamp2_func_set_workspace (self, instance, sampler)
    class(mci_vamp2_func_t), intent(inout) :: self
    class(mci_vamp2_instance_t), intent(inout), target :: instance

```

```

class(mci_sampler_t), intent(inout), target :: sampler
self%instance => instance
self%sampler => sampler
end subroutine mci_vamp2_func_set_workspace

```

Get the different channel probabilities.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: get_probabilities => mci_vamp2_func_get_probabilities

<MCI vamp2: procedures>+≡
  function mci_vamp2_func_get_probabilities (self) result (gi)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), dimension(self%n_channel) :: gi
    gi = self%gi
  end function mci_vamp2_func_get_probabilities

```

Get multi-channel weight.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: get_weight => mci_vamp2_func_get_weight

<MCI vamp2: procedures>+≡
  real(default) function mci_vamp2_func_get_weight (self) result (g)
    class(mci_vamp2_func_t), intent(in) :: self
    g = self%g
  end function mci_vamp2_func_get_weight

```

Set integrand.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: set_integrand => mci_vamp2_func_set_integrand

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_func_set_integrand (self, integrand)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), intent(in) :: integrand
    self%integrand = integrand
  end subroutine mci_vamp2_func_set_integrand

```

Evaluate the mappings.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: evaluate_maps => mci_vamp2_func_evaluate_maps

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_func_evaluate_maps (self, x)
    class(mci_vamp2_func_t), intent(inout) :: self
    real(default), dimension(:), intent(in) :: x
    select type (self)
    type is (mci_vamp2_func_t)
      call self%instance%evaluate (self%sampler, self%current_channel, x)
    end select
    self%valid_x = self%instance%valid
    self%xi = self%instance%x
    self%det = self%instance%f
  end subroutine mci_vamp2_func_evaluate_maps

```

Evaluate the function, more or less.

```

<MCI vamp2: mci vamp2 func: TBP>+≡
  procedure, public :: evaluate_func => mci_vamp2_func_evaluate_func

<MCI vamp2: procedures>+≡
  real(default) function mci_vamp2_func_evaluate_func (self, x) result (f)
    class(mci_vamp2_func_t), intent(in) :: self
    real(default), dimension(:), intent(in) :: x
    f = self%integrand
    if (signal_is_pending ()) then
      call msg_message ("VAMP2: function evaluate_func: signal received")
      call terminate_now_if_signal ()
    end if
    call terminate_now_if_single_event ()
  end function mci_vamp2_func_evaluate_func

```

21.7.2 Type: mci_vamp2_config_t

We extend vamp2_config_t.

```

<MCI vamp2: public>≡
  public :: mci_vamp2_config_t

<MCI vamp2: types>+≡
  type, extends (vamp2_config_t) :: mci_vamp2_config_t
  !
  end type mci_vamp2_config_t

```

21.7.3 Integration pass

The list of passes is organized in a separate container. We store the parameters and results for each integration pass in `pass_t` and the linked list is stored in `list_pass_t`.

```

<MCI vamp2: types>+≡
  type :: list_pass_t
    type(pass_t), pointer :: first => null ()
    type(pass_t), pointer :: current => null ()
    contains
    <MCI vamp2: list pass: TBP>
  end type list_pass_t

```

Finalizer. Deallocate each element of the list beginning by the first.

```

<MCI vamp2: list pass: TBP>≡
  procedure :: final => list_pass_final

<MCI vamp2: procedures>+≡
  subroutine list_pass_final (self)
    class(list_pass_t), intent(inout) :: self
    type(pass_t), pointer :: current
    current => self%first
    do while (associated (current))
      self%first => current%next
    end do
  end subroutine list_pass_final

```

```

        deallocate (current)
        current => self%first
    end do
end subroutine list_pass_final

```

Add a new pass.

```

<MCI vamp2: list pass: TBP>+≡
    procedure :: add => list_pass_add

<MCI vamp2: procedures>+≡
    subroutine list_pass_add (self, adapt_grids, adapt_weights, final_pass)
        class(list_pass_t), intent(inout) :: self
        logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
        type(pass_t), pointer :: new_pass
        allocate (new_pass)
        new_pass%i_pass = 1
        new_pass%i_first_it = 1
        new_pass%adapt_grids = .false.; if (present (adapt_grids)) &
            & new_pass%adapt_grids = adapt_grids
        new_pass%adapt_weights = .false.; if (present (adapt_weights)) &
            & new_pass%adapt_weights = adapt_weights
        new_pass%is_final_pass = .false.; if (present (final_pass)) &
            & new_pass%is_final_pass = final_pass
        if (.not. associated (self%first)) then
            self%first => new_pass
        else
            new_pass%i_pass = new_pass%i_pass + self%current%i_pass
            new_pass%i_first_it = self%current%i_first_it + self%current%n_it
            self%current%next => new_pass
        end if
        self%current => new_pass
    end subroutine list_pass_add

```

Update list from a reference. All passes except for the last one must match exactly. For the last one, integration results are updated. The reference output may contain extra passes, these are ignored.

```

<MCI vamp2: list pass: TBP>+≡
    procedure :: update_from_ref => list_pass_update_from_ref

<MCI vamp2: procedures>+≡
    subroutine list_pass_update_from_ref (self, ref, success)
        class(list_pass_t), intent(inout) :: self
        type(list_pass_t), intent(in) :: ref
        logical, intent(out) :: success
        type(pass_t), pointer :: current, ref_current
        current => self%first
        ref_current => ref%first
        success = .true.
        do while (success .and. associated (current))
            if (associated (ref_current)) then
                if (associated (current%next)) then
                    success = current .matches. ref_current
                else
                    call current%update (ref_current, success)
                end if
            end if
            current => current%next
            ref_current => ref_current%next
        end do
    end subroutine list_pass_update_from_ref

```

```

        end if
        current => current%next
        ref_current => ref_current%next
    else
        success = .false.
    end if
end do
end subroutine list_pass_update_from_ref

```

<MCI vamp2: list pass: TBP>+≡

```

    procedure :: has_last_integral => list_pass_has_last_integral
    procedure :: get_last_integral => list_pass_get_last_integral

```

<MCI vamp2: procedures>+≡

```

function list_pass_has_last_integral(self) result (flag)
    class(list_pass_t), intent(in) :: self
    logical :: flag
    flag = associated(self%current)
    if (flag) flag = self%current%integral_defined
end function list_pass_has_last_integral

```

```

subroutine list_pass_get_last_integral(self, integral, error, efficiency)
    class(list_pass_t), intent(in) :: self
    real(default), intent(out) :: integral
    real(default), intent(out) :: error
    real(default), intent(out) :: efficiency
    if (self%has_last_integral()) then
        integral = self%current%get_integral()
        error = self%current%get_error()
        efficiency = self%current%get_efficiency()
    else
        integral = 0
        error = 0
        efficiency = 0
    end if
end subroutine list_pass_get_last_integral

```

Output. Write the complete linked list to the specified unit.

<MCI vamp2: list pass: TBP>+≡

```

    procedure :: write => list_pass_write

```

<MCI vamp2: procedures>+≡

```

subroutine list_pass_write (self, unit, pacify)
    class(list_pass_t), intent(in) :: self
    integer, intent(in) :: unit
    logical, intent(in), optional :: pacify
    type(pass_t), pointer :: current
    current => self%first
    do while (associated (current))
        write (unit, "(1X,A)") "Integration pass:"
        call current%write (unit, pacify)
        current => current%next
    end do
end subroutine list_pass_write

```

The parameters and results are stored in the nodes `pass_t` of the linked list.

```

(MCI vamp2: types)+≡
  type :: pass_t
    integer :: i_pass = 0
    integer :: i_first_it = 0
    integer :: n_it = 0
    integer :: n_calls = 0
    logical :: adapt_grids = .false.
    logical :: adapt_weights = .false.
    logical :: is_final_pass = .false.
    logical :: integral_defined = .false.
    integer, dimension(:), allocatable :: calls
    integer, dimension(:), allocatable :: calls_valid
    real(default), dimension(:), allocatable :: integral
    real(default), dimension(:), allocatable :: error
    real(default), dimension(:), allocatable :: efficiency
    type(pass_t), pointer :: next => null ()
  contains
    (MCI vamp2: pass: TBP)
  end type pass_t

```

Output. Note that the precision of the numerical values should match the precision for comparing output from file with data.

```

(MCI vamp2: pass: TBP)≡
  procedure :: write => pass_write

(MCI vamp2: procedures)+≡
  subroutine pass_write (self, unit, pacify)
    class(pass_t), intent(in) :: self
    integer, intent(in) :: unit
    logical, intent(in), optional :: pacify
    integer :: u, i
    real(default) :: pac_error
    character(len=7) :: fmt
    call pac_fmt (fmt, FMT_17, FMT_14, pacify)
    u = given_output_unit (unit)
    write (u, "(3X,A,I0)") "n_it          = ", self%n_it
    write (u, "(3X,A,I0)") "n_calls       = ", self%n_calls
    write (u, "(3X,A,L1)") "adapt grids  = ", self%adapt_grids
    write (u, "(3X,A,L1)") "adapt weights = ", self%adapt_weights
    if (self%integral_defined) then
      write (u, "(3X,A)") "Results: [it, calls, valid, integral, error, efficiency]"
      do i = 1, self%n_it
        if (abs (self%error(i)) > tiny_13) then
          pac_error = self%error(i)
        else
          pac_error = 0
        end if
        write (u, "(5x,I0,2(1x,I0),3(1x," // fmt // "))" &
              i, self%calls(i), self%calls_valid(i), self%integral(i), &
              pac_error, self%efficiency(i)
      end do
    else
      write (u, "(3x,A)") "Results: [undefined]"
    end if
  end subroutine pass_write

```

```

        end if
    end subroutine pass_write

```

Read and reconstruct the pass.

(MCI vamp2: pass: TBP)+≡

```

    procedure :: read => pass_read

```

(MCI vamp2: procedures)+≡

```

    subroutine pass_read (self, u, n_pass, n_it)
        class(pass_t), intent(out) :: self
        integer, intent(in) :: u, n_pass, n_it
        integer :: i, j
        character(80) :: buffer
        self%i_pass = n_pass + 1
        self%i_first_it = n_it + 1
        call read_ival (u, self%n_it)
        call read_ival (u, self%n_calls)
        call read_lval (u, self%adapt_grids)
        call read_lval (u, self%adapt_weights)
        allocate (self%calls (self%n_it), source = 0)
        allocate (self%calls_valid (self%n_it), source = 0)
        allocate (self%integral (self%n_it), source = 0._default)
        allocate (self%error (self%n_it), source = 0._default)
        allocate (self%efficiency (self%n_it), source = 0._default)
        read (u, "(A)") buffer
        select case (trim (adjustl (buffer)))
        case ("Results: [it, calls, valid, integral, error, efficiency]")
            do i = 1, self%n_it
                read (u, *) &
                    j, self%calls(i), self%calls_valid(i), self%integral(i), self%error(i), &
                    self%efficiency(i)
            end do
            self%integral_defined = .true.
        case ("Results: [undefined]")
            self%integral_defined = .false.
        case default
            call msg_fatal ("Reading integration pass: corrupted file")
        end select
    end subroutine pass_read

```

Auxiliary: Read real, integer, string value. We search for an equals sign, the value must follow.

(MCI vamp2: procedures)+≡

```

    subroutine read_rval (u, rval)
        integer, intent(in) :: u
        real(default), intent(out) :: rval
        character(80) :: buffer
        read (u, "(A)") buffer
        buffer = adjustl (buffer(scan (buffer, "=") + 1:))
        read (buffer, *) rval
    end subroutine read_rval

    subroutine read_ival (u, ival)

```



```

integer, intent(in) :: u
integer, intent(out) :: ival
character(80) :: buffer
read (u, "(A)") buffer
buffer = adjustl (buffer(scan (buffer, "=") + 1:))
read (buffer, *) ival
end subroutine read_ival

subroutine read_sval (u, sval)
integer, intent(in) :: u
character(*), intent(out) :: sval
character(80) :: buffer
read (u, "(A)") buffer
buffer = adjustl (buffer(scan (buffer, "=") + 1:))
read (buffer, *) sval
end subroutine read_sval

subroutine read_lval (u, lval)
integer, intent(in) :: u
logical, intent(out) :: lval
character(80) :: buffer
read (u, "(A)") buffer
buffer = adjustl (buffer(scan (buffer, "=") + 1:))
read (buffer, *) lval
end subroutine read_lval

```

Configure. We adjust the number of `n_calls`, if it is lower than `n_calls_min_per_channel` times `b_channel`, and print a warning message.

```

<MCI vamp2: pass: TBP>+≡
  procedure :: configure => pass_configure

<MCI vamp2: procedures>+≡
  subroutine pass_configure (pass, n_it, n_calls, n_calls_min)
    class(pass_t), intent(inout) :: pass
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    integer, intent(in) :: n_calls_min
    pass%n_it = n_it
    pass%n_calls = max (n_calls, n_calls_min)
    if (pass%n_calls /= n_calls) then
      write (msg_buffer, "(A,I0)") "VAMP2: too few calls, resetting " &
        // "n_calls to ", pass%n_calls
      call msg_warning ()
    end if
    allocate (pass%calls (n_it), source = 0)
    allocate (pass%calls_valid (n_it), source = 0)
    allocate (pass%integral (n_it), source = 0._default)
    allocate (pass%error (n_it), source = 0._default)
    allocate (pass%efficiency (n_it), source = 0._default)
  end subroutine pass_configure

```

Given two pass objects, compare them. All parameters must match. Where integrations are done in both (number of calls nonzero), the results must be equal (up to numerical noise).

The allocated array sizes might be different, but should match up to the common `n_it` value.

```

(MCI vamp2: interfaces)≡
  interface operator (.matches.)
    module procedure pass_matches
  end interface operator (.matches.)

(MCI vamp2: procedures)+≡
  function pass_matches (pass, ref) result (ok)
    type(pass_t), intent(in) :: pass, ref
    integer :: n
    logical :: ok
    ok = .true.
    if (ok) ok = pass%i_pass == ref%i_pass
    if (ok) ok = pass%i_first_it == ref%i_first_it
    if (ok) ok = pass%n_it == ref%n_it
    if (ok) ok = pass%n_calls == ref%n_calls
    if (ok) ok = pass%adapt_grids .eqv. ref%adapt_grids
    if (ok) ok = pass%adapt_weights .eqv. ref%adapt_weights
    if (ok) ok = pass%integral_defined .eqv. ref%integral_defined
    if (pass%integral_defined) then
      n = pass%n_it
      if (ok) ok = all (pass%calls(:n) == ref%calls(:n))
      if (ok) ok = all (pass%calls_valid(:n) == ref%calls_valid(:n))
      if (ok) ok = all (pass%integral(:n) .matches. ref%integral(:n))
      if (ok) ok = all (pass%error(:n) .matches. ref%error(:n))
      if (ok) ok = all (pass%efficiency(:n) .matches. ref%efficiency(:n))
    end if
  end function pass_matches

```

Update a pass object, given a reference. The parameters must match, except for the `n_it` entry. The number of complete iterations must be less or equal to the reference, and the number of complete iterations in the reference must be no larger than `n_it`. Where results are present in both passes, they must match. Where results are present in the reference only, the pass is updated accordingly.

```

(MCI vamp2: pass: TBP)+≡
  procedure :: update => pass_update

(MCI vamp2: procedures)+≡
  subroutine pass_update (pass, ref, ok)
    class(pass_t), intent(inout) :: pass
    type(pass_t), intent(in) :: ref
    logical, intent(out) :: ok
    integer :: n, n_ref
    ok = .true.
    if (ok) ok = pass%i_pass == ref%i_pass
    if (ok) ok = pass%i_first_it == ref%i_first_it
    if (ok) ok = pass%n_calls == ref%n_calls
    if (ok) ok = pass%adapt_grids .eqv. ref%adapt_grids
    if (ok) ok = pass%adapt_weights .eqv. ref%adapt_weights
    if (ok) then
      if (ref%integral_defined) then
        if (.not. allocated (pass%calls)) then
          allocate (pass%calls (pass%n_it), source = 0)
          allocate (pass%calls_valid (pass%n_it), source = 0)

```

```

        allocate (pass%integral (pass%n_it), source = 0._default)
        allocate (pass%error (pass%n_it), source = 0._default)
        allocate (pass%efficiency (pass%n_it), source = 0._default)
    end if
    n = count (pass%calls /= 0)
    n_ref = count (ref%calls /= 0)
    ok = n <= n_ref .and. n_ref <= pass%n_it
    if (ok) ok = all (pass%calls(:n) == ref%calls(:n))
    if (ok) ok = all (pass%calls_valid(:n) == ref%calls_valid(:n))
    if (ok) ok = all (pass%integral(:n) .matches. ref%integral(:n))
    if (ok) ok = all (pass%error(:n) .matches. ref%error(:n))
    if (ok) ok = all (pass%efficiency(:n) .matches. ref%efficiency(:n))
    if (ok) then
        pass%calls(n+1:n_ref) = ref%calls(n+1:n_ref)
        pass%calls_valid(n+1:n_ref) = ref%calls_valid(n+1:n_ref)
        pass%integral(n+1:n_ref) = ref%integral(n+1:n_ref)
        pass%error(n+1:n_ref) = ref%error(n+1:n_ref)
        pass%efficiency(n+1:n_ref) = ref%efficiency(n+1:n_ref)
        pass%integral_defined = any (pass%calls /= 0)
    end if
end if
end if
end subroutine pass_update

```

Match two real numbers: they are equal up to a tolerance, which is 10^{-8} , matching the number of digits that are output by `pass_write`. In particular, if one number is exactly zero, the other one must also be zero.

```

<MCI vamp2: interfaces>+≡
    interface operator (.matches.)
        module procedure real_matches
    end interface operator (.matches.)

<MCI vamp2: procedures>+≡
    elemental function real_matches (x, y) result (ok)
        real(default), intent(in) :: x, y
        logical :: ok
        real(default), parameter :: tolerance = 1.e-8_default
        ok = abs (x - y) <= tolerance * max (abs (x), abs (y))
    end function real_matches

```

Return the index of the most recent complete integration. If there is none, return zero.

```

<MCI vamp2: pass: TBP>+≡
    procedure :: get_integration_index => pass_get_integration_index

<MCI vamp2: procedures>+≡
    function pass_get_integration_index (pass) result (n)
        class (pass_t), intent(in) :: pass
        integer :: n
        integer :: i
        n = 0
        if (allocated (pass%calls)) then
            do i = 1, pass%n_it
                if (pass%calls(i) == 0) exit
            end do
        end if
    end function pass_get_integration_index

```

```

        n = i
    end do
end if
end function pass_get_integration_index

```

Return the most recent integral and error, if available.

```

(MCI vamp2: pass: TBP)+≡
    procedure :: get_calls => pass_get_calls
    procedure :: get_calls_valid => pass_get_calls_valid
    procedure :: get_integral => pass_get_integral
    procedure :: get_error => pass_get_error
    procedure :: get_efficiency => pass_get_efficiency

(MCI vamp2: procedures)+≡
    function pass_get_calls (pass) result (calls)
        class(pass_t), intent(in) :: pass
        integer :: calls
        integer :: n
        n = pass%get_integration_index ()
        calls = 0
        if (n /= 0) then
            calls = pass%calls(n)
        end if
    end function pass_get_calls

    function pass_get_calls_valid (pass) result (valid)
        class(pass_t), intent(in) :: pass
        integer :: valid
        integer :: n
        n = pass%get_integration_index ()
        valid = 0
        if (n /= 0) then
            valid = pass%calls_valid(n)
        end if
    end function pass_get_calls_valid

    function pass_get_integral (pass) result (integral)
        class(pass_t), intent(in) :: pass
        real(default) :: integral
        integer :: n
        n = pass%get_integration_index ()
        integral = 0
        if (n /= 0) then
            integral = pass%integral(n)
        end if
    end function pass_get_integral

    function pass_get_error (pass) result (error)
        class(pass_t), intent(in) :: pass
        real(default) :: error
        integer :: n
        n = pass%get_integration_index ()
        error = 0
        if (n /= 0) then

```

```

        error = pass%error(n)
    end if
end function pass_get_error

function pass_get_efficiency (pass) result (efficiency)
    class(pass_t), intent(in) :: pass
    real(default) :: efficiency
    integer :: n
    n = pass%get_integration_index ()
    efficiency = 0
    if (n /= 0) then
        efficiency = pass%efficiency(n)
    end if
end function pass_get_efficiency

```

21.7.4 Integrator

We store the different passes of integration, adaptation and actual sampling, in a linked list.

We store the total number of calls `n_calls` and the minimal number of calls `n_calls_min`. The latter is calculated based on `n_channel` and `min_calls_per_channel`. If `n_calls` is smaller than `n_calls_min`, then we replace `n_calls` with `n_min_calls`.

```

<MCI vamp2: public>+≡
    public :: mci_vamp2_t

<MCI vamp2: types>+≡
    type, extends(mci_t) :: mci_vamp2_t
        type(mci_vamp2_config_t) :: config
        type(vamp2_t) :: integrator
        type(vamp2_equivalences_t) :: equivalences
        logical :: integrator_defined = .false.
        logical :: integrator_from_file = .false.
        logical :: adapt_grids = .false.
        logical :: adapt_weights = .false.
        integer :: n_adapt_grids = 0
        integer :: n_adapt_weights = 0
        integer :: n_calls = 0
        type(list_pass_t) :: list_pass
        logical :: rebuild = .true.
        logical :: check_grid_file = .true.
        logical :: grid_filename_set = .false.
        logical :: negative_weights = .false.
        logical :: verbose = .false.
        logical :: pass_complete = .false.
        logical :: it_complete = .false.
        type(string_t) :: grid_filename
        integer :: grid_checkpoint = 1
        logical :: binary_grid_format = .false.
        type(string_t) :: parallel_method
        character(32) :: md5sum_adapted = ""
    contains
    <MCI vamp2: mci vamp2: TBP>

```

```
end type mci_vamp2_t
```

Finalizer: call to base and list finalizer.

```
<MCI vamp2: mci vamp2: TBP>≡
  procedure, public :: final => mci_vamp2_final

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_final (object)
    class(mci_vamp2_t), intent(inout) :: object
    call object%list_pass%final ()
    call object%base_final ()
  end subroutine mci_vamp2_final
```

Output. Do not output the grids themselves, this may result in tons of data.

```
<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: write => mci_vamp2_write

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_write (object, unit, pacify, md5sum_version)
    class(mci_vamp2_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    logical, intent(in), optional :: md5sum_version
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1X,A)") "VAMP2 integrator:"
    call object%base_write (u, pacify, md5sum_version)
    write (u, "(1X,A)") "Grid config:"
    call object%config%write (u)
    write (u, "(3X,A,L1)") "Integrator defined      = ", object%integrator_defined
    write (u, "(3X,A,L1)") "Integrator from file = ", object%integrator_from_file
    write (u, "(3X,A,L1)") "Adapt grids          = ", object%adapt_grids
    write (u, "(3X,A,L1)") "Adapt weights        = ", object%adapt_weights
    write (u, "(3X,A,I0)") "No. of adapt grids   = ", object%n_adapt_grids
    write (u, "(3X,A,I0)") "No. of adapt weights = ", object%n_adapt_weights
    write (u, "(3X,A,L1)") "Verbose              = ", object%verbose
    if (object%config%equivalences) then
      call object%equivalences%write (u)
    end if
    call object%list_pass%write (u, pacify)
    if (object%md5sum_adapted /= "") then
      write (u, "(1X,A,A,A)") "MD5 sum (including results) = '", &
        & object%md5sum_adapted, "'"
    end if
  end subroutine mci_vamp2_write
```

Compute the (adapted) MD5 sum, including the configuration MD5 sum and the printout, which incorporates the current results.

```
<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: compute_md5sum => mci_vamp2_compute_md5sum

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_compute_md5sum (mci, pacify)
```

```

class(mci_vamp2_t), intent(inout) :: mci
logical, intent(in), optional :: pacify
integer :: u
mci%md5sum_adapted = ""
u = free_unit ()
open (u, status = "scratch", action = "readwrite")
write (u, "(A)") mci%md5sum
call mci%write (u, pacify, md5sum_version = .true.)
rewind (u)
mci%md5sum_adapted = md5sum (u)
close (u)
end subroutine mci_vamp2_compute_md5sum

```

Return the MD5 sum: If available, return the adapted one.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: get_md5sum => mci_vamp2_get_md5sum

<MCI vamp2: procedures>+≡
  pure function mci_vamp2_get_md5sum (mci) result (md5sum)
    class(mci_vamp2_t), intent(in) :: mci
    character(32) :: md5sum
    if (mci%md5sum_adapted /= "") then
      md5sum = mci%md5sum_adapted
    else
      md5sum = mci%md5sum
    end if
  end function mci_vamp2_get_md5sum

```

Startup message: short version. Make a call to the base function and print additional information about the multi-channel parameters.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: startup_message => mci_vamp2_startup_message

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_startup_message (mci, unit, n_calls)
    class(mci_vamp2_t), intent(in) :: mci
    integer, intent(in), optional :: unit, n_calls
    integer :: num_calls, n_bins
    num_calls = 0; if (present (n_calls)) num_calls = n_calls
    n_bins = mci%config%n_bins_max
    call mci%base_startup_message (unit = unit, n_calls = n_calls)
    if (mci%config%equivalences) then
      write (msg_buffer, "(A)") &
        "Integrator: Using VAMP2 channel equivalences"
      call msg_message (unit = unit)
    end if
    if (mci%binary_grid_format) then
      write (msg_buffer, "(A,A,A,A)") &
        "Integrator: Write grid header to '" // char (mci%get_grid_filename ()) // &
        "' and grids to '" // char (mci%get_grid_filename (binary_grid_format = .true.)) // "
    else
      write (msg_buffer, "(A,A,A)") &
        "Integrator: Write grid header and grids to '" // char (mci%get_grid_filename ()) // "
    end if
  end subroutine mci_vamp2_startup_message

```

```

call msg_message (unit = unit)
select case (mci%grid_checkpoint)
case (0)
  write (msg_buffer, "(A)") &
    "Integrator: Grid checkpoint after each pass"
case (1)
  write (msg_buffer, "(A)") &
    "Integrator: Grid checkpoint after each iteration"
case (2:)
  write (msg_buffer, "(A,1X,I0,1X,A)") &
    "Integrator: Grid checkpoint after", mci%grid_checkpoint, &
    "iterations and after each pass"
case default
  call msg_bug ("Integrator: Cannot assign grid checkpoint (value is negative).")
end select
call msg_message (unit = unit)
write (msg_buffer, "(A,2(1x,I0,1x,A),L1)") &
  "Integrator:", num_calls, &
  "initial calls,", n_bins, &
  "max. bins, stratified = ", &
  mci%config%stratified
call msg_message (unit = unit)
write (msg_buffer, "(A,2(1x,I0,1x,A))") &
  "Integrator: VAMP2"
call msg_message (unit = unit)
end subroutine mci_vamp2_startup_message

```

Log entry: just headline.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: write_log_entry => mci_vamp2_write_log_entry

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_write_log_entry (mci, u)
    class(mci_vamp2_t), intent(in) :: mci
    integer, intent(in) :: u
    write (u, "(1x,A)") "MC Integrator is VAMP2"
    call write_separator (u)
    if (mci%config%equivalences) then
      call mci%equivalences%write (u)
    else
      write (u, "(3x,A)") "No channel equivalences have been used."
    end if
    call write_separator (u)
    call mci%write_chain_weights (u)
  end subroutine mci_vamp2_write_log_entry

```

Set the MCI index (necessary for processes with multiple components). We append the index to the grid filename, just before the final dotted suffix.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: record_index => mci_vamp2_record_index

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_record_index (mci, i_mci)
    class(mci_vamp2_t), intent(inout) :: mci

```



```

integer, intent(in) :: i_mci
type(string_t) :: basename, suffix
character(32) :: buffer
if (mci%grid_filename_set) then
    write (buffer, "(I0)") i_mci
    mci%grid_filename = mci%grid_filename // ".m" // trim (buffer)
end if
end subroutine mci_vamp2_record_index

```

Set the configuration object. We adjust the maximum number of bins `n_bins_max` according to `n_calls`

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: set_config => mci_vamp2_set_config

<MCI vamp2: procedures>+≡
    subroutine mci_vamp2_set_config (mci, config)
        class(mci_vamp2_t), intent(inout) :: mci
        type(mci_vamp2_config_t), intent(in) :: config
        mci%config = config
    end subroutine mci_vamp2_set_config

```

Set the the rebuild flag, also the for checking the grid.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: set_rebuild_flag => mci_vamp2_set_rebuild_flag

<MCI vamp2: procedures>+≡
    subroutine mci_vamp2_set_rebuild_flag (mci, rebuild, check_grid_file)
        class(mci_vamp2_t), intent(inout) :: mci
        logical, intent(in) :: rebuild
        logical, intent(in) :: check_grid_file
        mci%rebuild = rebuild
        mci%check_grid_file = check_grid_file
    end subroutine mci_vamp2_set_rebuild_flag

```

Set the filename.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: set_grid_filename => mci_vamp2_set_grid_filename
    procedure, public :: get_grid_filename => mci_vamp2_get_grid_filename

<MCI vamp2: procedures>+≡
    subroutine mci_vamp2_set_grid_filename (mci, name, run_id)
        class(mci_vamp2_t), intent(inout) :: mci
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: run_id
        mci%grid_filename = name
        if (present (run_id)) then
            mci%grid_filename = name // "." // run_id
        end if
        mci%grid_filename_set = .true.
    end subroutine mci_vamp2_set_grid_filename

type(string_t) function mci_vamp2_get_grid_filename (mci, binary_grid_format) &
    result (filename)

```

```

class(mci_vamp2_t), intent(in) :: mci
logical, intent(in), optional :: binary_grid_format
filename = mci%grid_filename // ".vg2"
if (present (binary_grid_format)) then
  if (binary_grid_format) then
    filename = mci%grid_filename // ".vgx2"
  end if
end if
end function mci_vamp2_get_grid_filename

```

To simplify the interface, we prepend a grid path in a separate subroutine.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure :: prepend_grid_path => mci_vamp2_prepend_grid_path

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_prepend_grid_path (mci, prefix)
    class(mci_vamp2_t), intent(inout) :: mci
    type(string_t), intent(in) :: prefix
    if (.not. mci%grid_filename_set) then
      call msg_warning ("VAMP2: Cannot add prefix to invalid integrator filename!")
    end if
    mci%grid_filename = prefix // "/" // mci%grid_filename
  end subroutine mci_vamp2_prepend_grid_path

```

Not implemented.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: declare_flat_dimensions => mci_vamp2_declare_flat_dimensions

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_declare_flat_dimensions (mci, dim_flat)
    class(mci_vamp2_t), intent(inout) :: mci
    integer, dimension(:), intent(in) :: dim_flat
  end subroutine mci_vamp2_declare_flat_dimensions

```

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: declare_equivalences => mci_vamp2_declare_equivalences

```

```

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_declare_equivalences (mci, channel, dim_offset)
    class(mci_vamp2_t), intent(inout) :: mci
    type(phs_channel_t), dimension(:), intent(in) :: channel
    integer, intent(in) :: dim_offset
    integer, dimension(:), allocatable :: perm, mode
    integer :: n_channels, n_dim, n_equivalences
    integer :: c, i, j, dest, src
    integer :: n_dim_perm
    n_channels = mci%n_channel
    n_dim = mci%n_dim
    n_equivalences = 0
    do c = 1, n_channels
      n_equivalences = n_equivalences + size (channel(c)%eq)
    end do
    mci%equivalences = vamp2_equivalences_t (&
      n_eqv = n_equivalences, n_channel = n_channels, n_dim = n_dim)
  end subroutine mci_vamp2_declare_equivalences

```

```

allocate (perm (n_dim))
allocate (mode (n_dim))
perm = [(i, i = 1, n_dim)]
mode = 0
c = 1
j = 0
do i = 1, n_equivalences
  if (j < size (channel(c)%eq)) then
    j = j + 1
  else
    c = c + 1
    j = 1
  end if
  associate (eq => channel(c)%eq(j))
    dest = c
    src = eq%c
    n_dim_perm = size (eq%perm)
    perm(dim_offset+1:dim_offset+n_dim_perm) = eq%perm + dim_offset
    mode(dim_offset+1:dim_offset+n_dim_perm) = eq%mode
    call mci%equivalences%set_equivalence &
      (i, dest, src, perm, mode)
  end associate
end do
call mci%equivalences%freeze ()
end subroutine mci_vamp2_declare_equivalences

```

Allocate instance with matching type.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: allocate_instance => mci_vamp2_allocate_instance

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_allocate_instance (mci, mci_instance)
    class(mci_vamp2_t), intent(in) :: mci
    class(mci_instance_t), intent(out), pointer :: mci_instance
    allocate (mci_vamp2_instance_t :: mci_instance)
  end subroutine mci_vamp2_allocate_instance

```

Allocate a new integration pass. We can preset everything that does not depend on the number of iterations and calls. This is postponed to the integrate method.

In the final pass, we do not check accuracy goal etc., since we can assume that the user wants to perform and average all iterations in this pass.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: add_pass => mci_vamp2_add_pass

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_add_pass (mci, adapt_grids, adapt_weights, final_pass)
    class(mci_vamp2_t), intent(inout) :: mci
    logical, intent(in), optional :: adapt_grids, adapt_weights, final_pass
    call mci%list_pass%add (adapt_grids, adapt_weights, final_pass)
  end subroutine mci_vamp2_add_pass

```

Update the list of integration passes.

```

<MCI vamp2: mci vamp2: TBP>+≡
  procedure, public :: update_from_ref => mci_vamp2_update_from_ref

```

```

<MCI vamp2: procedures>+≡
subroutine mci_vamp2_update_from_ref (mci, mci_ref, success)
  class(mci_vamp2_t), intent(inout) :: mci
  class(mci_t), intent(in) :: mci_ref
  logical, intent(out) :: success
  select type (mci_ref)
  type is (mci_vamp2_t)
    call mci%list_pass%update_from_ref (mci_ref%list_pass, success)
    if (mci%list_pass%has_last_integral()) then
      call mci%list_pass%get_last_integral( &
        integral = mci%integral, &
        error = mci%error, &
        efficiency = mci%efficiency)
      mci%integral_known = .true.
      mci%error_known = .true.
      mci%efficiency_known = .true.
    end if
  end select
end subroutine mci_vamp2_update_from_ref

```

Update the MCI record (i.e., the integration passes) by reading from input stream. The stream should contain a write output from a previous run. We first check the MD5 sum of the configuration parameters. If that matches, we proceed directly to the stored integration passes. If successful, we may continue to read the file; the position will be after a blank line that must follow the MCI record.

```

<MCI vamp2: mci vamp2: TBP>+≡
procedure, public :: update => mci_vamp2_update
<MCI vamp2: procedures>+≡
subroutine mci_vamp2_update (mci, u, success)
  class(mci_vamp2_t), intent(inout) :: mci
  integer, intent(in) :: u
  logical, intent(out) :: success
  character(80) :: buffer
  character(32) :: md5sum_file
  type(mci_vamp2_t) :: mci_file
  integer :: n_pass, n_it
  call read_sval (u, md5sum_file)
  success = .true.; if (mci%check_grid_file) &
    & success = (md5sum_file == mci%md5sum)
  if (success) then
    read (u, *)
    read (u, "(A)") buffer
    if (trim (adjustl (buffer)) /= "VAMP2 integrator:") then
      call msg_fatal ("VAMP2: reading grid file: corrupted data")
    end if
    n_pass = 0
    n_it = 0
    do
      read (u, "(A)") buffer
      select case (trim (adjustl (buffer)))
      case ("")
        exit
      end select
    end do
  end if

```

```

        case ("Integration pass:")
            call mci_file%list_pass%add ()
            call mci_file%list_pass%current%read (u, n_pass, n_it)
            n_pass = n_pass + 1
            n_it = n_it + mci_file%list_pass%current%n_it
        end select
    end do
    call mci%update_from_ref (mci_file, success)
    call mci_file%final ()
end if
end subroutine mci_vamp2_update

```

Read / write grids from / to file.

We split the reading process in two parts. First, we check on the header where we check (and update) all relevant pass data using `mci_vamp2_update`. In the second part we only read the integrator data. We implement `mci_vamp2_read` for completeness.

The writing of the MCI object is split into two parts, a header with the relevant process configuration regarding the integration and the results of the different passes and their iterations. The other part is the actual grid. The header will always be written in ASCII format, including a md5 hash, in order to testify against unwilling changes to the setup. The grid part can be either added to the ASCII file, or to an additional binary file.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure :: write_grids => mci_vamp2_write_grids
    procedure :: read_header => mci_vamp2_read_header
    procedure :: read_data => mci_vamp2_read_data
    procedure, private :: advance_to_data => mci_vamp2_advance_to_data

<MCI vamp2: procedures>+≡
    subroutine mci_vamp2_write_grids (mci)
        class(mci_vamp2_t), intent(in) :: mci
        integer :: u
        if (.not. mci%grid_filename_set) then
            call msg_bug ("VAMP2: write grids: filename undefined")
        end if
        if (.not. mci%integrator_defined) then
            call msg_bug ("VAMP2: write grids: grids undefined")
        end if
        open (newunit = u, file = char (mci%get_grid_filename ()), &
            action = "write", status = "replace")
        write (u, "(1X,A,A,A)") "MD5sum = '", mci%md5sum, "'"
        write (u, *)
        call mci%write (u)
        write (u, *)
        if (mci%binary_grid_format) then
            write (u, "(1X,2A)") "VAMP2 grids: binary file: ", &
                char (mci%get_grid_filename (binary_grid_format = .true.))
            close (u)
            open (newunit = u, &
                file = char (mci%get_grid_filename (binary_grid_format = .true.)), &
                action = "write", &
                access = "stream", &

```

```

        form = "unformatted", &
        status = "replace")
    call mci%integrator%write_binary_grids (u)
else
    write (u, "(1X,A)") "VAMP2 grids:"
    call mci%integrator%write_grids (u)
end if
close (u)
end subroutine mci_vamp2_write_grids

subroutine mci_vamp2_read_header (mci, success)
    class(mci_vamp2_t), intent(inout) :: mci
    logical, intent(out) :: success
    logical :: exist, binary_grid_format, exist_binary
    integer :: u
    success = .false.
    if (.not. mci%grid_filename_set) then
        call msg_bug ("VAMP2: read grids: filename undefined")
    end if
    !! First, check for existence of the (usual) grid file.
    inquire (file = char (mci%get_grid_filename ()), exist = exist)
    if (.not. exist) return !! success = .false.
    open (newunit = u, file = char (mci%get_grid_filename ()), &
        action = "read", status = "old")
    !! Second, check for existence of a (possible) binary grid file.
    call mci%advance_to_data (u, binary_grid_format)
    rewind (u) !! Rewind header file, after line search.
    if (binary_grid_format) then
        inquire (file = char (mci%get_grid_filename (binary_grid_format = .true.)), &
            exist = exist)
        if (.not. exist) then
            write (msg_buffer, "(3A)") &
                "VAMP2: header: binary grid file not found, discarding grid file '", &
                char (mci%get_grid_filename ()), "'."
            call msg_message ()
            return !! success = .false.
        end if
    end if
    !! The grid file (ending *.vg) exists and, if binary file is listed, it exists, too.
    call mci%update (u, success)
    close (u)
    if (.not. success) then
        write (msg_buffer, "(A,A,A)") &
            "VAMP2: header: parameter mismatch, discarding pass from file '", &
            char (mci%get_grid_filename ()), "'."
        call msg_message ()
    end if
end subroutine mci_vamp2_read_header

subroutine mci_vamp2_read_data (mci)
    class(mci_vamp2_t), intent(inout) :: mci
    integer :: u
    logical :: binary_grid_format
    if (mci%integrator_defined) then

```

```

        call msg_bug ("VAMP2: read grids: grids already defined")
    end if
    open (newunit = u, &
        file = char (mci%get_grid_filename ()), &
        action = "read", &
        status = "old")
    call mci%advance_to_data (u, binary_grid_format)
    if (binary_grid_format) then
        close (u)
        write (msg_buffer, "(3A)") &
            "VAMP2: Reading from binary grid file '", &
            char (mci%get_grid_filename (binary_grid_format = .true.)), "'"
        call msg_message ()
        open (newunit = u, &
            file = char (mci%get_grid_filename (binary_grid_format = .true.)), &
            action = "read", &
            access = "stream", &
            form = "unformatted", &
            status = "old")
        call mci%integrator%read_binary_grids (u)
    else
        call mci%integrator%read_grids (u)
    end if
    mci%integrator_defined = .true.
    close (u)
end subroutine mci_vamp2_read_data

subroutine mci_vamp2_advance_to_data (mci, u, binary_grid_format)
    class(mci_vamp2_t), intent(in) :: mci
    integer, intent(in) :: u
    logical, intent(out) :: binary_grid_format
    character(80) :: buffer
    type(string_t) :: search_string_binary, search_string_ascii
    search_string_binary = "VAMP2 grids: binary file: " // &
        mci%get_grid_filename (binary_grid_format = .true.)
    search_string_ascii = "VAMP2 grids:"
    SEARCH: do
        read (u, "(A)") buffer
        if (trim (adjustl (buffer)) == char (search_string_binary)) then
            binary_grid_format = .true.
            exit SEARCH
        else if (trim (adjustl (buffer)) == char (search_string_ascii)) then
            binary_grid_format = .false.
            exit SEARCH
        end if
    end do SEARCH
end subroutine mci_vamp2_advance_to_data

```

Interface: VAMP2

We define the interfacing procedures, as such, initialising the VAMP2 integrator or resetting the results.

Initialise the VAMP2 integrator which is stored within the `mci` object, using the data of the current integration pass. Furthermore, reset the counters that track this set of integrator.

```

(MCI vamp2: mci vamp2: TBP)+≡
  procedure, public :: init_integrator => mci_vamp2_init_integrator

(MCI vamp2: procedures)+≡
  subroutine mci_vamp2_init_integrator (mci)
    class(mci_vamp2_t), intent(inout) :: mci
    type (pass_t), pointer :: current
    integer :: ch, vegas_mode
    current => mci%list_pass%current
    vegas_mode = merge (VEGAS_MODE_IMPORTANCE, VEGAS_MODE_IMPORTANCE_ONLY, &
      & mci%config%stratified)
    mci%n_adapt_grids = 0
    mci%n_adapt_weights = 0
    if (mci%integrator_defined) then
      call msg_bug ("VAMP2: init integrator: &
        & integrator is already initialised.")
    end if
    mci%integrator = vamp2_t (mci%n_channel, mci%n_dim, &
      & n_bins_max = mci%config%n_bins_max, &
      & iterations = 1, &
      & mode = vegas_mode)
    if (mci%has_chains ()) call mci%integrator%set_chain (mci%n_chain, mci%chain)
    call mci%integrator%set_config (mci%config)
    mci%integrator_defined = .true.
  end subroutine mci_vamp2_init_integrator

```

Reset a grid set. Purge the accumulated results.

```

(MCI vamp2: mci vamp2: TBP)+≡
  procedure, public :: reset_result => mci_vamp2_reset_result

(MCI vamp2: procedures)+≡
  subroutine mci_vamp2_reset_result (mci)
    class(mci_vamp2_t), intent(inout) :: mci
    if (.not. mci%integrator_defined) then
      call msg_bug ("VAMP2: reset results: integrator undefined")
    end if
    call mci%integrator%reset_result ()
  end subroutine mci_vamp2_reset_result

```

Set calls per channel. The number of calls to each channel is defined by the channel weight

$$\alpha_i = \frac{N_i}{\sum N_i}. \quad (21.18)$$

```

(MCI vamp2: mci vamp2: TBP)+≡
  procedure, public :: set_calls => mci_vamp2_set_calls

(MCI vamp2: procedures)+≡
  subroutine mci_vamp2_set_calls (mci, n_calls)
    class(mci_vamp2_t), intent(inout) :: mci
    integer :: n_calls

```



```

    if (.not. mci%integrator_defined) then
        call msg_bug ("VAMP2: set calls: grids undefined")
    end if
    call mci%integrator%set_calls (n_calls)
end subroutine mci_vamp2_set_calls

```

Integration

Initialize. We prepare the integrator from a previous pass, or from file, or with new objects.

At the end, we update the number of calls either when we got the integration grids from file and we added new iterations to the current pass, or we allocated a new integrator.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, private :: init_integration => mci_vamp2_init_integration

<MCI vamp2: procedures>+≡
    subroutine mci_vamp2_init_integration (mci, n_it, n_calls, instance)
        class(mci_vamp2_t), intent(inout) :: mci
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
        class(mci_instance_t), intent(inout) :: instance
        logical :: from_file, success
        if (.not. associated (mci%list_pass%current)) then
            call msg_bug ("MCI integrate: current_pass object not allocated")
        end if
        associate (current_pass => mci%list_pass%current)
            current_pass%integral_defined = .false.
            mci%config%n_calls_min = mci%config%n_calls_min_per_channel * mci%config%n_channel
            call current_pass%configure (n_it, n_calls, mci%config%n_calls_min)
            mci%adapt_grids = current_pass%adapt_grids
            mci%adapt_weights = current_pass%adapt_weights
            mci%pass_complete = .false.
            mci%it_complete = .false.
            from_file = .false.
            if (.not. mci%integrator_defined .or. mci%integrator_from_file) then
                if (mci%grid_filename_set .and. .not. mci%rebuild) then
                    call mci%read_header (success)
                    from_file = success
                    if (.not. mci%integrator_defined .and. success) &
                        call mci%read_data ()
                end if
            end if
            if (from_file) then
                if (.not. mci%check_grid_file) &
                    & call msg_warning ("Reading grid file: MD5 sum check disabled")
                call msg_message ("VAMP2: " &
                    // "Using grids and results from file '" &
                    // char (mci%get_grid_filename ()) // "'.")
            else if (.not. mci%integrator_defined) then
                call msg_message ("VAMP2: " &
                    // "Initialize new grids and write to file '" &
                    // char (mci%get_grid_filename ()) // "'.")
            end if
        end associate
    end subroutine

```

```

        call mci%init_integrator ()
    end if
    mci%integrator_from_file = from_file
    if (.not. mci%integrator_from_file .or. (n_it > current_pass%get_integration_index ())) then
        call mci%integrator%set_calls (current_pass%n_calls)
    end if
    call mci%integrator%set_equivalences (mci%equivalences)
end associate
<MCI vamp2: mci vamp2 init integration: allocate request>
end subroutine mci_vamp2_init_integration

```

Allocate request object and load into integrator object.

```

<MPI: MCI vamp2: mci vamp2 init integration: allocate request>≡
    if (mci%parallel_method /= "") then
        call mci%integrator%allocate_request (method = char (mci%parallel_method))
    else
        call msg_message ("VAMP2: Use default parallel method: simple.")
        call mci%integrator%allocate_request (method = "simple")
    end if

```

Integrate. Perform a new integration pass (possibly reusing previous results), which may consist of several iterations. We reinitialise the sampling new each time and set the workspace again. Note: we record the integral once per iteration. The integral stored in the mci record itself is the last integral of the current iteration, no averaging done. The results record may average results. Note: recording the efficiency is not supported yet.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: integrate => mci_vamp2_integrate

<MCI vamp2: procedures>+≡
    subroutine mci_vamp2_integrate (mci, instance, sampler, &
        n_it, n_calls, results, pacify)
        class(mci_vamp2_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout), target :: instance
        class(mci_sampler_t), intent(inout), target :: sampler
        integer, intent(in) :: n_it
        integer, intent(in) :: n_calls
        class(mci_results_t), intent(inout), optional :: results
        logical, intent(in), optional :: pacify
        integer :: it
        logical :: from_file, success
    <MCI vamp2: mci vamp2 integrate: variables>
    <MCI vamp2: mci vamp2 integrate: initialization>
        call mci%init_integration (n_it, n_calls, instance)
        from_file = mci%integrator_from_file
        select type (instance)
            type is (mci_vamp2_instance_t)
                call instance%set_workspace (sampler)
            end select
        associate (current_pass => mci%list_pass%current)
            do it = 1, current_pass%n_it
                if (signal_is_pending ()) return
                mci%integrator_from_file = from_file .and. &
                    it <= current_pass%get_integration_index ()
            end do
        end associate
    end subroutine

```

```

if (.not. mci%integrator_from_file) then
  mci%it_complete = .false.
  select type (instance)
  type is (mci_vamp2_instance_t)
    call mci%integrator%integrate (instance%func, mci%rng, &
      & iterations = 1, &
      & reset_result = .true., &
      & refine_grids = mci%adapt_grids, &
      & adapt_weights = mci%adapt_weights, &
      & verbose = mci%verbose)
  end select
  if (signal_is_pending ()) return
  mci%it_complete = .true.
  integral = mci%integrator%get_integral ()
  calls = mci%integrator%get_n_calls ()
  select type (instance)
  type is (mci_vamp2_instance_t)
    calls_valid = instance%func%get_n_calls ()
    call instance%func%reset_n_calls ()
  end select
  error = sqrt (mci%integrator%get_variance ())
  efficiency = mci%integrator%get_efficiency ()
  (MCI vamp2: mci vamp2 integrate: sampling)
  if (integral /= 0) then
    current_pass%integral(it) = integral
    current_pass%calls(it) = calls
    current_pass%calls_valid(it) = calls_valid
    current_pass%error(it) = error
    current_pass%efficiency(it) = efficiency
  end if
  current_pass%integral_defined = .true.
end if
if (present (results)) then
  if (mci%has_chains ()) then
    call mci%collect_chain_weights (instance%w)
    call results%record (1, &
      n_calls = current_pass%calls(it), &
      n_calls_valid = current_pass%calls_valid(it), &
      integral = current_pass%integral(it), &
      error = current_pass%error(it), &
      efficiency = current_pass%efficiency(it), &
      efficiency_pos = current_pass%efficiency(it), &
      efficiency_neg = 0._default, &
      chain_weights = mci%chain_weights, &
      suppress = pacify)
  else
    call results%record (1, &
      n_calls = current_pass%calls(it), &
      n_calls_valid = current_pass%calls_valid(it), &
      integral = current_pass%integral(it), &
      error = current_pass%error(it), &
      efficiency = current_pass%efficiency(it), &
      efficiency_pos = current_pass%efficiency(it), &
      efficiency_neg = 0._default, &

```

```

        suppress = pacify)
    end if
end if
if (.not. mci%integrator_from_file &
    .and. mci%grid_filename_set) then
    <MCI vamp2: mci vamp2 integrate: post sampling>
    call checkpoint_and_write_grids (it = it, &
        final_it = (it == current_pass%n_it))
    end if
    if (.not. current_pass%is_final_pass) then
        call check_goals (it, success)
        if (success) exit
    end if
end do
if (signal_is_pending ()) return
mci%pass_complete = .true.
mci%integral = current_pass%get_integral()
mci%error = current_pass%get_error()
mci%efficiency = current_pass%get_efficiency()
mci%integral_known = .true.
mci%error_known = .true.
mci%efficiency_known = .true.
call mci%compute_md5sum (pacify)
end associate
contains
    <MCI vamp2: mci vamp2 integrate: procedures>
end subroutine mci_vamp2_integrate

```

```

<MCI vamp2: mci vamp2 integrate: variables>≡
    real(default) :: integral, error, efficiency
    integer :: calls, calls_valid

```

```

<MCI vamp2: mci vamp2 integrate: initialization>≡

```

```

<MCI vamp2: mci vamp2 integrate: sampling>≡

```

```

<MCI vamp2: mci vamp2 integrate: post sampling>≡

```

```

<MPI: MCI vamp2: mci vamp2 integrate: variables>≡
    integer :: rank, n_size
    type(MPI_Request), dimension(6) :: request

```

MPI procedure-specific initialization.

```

<MPI: MCI vamp2: mci vamp2 integrate: initialization>≡
    call MPI_Comm_size (MPI_COMM_WORLD, n_size)
    call MPI_Comm_rank (MPI_COMM_WORLD, rank)

```

We broadcast the current results to all worker, such that they can store them in to the pass list.

```

<MPI: MCI vamp2: mci vamp2 integrate: sampling>≡
    call MPI_Ibcast (integral, 1, MPI_DOUBLE_PRECISION, 0, MPI_COMM_WORLD, request(1))
    call MPI_Ibcast (calls, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, request(2))
    call MPI_Ibcast (calls_valid, 1, MPI_INTEGER, 0, MPI_COMM_WORLD, request(3))
    call MPI_Ibcast (error, 1, MPI_DOUBLE_PRECISION, 0, MPI_COMM_WORLD, request(4))
    call MPI_Ibcast (efficiency, 1, MPI_DOUBLE_PRECISION, 0, MPI_COMM_WORLD, request(5))
    call MPI_Waitall (5, request, MPI_STATUSES_IGNORE)

```

We only allow the master to write the grids to file.

```
(MPI: MCI vamp2: mci vamp2 integrate: post sampling)≡
  if (rank == 0) &
```

Write grids to `grid_filename` at a given checkpoint.

We qualify each iteration and pass as possible checkpoint. However, we allow the user to alter the checkpoint behavior:

- after every iteration,
- after every pass,
- after a N iterations and every pass.

The user sets the Sindarin variable `vamp_grid_checkpoint` to an integer value where the value 0 represents each pass, value 1 each iteration, and a value > 1 means after N iterations (or at the last iteration of a pass).

```
(MCI vamp2: mci vamp2 integrate: procedures)≡
  subroutine checkpoint_and_write_grids (it, final_it)
    integer, intent(in) :: it
    logical, intent(in) :: final_it
    select case (mci%grid_checkpoint)
    case (0)
      if (.not. final_it) return
    case (1)
    case(2:)
      if (.not. (final_it &
        .or. mod (it, mci%grid_checkpoint) == 0)) return
    case default
      call msg_bug ("VAMP2: Grid checkpoint must be a positive integer.")
    end select
    call mci%write_grids ()
  end subroutine checkpoint_and_write_grids
```

Check whether we are already finished with this pass.

```
(MCI vamp2: mci vamp2 integrate: procedures)+≡
  subroutine check_goals (it, success)
    integer, intent(in) :: it
    logical, intent(out) :: success
    success = .false.
    associate (current_pass => mci%list_pass%current)
      if (error_reached (it)) then
        current_pass%n_it = it
        call msg_message ("VAMP2: error goal reached; &
          &skipping iterations")
        success = .true.
        return
      end if
      if (rel_error_reached (it)) then
        current_pass%n_it = it
        call msg_message ("VAMP2: relative error goal reached; &
          &skipping iterations")
        success = .true.
        return
      end if
    end associate
  end subroutine check_goals
```

```

end if
if (accuracy_reached (it)) then
    current_pass%n_it = it
    call msg_message ("VAMP2: accuracy goal reached; &
        &skipping iterations")
    success = .true.
    return
end if
end associate
end subroutine check_goals

```

Return true if the error, relative error or accuracy goals have been reached, if any.

(MCI vamp2: mci vamp2 integrate: procedures)+≡

```

function error_reached (it) result (flag)
    integer, intent(in) :: it
    logical :: flag
    real(default) :: error_goal, error
    error_goal = mci%config%error_goal
    flag = .false.
    associate (current_pass => mci%list_pass%current)
        if (error_goal > 0 .and. current_pass%integral_defined) then
            error = abs (current_pass%error(it))
            flag = error < error_goal
        end if
    end associate
end function error_reached

function rel_error_reached (it) result (flag)
    integer, intent(in) :: it
    logical :: flag
    real(default) :: rel_error_goal, rel_error
    rel_error_goal = mci%config%rel_error_goal
    flag = .false.
    associate (current_pass => mci%list_pass%current)
        if (rel_error_goal > 0 .and. current_pass%integral_defined) then
            rel_error = abs (current_pass%error(it) / current_pass%integral(it))
            flag = rel_error < rel_error_goal
        end if
    end associate
end function rel_error_reached

function accuracy_reached (it) result (flag)
    integer, intent(in) :: it
    logical :: flag
    real(default) :: accuracy_goal, accuracy
    accuracy_goal = mci%config%accuracy_goal
    flag = .false.
    associate (current_pass => mci%list_pass%current)
        if (accuracy_goal > 0 .and. current_pass%integral_defined) then
            if (current_pass%integral(it) /= 0) then
                accuracy = abs (current_pass%error(it) / current_pass%integral(it)) &
                    * sqrt (real (current_pass%calls(it), default))
            end if
        end if
    end associate
end function accuracy_reached

```

```

        flag = accuracy < accuracy_goal
    else
        flag = .true.
    end if
end if
end associate
end function accuracy_reached

```

21.7.5 Event generation

Prepare simulation. We check the grids and reread them from file, if necessary.

```

<MCI vamp2: mci vamp2: TBP>+≡
    procedure, public :: prepare_simulation => mci_vamp2_prepare_simulation

<MCI vamp2: procedures>+≡
    subroutine mci_vamp2_prepare_simulation (mci)
        class(mci_vamp2_t), intent(inout) :: mci
        logical :: success
        if (.not. mci%grid_filename_set) then
            call msg_bug ("VAMP2: preapre simulation: integrator filename not set.")
        end if
        call mci%read_header (success)
        call mci%compute_md5sum ()
        if (.not. success) then
            call msg_fatal ("Simulate: " &
                // "reading integration grids from file '" &
                // char (mci%get_grid_filename ()) // "' failed")
        end if
        if (.not. mci%integrator_defined) then
            call mci%read_data ()
        end if
        call groom_rng (mci%rng)
contains
        subroutine groom_rng (rng)
            class(rng_t), intent(inout) :: rng
            integer :: i, rank, n_size
            call mpi_get_comm_id (n_size, rank)
            do i = 2, rank + 1
                select type (rng)
                type is (rng_stream_t)
                    call rng%next_substream ()
                    if (i == rank) &
                        call msg_message ("MCI: Advance RNG for parallel event simulation")
                class default
                    call msg_bug ("Use of any random number generator &
                        &beside rng_stream for parallel event generation not supported.")
                end select
            end do
        end subroutine groom_rng
    end subroutine mci_vamp2_prepare_simulation

```

Generate an unweighted event. We only set the workspace again before generating an event.

```

(MCI vamp2: mci vamp2: TBP)+≡
  procedure, public :: generate_weighted_event => mci_vamp2_generate_weighted_event

(MCI vamp2: procedures)+≡
  subroutine mci_vamp2_generate_weighted_event (mci, instance, sampler)
    class(mci_vamp2_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    if (.not. mci%integrator_defined) then
      call msg_bug ("VAMP2: generate weighted event: undefined integrator")
    end if
    select type (instance)
    type is (mci_vamp2_instance_t)
      instance%event_generated = .false.
      call instance%set_workspace (sampler)
      call mci%integrator%generate_weighted (&
        & instance%func, mci%rng, instance%event_x)
      instance%event_weight = mci%integrator%get_evt_weight ()
      instance%event_excess = 0
      instance%n_events = instance%n_events + 1
      instance%event_generated = .true.
    end select
  end subroutine mci_vamp2_generate_weighted_event

```

We apply an additional rescaling factor for `f_max` (either for the positive or negative distribution).

```

(MCI vamp2: mci vamp2: TBP)+≡
  procedure, public :: generate_unweighted_event => mci_vamp2_generate_unweighted_event

(MCI vamp2: procedures)+≡
  subroutine mci_vamp2_generate_unweighted_event (mci, instance, sampler)
    class(mci_vamp2_t), intent(inout) :: mci
    class(mci_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    if (.not. mci%integrator_defined) then
      call msg_bug ("VAMP2: generate unweighted event: undefined integrator")
    end if
    select type (instance)
    type is (mci_vamp2_instance_t)
      instance%event_generated = .false.
      call instance%set_workspace (sampler)
      generate: do
        call mci%integrator%generate_unweighted (&
          & instance%func, mci%rng, instance%event_x, &
          & opt_event_rescale = instance%event_rescale_f_max)
        instance%event_excess = mci%integrator%get_evt_weight_excess ()
        if (signal_is_pending ()) return
        if (sampler%is_valid ()) exit generate
      end do generate
      if (mci%integrator%get_evt_weight () < 0.) then
        if (.not. mci%negative_weights) then
          call msg_fatal ("VAMP2: cannot sample negative weights!")
        end if
      end if
    end select
  end subroutine mci_vamp2_generate_unweighted_event

```



```

        end if
        instance%event_weight = -1._default
    else
        instance%event_weight = 1._default
    end if
    instance%n_events = instance%n_events + 1
    instance%event_generated = .true.
end select
end subroutine mci_vamp2_generate_unweighted_event

```

```

⟨MCI vamp2: mci vamp2: TBP⟩+≡
    procedure, public :: rebuild_event => mci_vamp2_rebuild_event

⟨MCI vamp2: procedures⟩+≡
    subroutine mci_vamp2_rebuild_event (mci, instance, sampler, state)
        class(mci_vamp2_t), intent(inout) :: mci
        class(mci_instance_t), intent(inout) :: instance
        class(mci_sampler_t), intent(inout) :: sampler
        class(mci_state_t), intent(in) :: state
        call msg_bug ("VAMP2: rebuild event not implemented yet.")
    end subroutine mci_vamp2_rebuild_event

```

21.7.6 Integrator instance

We store all information relevant for simulation. The event weight is stored, when a weighted event is generated, and the event excess, when a larger weight occurs than actual stored max. weight.

We give the possibility to rescale the `f_max` within the integrator object with `event_rescale_f_max`.

```

⟨MCI vamp2: public⟩+≡
    public :: mci_vamp2_instance_t

⟨MCI vamp2: types⟩+≡
    type, extends (mci_instance_t) :: mci_vamp2_instance_t
        class(mci_vamp2_func_t), allocatable :: func
        real(default), dimension(:), allocatable :: gi
        integer :: n_events = 0
        logical :: event_generated = .false.
        real(default) :: event_weight = 0.
        real(default) :: event_excess = 0.
        real(default) :: event_rescale_f_max = 1.
        real(default), dimension(:), allocatable :: event_x
    contains
        ⟨MCI vamp2: mci vamp2 instance: TBP⟩
    end type mci_vamp2_instance_t

```

Output.

```

⟨MCI vamp2: mci vamp2 instance: TBP⟩≡
    procedure, public :: write => mci_vamp2_instance_write

```

<MCI vamp2: procedures>+≡

```

subroutine mci_vamp2_instance_write (object, unit, pacify)
  class(mci_vamp2_instance_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: pacify
  integer :: u, ch, j
  character(len=7) :: fmt
  call pac_fmt (fmt, FMT_17, FMT_14, pacify)
  u = given_output_unit (unit)
  write (u, "(1X,A)") "MCI VAMP2 instance:"
  write (u, "(1X,A,I0)") &
    & "Selected channel          = ", object%selected_channel
  write (u, "(1X,A25,1X," // fmt // ")") &
    & "Integrand                = ", object%integrand
  write (u, "(1X,A25,1X," // fmt // ")") &
    & "MCI weight                = ", object%mc_i_weight
  write (u, "(1X,A,L1)") &
    & "Valid                      = ", object%valid
  write (u, "(1X,A)") "MCI a-priori weight:"
  do ch = 1, size (object%w)
    write (u, "(3X,I25,1X," // fmt // ")") ch, object%w(ch)
  end do
  write (u, "(1X,A)") "MCI jacobian:"
  do ch = 1, size (object%w)
    write (u, "(3X,I25,1X," // fmt // ")") ch, object%f(ch)
  end do
  write (u, "(1X,A)") "MCI mapped x:"
  do ch = 1, size (object%w)
    do j = 1, size (object%x, 1)
      write (u, "(3X,2(1X,I8),1X," // fmt // ")") j, ch, object%x(j, ch)
    end do
  end do
  write (u, "(1X,A)") "MCI channel weight:"
  do ch = 1, size (object%w)
    write (u, "(3X,I25,1X," // fmt // ")") ch, object%gi(ch)
  end do
  write (u, "(1X,A,I0)") &
    & "Number of event          = ", object%n_events
  write (u, "(1X,A,L1)") &
    & "Event generated          = ", object%event_generated
  write (u, "(1X,A25,1X," // fmt // ")") &
    & "Event weight            = ", object%event_weight
  write (u, "(1X,A25,1X," // fmt // ")") &
    & "Event excess            = ", object%event_excess
  write (u, "(1X,A25,1X," // fmt // ")") &
    & "Event rescale f max      = ", object%event_rescale_f_max
  write (u, "(1X,A,L1)") &
    & "Negative (event) weight = ", object%negative_weights
  write (u, "(1X,A)") "MCI event"
  do j = 1, size (object%event_x)
    write (u, "(3X,I25,1X," // fmt // ")") j, object%event_x(j)
  end do
end subroutine mci_vamp2_instance_write

```

Finalizer. We are only using allocatable, so there is nothing to do here.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: final => mci_vamp2_instance_final

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_instance_final (object)
    class(mci_vamp2_instance_t), intent(inout) :: object
    !
  end subroutine mci_vamp2_instance_final

```

Initializer.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: init => mci_vamp2_instance_init

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_instance_init (mci_instance, mci)
    class(mci_vamp2_instance_t), intent(out) :: mci_instance
    class(mci_t), intent(in), target :: mci
    call mci_instance%base_init (mci)
    allocate (mci_instance%gi(mci%n_channel), source=0._default)
    allocate (mci_instance%event_x(mci%n_dim), source=0._default)
    allocate (mci_vamp2_func_t :: mci_instance%func)
    call mci_instance%func%init (n_dim = mci%n_dim, n_channel = mci%n_channel)
  end subroutine mci_vamp2_instance_init

```

Set workspace for mci_vamp2_func_t.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: set_workspace => mci_vamp2_instance_set_workspace

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_instance_set_workspace (instance, sampler)
    class(mci_vamp2_instance_t), intent(inout), target :: instance
    class(mci_sampler_t), intent(inout), target :: sampler
    call instance%func%set_workspace (instance, sampler)
  end subroutine mci_vamp2_instance_set_workspace

```

Evaluation

Compute multi-channel weight. The computation of the multi-channel weight is done by the VAMP2 function. We retrieve the information.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: compute_weight => mci_vamp2_instance_compute_weight

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_instance_compute_weight (mci, c)
    class(mci_vamp2_instance_t), intent(inout) :: mci
    integer, intent(in) :: c
    mci%gi = mci%func%get_probabilities ()
    mci%weight = mci%func%get_weight ()
  end subroutine mci_vamp2_instance_compute_weight

```

Record the integrand.

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: record_integrand => mci_vamp2_instance_record_integrand

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_instance_record_integrand (mci, integrand)
    class(mci_vamp2_instance_t), intent(inout) :: mci
    real(default), intent(in) :: integrand
    mci%integrand = integrand
    call mci%func%set_integrand (integrand)
  end subroutine mci_vamp2_instance_record_integrand

```

Event simulation

In contrast to VAMP, we reset only counters and set the safety factor, which will then be applied each time an event is generated. In that way we do not rescale the actual values in the integrator, but more the current value!

```

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: init_simulation => mci_vamp2_instance_init_simulation

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_instance_init_simulation (instance, safety_factor)
    class(mci_vamp2_instance_t), intent(inout) :: instance
    real(default), intent(in), optional :: safety_factor
    if (present (safety_factor)) instance%event_rescale_f_max = safety_factor
    instance%n_events = 0
    instance%event_generated = .false.
    if (instance%event_rescale_f_max /= 1) then
      write (msg_buffer, "(A,ES10.3,A)") "Simulate: &
        &applying safety factor ", instance%event_rescale_f_max, &
        & " to event rejection."
      call msg_message ()
    end if
  end subroutine mci_vamp2_instance_init_simulation

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: final_simulation => mci_vamp2_instance_final_simulation

<MCI vamp2: procedures>+≡
  subroutine mci_vamp2_instance_final_simulation (instance)
    class(mci_vamp2_instance_t), intent(inout) :: instance
    !
  end subroutine mci_vamp2_instance_final_simulation

<MCI vamp2: mci vamp2 instance: TBP>+≡
  procedure, public :: get_event_weight => mci_vamp2_instance_get_event_weight

<MCI vamp2: procedures>+≡
  function mci_vamp2_instance_get_event_weight (mci) result (weight)
    class(mci_vamp2_instance_t), intent(in) :: mci
    real(default) :: weight
    if (.not. mci%event_generated) then
      call msg_bug ("VAMP2: get event weight: no event generated")
    end if
  end function mci_vamp2_instance_get_event_weight

```

```

        end if
        weight = mci%event_weight
    end function mci_vamp2_instance_get_event_weight

<MCI vamp2: mci vamp2 instance: TBP>+≡
    procedure, public :: get_event_excess => mci_vamp2_instance_get_event_excess

<MCI vamp2: procedures>+≡
    function mci_vamp2_instance_get_event_excess (mci) result (excess)
        class(mci_vamp2_instance_t), intent(in) :: mci
        real(default) :: excess
        if (.not. mci%event_generated) then
            call msg_bug ("VAMP2: get event excess: no event generated")
        end if
        excess = mci%event_excess
    end function mci_vamp2_instance_get_event_excess

```

21.7.7 Unit tests

Test module, followed by the corresponding implementation module.

```
<mci_vamp2_ut.f90>≡  
  <File header>  
  
  module mci_vamp2_ut  
    use unit_tests  
    use mci_vamp2_uti  
  
    <Standard module head>  
  
    <MCI vamp2: public test>  
  
    contains  
  
    <MCI vamp2: test driver>  
  
  end module mci_vamp2_ut  
<mci_vamp2_uti.f90>≡  
  <File header>  
  
  module mci_vamp2_uti  
  
    <Use kinds>  
    <Use strings>  
  
    use io_units  
    use constants, only: PI, TWOPI  
    use rng_base  
    use rng_tao  
    use rng_stream  
    use mci_base  
  
    use mci_vamp2  
  
    <Standard module head>  
  
    <MCI vamp2: test declarations>  
  
    <MCI vamp2: test types>  
  
    contains  
  
    <MCI vamp2: tests>  
  
  end module mci_vamp2_uti  
API: driver for the unit tests below.  
<MCI vamp2: public test>≡  
  public :: mci_vamp2_test  
<MCI vamp2: test driver>≡  
  subroutine mci_vamp2_test (u, results)  
    integer, intent(in) :: u
```

```

    type(test_results_t), intent(inout) :: results
  <MCI vamp2: execute tests>
end subroutine mci_vamp2_test

```

Test sampler

A test sampler object should implement a function with known integral that we can use to check the integrator.

In mode 1, the function is $f(x) = 3x^2$ with integral $\int_0^1 f(x) dx = 1$ and maximum $f(1) = 3$. If the integration dimension is greater than one, the function is extended as a constant in the other dimension(s).

In mode 2, the function is $11x^{10}$, also with integral 1.

Mode 4 includes ranges of zero and negative function value, the integral is negative. The results should be identical to the results of `mci_midpoint_4`, where the same function is evaluated. The function is $f(x) = (1 - 3x^2)\theta(x - 1/2)$ with integral $\int_0^1 f(x) dx = -3/8$, minimum $f(1) = -2$ and maximum $f(1/2) = 1/4$.

```

<MCI vamp2: test types>≡
  type, extends (mci_sampler_t) :: test_sampler_1_t
    real(default), dimension(:), allocatable :: x
    real(default) :: val
    integer :: mode = 1
  contains
    <MCI vamp2: test sampler 1: TBP>
  end type test_sampler_1_t

```

Output: There is nothing stored inside, so just print an informative line.

```

<MCI vamp2: test sampler 1: TBP>≡
  procedure, public :: write => test_sampler_1_write
<MCI vamp2: tests>≡
  subroutine test_sampler_1_write (object, unit, testflag)
    class(test_sampler_1_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    select case (object%mode)
    case (1)
      write (u, "(1x,A)") "Test sampler: f(x) = 3 x^2"
    case (2)
      write (u, "(1x,A)") "Test sampler: f(x) = 11 x^10"
    case (3)
      write (u, "(1x,A)") "Test sampler: f(x) = 11 x^10 * 2 * cos^2 (2 pi y)"
    case (4)
      write (u, "(1x,A)") "Test sampler: f(x) = (1 - 3 x^2) theta(x - 1/2)"
    end select
  end subroutine test_sampler_1_write

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

<MCI vamp2: test sampler 1: TBP>+≡

```

```

    procedure, public :: evaluate => test_sampler_1_evaluate
<MCI vamp2: tests>+≡
    subroutine test_sampler_1_evaluate (sampler, c, x_in, val, x, f)
        class(test_sampler_1_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        if (allocated (sampler%x)) deallocate (sampler%x)
        allocate (sampler%x (size (x_in)))
        sampler%x = x_in
        select case (sampler%mode)
        case (1)
            sampler%val = 3 * x_in(1) ** 2
        case (2)
            sampler%val = 11 * x_in(1) ** 10
        case (3)
            sampler%val = 11 * x_in(1) ** 10 * 2 * cos (twopi * x_in(2)) ** 2
        case (4)
            if (x_in(1) >= .5_default) then
                sampler%val = 1 - 3 * x_in(1) ** 2
            else
                sampler%val = 0
            end if
        end select
        call sampler%fetch (val, x, f)
    end subroutine test_sampler_1_evaluate

```

The point is always valid.

```

<MCI vamp2: test sampler 1: TBP>+≡
    procedure, public :: is_valid => test_sampler_1_is_valid
<MCI vamp2: tests>+≡
    function test_sampler_1_is_valid (sampler) result (valid)
        class(test_sampler_1_t), intent(in) :: sampler
        logical :: valid
        valid = .true.
    end function test_sampler_1_is_valid

```

Rebuild: compute all but the function value.

```

<MCI vamp2: test sampler 1: TBP>+≡
    procedure, public :: rebuild => test_sampler_1_rebuild
<MCI vamp2: tests>+≡
    subroutine test_sampler_1_rebuild (sampler, c, x_in, val, x, f)
        class(test_sampler_1_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(in) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        if (allocated (sampler%x)) deallocate (sampler%x)

```



```

allocate (sampler%x (size (x_in)))
sampler%x = x_in
sampler%val = val
x(:,1) = sampler%x
f = 1
end subroutine test_sampler_1_rebuild

```

Extract the results.

```

⟨MCI vamp2: test sampler 1: TBP⟩+≡
  procedure, public :: fetch => test_sampler_1_fetch
⟨MCI vamp2: tests⟩+≡
  subroutine test_sampler_1_fetch (sampler, val, x, f)
    class(test_sampler_1_t), intent(in) :: sampler
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    val = sampler%val
    x(:,1) = sampler%x
    f = 1
  end subroutine test_sampler_1_fetch

```

Two-channel, two dimension test sampler

This sampler implements the function

$$f(x, y) = 4 \sin^2(\pi x) \sin^2(\pi y) + 2 \sin^2(\pi v) \quad (21.19)$$

where

$$x = u^v \quad u = xy \quad (21.20)$$

$$y = u^{(1-v)} \quad v = \frac{1}{2} \left(1 + \frac{\log(x/y)}{\log xy} \right) \quad (21.21)$$

Each term contributes 1 to the integral. The first term in the function is peaked along a cross aligned to the coordinates x and y , while the second term is peaked along the diagonal $x = y$.

The Jacobian is

$$\frac{\partial(x, y)}{\partial(u, v)} = |\log u| \quad (21.22)$$

```

⟨MCI vamp2: test types⟩+≡
  type, extends (mci_sampler_t) :: test_sampler_2_t
    real(default), dimension(:,:), allocatable :: x
    real(default), dimension(:), allocatable :: f
    real(default) :: val
  contains
    ⟨MCI vamp2: test sampler 2: TBP⟩
  end type test_sampler_2_t

```

Output: There is nothing stored inside, so just print an informative line.

```

⟨MCI vamp2: test sampler 2: TBP⟩≡
  procedure, public :: write => test_sampler_2_write

```

```

(MCI vamp2: tests)+≡
subroutine test_sampler_2_write (object, unit, testflag)
  class(test_sampler_2_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Two-channel test sampler 2"
end subroutine test_sampler_2_write

```

Kinematics: compute x and Jacobians, given the input parameter array.

```

(MCI vamp2: test_sampler_2: TBP)+≡
  procedure, public :: compute => test_sampler_2_compute

(MCI vamp2: tests)+≡
subroutine test_sampler_2_compute (sampler, c, x_in)
  class(test_sampler_2_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default) :: xx, yy, uu, vv
  if (.not. allocated (sampler%x)) &
    allocate (sampler%x (size (x_in), 2))
  if (.not. allocated (sampler%f)) &
    allocate (sampler%f (2))
  select case (c)
  case (1)
    xx = x_in(1)
    yy = x_in(2)
    uu = xx * yy
    vv = (1 + log (xx/yy) / log (xx*yy)) / 2
  case (2)
    uu = x_in(1)
    vv = x_in(2)
    xx = uu ** vv
    yy = uu ** (1 - vv)
  end select
  sampler%val = (2 * sin (pi * xx) * sin (pi * yy)) ** 2 &
    + 2 * sin (pi * vv) ** 2
  sampler%f(1) = 1
  sampler%f(2) = abs (log (uu))
  sampler%x(:,1) = [xx, yy]
  sampler%x(:,2) = [uu, vv]
end subroutine test_sampler_2_compute

```

Evaluation: compute the function value. The output x parameter (only one channel) is identical to the input x , and the Jacobian is 1.

```

(MCI vamp2: test_sampler_2: TBP)+≡
  procedure, public :: evaluate => test_sampler_2_evaluate

(MCI vamp2: tests)+≡
subroutine test_sampler_2_evaluate (sampler, c, x_in, val, x, f)
  class(test_sampler_2_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in

```

```

    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    call sampler%compute (c, x_in)
    call sampler%fetch (val, x, f)
end subroutine test_sampler_2_evaluate

```

The point is always valid.

```

<MCI vamp2: test_sampler_2: TBP>+≡
    procedure, public :: is_valid => test_sampler_2_is_valid

<MCI vamp2: tests>+≡
    function test_sampler_2_is_valid (sampler) result (valid)
        class(test_sampler_2_t), intent(in) :: sampler
        logical :: valid
        valid = .true.
    end function test_sampler_2_is_valid

```

Rebuild: compute all but the function value.

```

<MCI vamp2: test_sampler_2: TBP>+≡
    procedure, public :: rebuild => test_sampler_2_rebuild

<MCI vamp2: tests>+≡
    subroutine test_sampler_2_rebuild (sampler, c, x_in, val, x, f)
        class(test_sampler_2_t), intent(inout) :: sampler
        integer, intent(in) :: c
        real(default), dimension(:), intent(in) :: x_in
        real(default), intent(in) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        call sampler%compute (c, x_in)
        x = sampler%x
        f = sampler%f
    end subroutine test_sampler_2_rebuild

```

Extract the results.

```

<MCI vamp2: test_sampler_2: TBP>+≡
    procedure, public :: fetch => test_sampler_2_fetch

<MCI vamp2: tests>+≡
    subroutine test_sampler_2_fetch (sampler, val, x, f)
        class(test_sampler_2_t), intent(in) :: sampler
        real(default), intent(out) :: val
        real(default), dimension(:,:), intent(out) :: x
        real(default), dimension(:), intent(out) :: f
        val = sampler%val
        x = sampler%x
        f = sampler%f
    end subroutine test_sampler_2_fetch

```

One-dimensional integration

Construct an integrator and use it for a one-dimensional sampler.

```
<MCI vamp2: execute tests>≡
    call test (mci_vamp2_1, "mci_vamp2_1", "one-dimensional integral", u, results)

<MCI vamp2: test declarations>≡
    public :: mci_vamp2_1

<MCI vamp2: tests>+≡
    subroutine mci_vamp2_1 (u)
        integer, intent(in) :: u
        type(mci_vamp2_config_t) :: config
        class(mci_t), allocatable, target :: mci
        class(mci_instance_t), pointer :: mci_instance => null ()
        class(mci_sampler_t), allocatable, target :: mci_sampler
        class(rng_t), allocatable :: rng
        type(string_t) :: filename

        write (u, "(A)") "* Test output: mci_vamp2_1"
        write (u, "(A)") "* Purpose: integrate function in one dimension (single channel)"

        write (u, "(A)")
        write (u, "(A)") "* Initialise integrator"
        write (u, "(A)")

        allocate (mci_vamp2_t :: mci)
        call mci%set_dimensions (1, 1)

        filename = "mci_vamp2_1"
        select type (mci)
            type is (mci_vamp2_t)
                call mci%set_config (config)
                call mci%set_grid_filename (filename)
            end select

        allocate (rng_stream_t :: rng)
        call rng%init ()
        call mci%import_rng (rng)

        call mci%write (u, pacify = .true.)

        write (u, "(A)")
        write (u, "(A)") "* Initialise instance"
        write (u, "(A)")

        call mci%allocate_instance (mci_instance)
        call mci_instance%init (mci)

        write (u, "(A)")
        write (u, "(A)") "* Initialise test sampler"
        write (u, "(A)")

        allocate (test_sampler_1_t :: mci_sampler)
        call mci_sampler%write (u)
```

```

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_calls = 1000"
write (u, "(A)")  "  (lower precision to avoid"
write (u, "(A)")  "    numerical noise)"
write (u, "(A)")

select type (mci)
type is (mci_vamp2_t)
  call mci%add_pass ()
end select
call mci%integrate (mci_instance, mci_sampler, 1, 1000, pacify = .true.)
call mci%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Dump channel weights and grids to file"
write (u, "(A)")

mci%md5sum = "1234567890abcdef1234567890abcdef"
select type (mci)
type is (mci_vamp2_t)
  call mci%write_grids ()
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp2_1"

end subroutine mci_vamp2_1

```

Multiple iterations

Construct an integrator and use it for a one-dimensional sampler. Integrate with five iterations without grid adaptation.

```

<MCI vamp2: execute tests>+≡
  call test (mci_vamp2_2, "mci_vamp2_2", &
    "multiple iterations", &
    u, results)

<MCI vamp2: test declarations>+≡
  public :: mci_vamp2_2

```

(MCI vamp2: tests) +=

```
subroutine mci_vamp2_2 (u)
  type(mci_vamp2_config_t) :: config
  integer, intent(in) :: u
  class(mci_t), allocatable, target :: mci
  class(mci_instance_t), pointer :: mci_instance => null ()
  class(mci_sampler_t), allocatable :: sampler
  class(rng_t), allocatable :: rng
  type(string_t) :: filename

  write (u, "(A)")  "* Test output: mci_vamp2_2"
  write (u, "(A)")  "* Purpose: integrate function in one dimension &
    &(single channel), but multiple iterations."

  write (u, "(A)")
  write (u, "(A)")  "* Initialize integrator, sampler, instance"
  write (u, "(A)")

  allocate (mci_vamp2_t :: mci)
  call mci%set_dimensions (1, 1)
  filename = "mci_vamp2_2"
  select type (mci)
    type is (mci_vamp2_t)
      call mci%set_config (config)
      call mci%set_grid_filename (filename)
  end select

  allocate (rng_stream_t :: rng)
  call rng%init ()
  call mci%import_rng (rng)

  call mci%allocate_instance (mci_instance)
  call mci_instance%init (mci)

  allocate (test_sampler_1_t :: sampler)
  select type (sampler)
    type is (test_sampler_1_t)
      sampler%mode = 2
  end select
  call sampler%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 100"
  write (u, "(A)")

  select type (mci)
    type is (mci_vamp2_t)
      call mci%add_pass (adapt_grids = .false.)
  end select
  call mci%integrate (mci_instance, sampler, 3, 1000, pacify = .true.)
  call mci%write (u, pacify = .true.)

  write (u, "(A)")
  write (u, "(A)")  "* Contents of mci_instance:"
```

```

write (u, "(A)")

call mci_instance%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)") "* Dump channel weights and grids to file"
write (u, "(A)")

mci%md5sum = "1234567890abcdef1234567890abcdef"
select type (mci)
type is (mci_vamp2_t)
  call mci%write_grids ()
end select

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: mci_vamp2_2"

end subroutine mci_vamp2_2

```

Grid adaptation

Construct an integrator and use it for a one-dimensional sampler. Integrate with three iterations and in-between grid adaptations.

```

<MCI vamp2: execute tests>+≡
  call test (mci_vamp2_3, "mci_vamp2_3", &
    "grid adaptation", &
    u, results)

<MCI vamp2: test declarations>+≡
  public :: mci_vamp2_3

<MCI vamp2: tests>+≡
  subroutine mci_vamp2_3 (u)
    integer, intent(in) :: u
    type(mci_vamp2_config_t) :: config
    class(mci_t), allocatable, target :: mci
    class(mci_instance_t), pointer :: mci_instance => null ()
    class(mci_sampler_t), allocatable :: sampler
    class(rng_t), allocatable :: rng
    type(string_t) :: filename

    write (u, "(A)") "* Test output: mci_vamp2_3"
    write (u, "(A)") "* Purpose: integrate function in one dimension &
      &(single channel)"
    write (u, "(A)") "*           and adapt grid"

    write (u, "(A)")

```

```

write (u, "(A)")  "* Initialize integrator, sampler, instance"
write (u, "(A)")

allocate (mci_vamp2_t :: mci)
call mci%set_dimensions (1, 1)
filename = "mci_vamp2_3"
select type (mci)
type is (mci_vamp2_t)
    call mci%set_grid_filename (filename)
    call mci%set_config (config)
end select

allocate (rng_stream_t :: rng)
call rng%init ()
call mci%import_rng (rng)

call mci%allocate_instance (mci_instance)
call mci_instance%init (mci)

allocate (test_sampler_1_t :: sampler)
select type (sampler)
type is (test_sampler_1_t)
    sampler%mode = 2
end select
call sampler%write (u)

write (u, "(A)")
write (u, "(A)")  "* Integrate with n_it = 3 and n_calls = 100"
write (u, "(A)")

select type (mci)
type is (mci_vamp2_t)
    call mci%add_pass (adapt_grids = .true.)
end select
call mci%integrate (mci_instance, sampler, 3, 1000, pacify = .true.)
call mci%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Contents of mci_instance:"
write (u, "(A)")

call mci_instance%write (u, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Dump channel weights and grids to file"
write (u, "(A)")

mci%md5sum = "1234567890abcdef1234567890abcdef"
select type (mci)
type is (mci_vamp2_t)
    call mci%write_grids ()
end select

write (u, "(A)")

```



```

write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call mci_instance%final ()
call mci%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: mci_vamp2_3"

end subroutine mci_vamp2_3

```

21.8 Dispatch

<dispatch_mci.f90>≡

<File header>

```
module dispatch_mci
```

<Use strings>

```

use diagnostics
use os_interface
use variables

```

```

use mci_base
use mci_none
use mci_midpoint
use mci_vamp
use mci_vamp2

```

<Standard module head>

<Dispatch mci: public>

<Dispatch mci: parameters>

```
contains
```

<Dispatch mci: procedures>

```
end module dispatch_mci
```

Allocate an integrator according to the variable `$integration_method`.

<Dispatch mci: public>≡

```
public :: dispatch_mci_s
```

<Dispatch mci: procedures>≡

```

subroutine dispatch_mci_s (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
  type(string_t) :: run_id
  type(string_t) :: integration_method

```

```

type(grid_parameters_t) :: grid_par
type(history_parameters_t) :: history_par
type(mci_vamp2_config_t) :: mci_vamp2_config
integer :: grid_checkpoint
logical :: rebuild_grids, check_grid_file, negative_weights, verbose
logical :: dispatch_nlo, binary_grid_format
type(string_t) :: grid_path, parallel_method
dispatch_nlo = .false.; if (present (is_nlo)) dispatch_nlo = is_nlo
integration_method = &
    var_list%get_sval (var_str ("integration_method"))
select case (char (integration_method))
case ("none")
    allocate (mci_none_t :: mci)
case ("midpoint")
    allocate (mci_midpoint_t :: mci)
case ("vamp", "default")
    call unpack_options_vamp ()
    allocate (mci_vamp_t :: mci)
    select type (mci)
    type is (mci_vamp_t)
        call mci%set_grid_parameters (grid_par)
        if (run_id /= "") then
            call mci%set_grid_filename (process_id, run_id)
        else
            call mci%set_grid_filename (process_id)
        end if
        grid_path = var_list%get_sval (var_str ("integrate_workspace"))
        if (grid_path /= "") then
            call setup_grid_path (grid_path)
            call mci%prepend_grid_path (grid_path)
        end if
        call mci%set_history_parameters (history_par)
        call mci%set_rebuild_flag (rebuild_grids, check_grid_file)
        mci%negative_weights = negative_weights
        mci%verbose = verbose
    end select
case ("vamp2")
    call unpack_options_vamp2 ()
    allocate (mci_vamp2_t :: mci)
    select type (mci)
    type is (mci_vamp2_t)
        call mci%set_config (mci_vamp2_config)
        if (run_id /= "") then
            call mci%set_grid_filename (process_id, run_id)
        else
            call mci%set_grid_filename (process_id)
        end if
        grid_path = var_list%get_sval (var_str ("integrate_workspace"))
        if (grid_path /= "") then
            call setup_grid_path (grid_path)
            call mci%prepend_grid_path (grid_path)
        end if
        call mci%set_rebuild_flag (rebuild_grids, check_grid_file)
        mci%negative_weights = negative_weights

```

```

        mci%verbose = verbose
        mci%grid_checkpoint = grid_checkpoint
        mci%binary_grid_format = binary_grid_format
        mci%parallel_method = parallel_method
    end select
case default
    call msg_fatal ("Integrator '" &
        // char (integration_method) // "' not implemented")
end select
contains
    <Dispatch mci s: procedures>
end subroutine dispatch_mci_s

```

<Dispatch mci s: procedures>≡

```

subroutine unpack_options_vamp ()
    grid_par%threshold_calls = &
        var_list%get_ival (var_str ("threshold_calls"))
    grid_par%min_calls_per_channel = &
        var_list%get_ival (var_str ("min_calls_per_channel"))
    grid_par%min_calls_per_bin = &
        var_list%get_ival (var_str ("min_calls_per_bin"))
    grid_par%min_bins = &
        var_list%get_ival (var_str ("min_bins"))
    grid_par%max_bins = &
        var_list%get_ival (var_str ("max_bins"))
    grid_par%stratified = &
        var_list%get_lval (var_str ("?stratified"))
    select case (char (var_list%get_sval (var_str ("$_phs_method"))))
    case ("rambo")
        grid_par%use_vamp_equivalences = .false.
    case default
        grid_par%use_vamp_equivalences = &
            var_list%get_lval (var_str ("?use_vamp_equivalences"))
    end select
    grid_par%channel_weights_power = &
        var_list%get_rval (var_str ("channel_weights_power"))
    grid_par%accuracy_goal = &
        var_list%get_rval (var_str ("accuracy_goal"))
    grid_par%error_goal = &
        var_list%get_rval (var_str ("error_goal"))
    grid_par%rel_error_goal = &
        var_list%get_rval (var_str ("relative_error_goal"))
    history_par%global = &
        var_list%get_lval (var_str ("?vamp_history_global"))
    history_par%global_verbose = &
        var_list%get_lval (var_str ("?vamp_history_global_verbose"))
    history_par%channel = &
        var_list%get_lval (var_str ("?vamp_history_channels"))
    history_par%channel_verbose = &
        var_list%get_lval (var_str ("?vamp_history_channels_verbose"))
    verbose = &
        var_list%get_lval (var_str ("?vamp_verbose"))
    check_grid_file = &
        var_list%get_lval (var_str ("?check_grid_file"))

```

```

run_id = &
    var_list%get_sval (var_str ("$_run_id"))
rebuild_grids = &
    var_list%get_lval (var_str ("?rebuild_grids"))
negative_weights = &
    var_list%get_lval (var_str ("?negative_weights")) .or. dispatch_nlo
end subroutine unpack_options_vamp

subroutine unpack_options_vamp2 ()
    mci_vamp2_config%n_bins_max = &
        var_list%get_ival (var_str ("max_bins"))
    mci_vamp2_config%n_calls_min_per_channel = &
        var_list%get_ival (var_str ("min_calls_per_channel"))
    mci_vamp2_config%n_calls_threshold = &
        var_list%get_ival (var_str ("threshold_calls"))
    mci_vamp2_config%beta = &
        var_list%get_rval (var_str ("channel_weights_power"))
    mci_vamp2_config%stratified = &
        var_list%get_lval (var_str ("?stratified"))
    select case (char (var_list%get_sval (var_str ("$_phs_method"))))
    case ("rambo")
        mci_vamp2_config%equivalences = .false.
    case default
        mci_vamp2_config%equivalences = &
            var_list%get_lval (var_str ("?use_vamp_equivalences"))
    end select
    mci_vamp2_config%accuracy_goal = &
        var_list%get_rval (var_str ("accuracy_goal"))
    mci_vamp2_config%error_goal = &
        var_list%get_rval (var_str ("error_goal"))
    mci_vamp2_config%rel_error_goal = &
        var_list%get_rval (var_str ("relative_error_goal"))
    verbose = &
        var_list%get_lval (var_str ("?vamp_verbose"))
    check_grid_file = &
        var_list%get_lval (var_str ("?check_grid_file"))
    run_id = &
        var_list%get_sval (var_str ("$_run_id"))
    rebuild_grids = &
        var_list%get_lval (var_str ("?rebuild_grids"))
    negative_weights = &
        var_list%get_lval (var_str ("?negative_weights")) .or. dispatch_nlo
    grid_checkpoint = &
        var_list%get_ival (var_str ("vamp_grid_checkpoint"))
    select case (char (var_list%get_sval (var_str ("$_vamp_grid_format"))))
    case ("binary","Binary","BINARY")
        binary_grid_format = .true.
    case ("ascii","Ascii","ASCII")
        binary_grid_format = .false.
    case default
        binary_grid_format = .false.
    end select
    select case (char (var_list%get_sval (var_str ("$_vamp_parallel_method"))))
    case ("simple","Simple","SIMPLE")

```

```

        parallel_method = var_str ("simple")
    case ("load","Load","LOAD")
        parallel_method = var_str ("load")
    case default
        parallel_method = var_str ("simple")
    end select
end subroutine unpack_options_vamp2

```

Make sure that the VAMP grid subdirectory, if requested, exists before it is used. Also include a sanity check on the directory name.

```

⟨Dispatch mci: parameters⟩≡
    character(*), parameter :: ALLOWED_IN_DIRNAME = &
        "abcdefghijklmnopqrstuvwxyz&
        &ABCDEFGHIJKLMNOPQRSTUVWXYZ&
        &1234567890&
        &.,_-=
⟨Dispatch mci: public⟩+≡
    public :: setup_grid_path
⟨Dispatch mci: procedures⟩+≡
    subroutine setup_grid_path (grid_path)
        type(string_t), intent(in) :: grid_path
        if (verify (grid_path, ALLOWED_IN_DIRNAME) == 0) then
            call msg_message ("Integrator: preparing VAMP grid directory '" &
                // char (grid_path) // "'")
            call os_system_call ("mkdir -p '" // grid_path // "'")
        else
            call msg_fatal ("Integrator: VAMP grid_path '" &
                // char (grid_path) // "' contains illegal characters")
        end if
    end subroutine setup_grid_path

```

21.8.1 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨dispatch_mci_ut.f90⟩≡
    ⟨File header⟩

    module dispatch_mci_ut
        use unit_tests
        use dispatch_mci_util

    ⟨Standard module head⟩

    ⟨Dispatch mci: public test⟩

    contains

    ⟨Dispatch mci: test driver⟩

    end module dispatch_mci_ut

```

```

⟨dispatch_mci_util.f90⟩≡
  ⟨File header⟩

  module dispatch_mci_util

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use variables
    use mci_base
    use mci_none
    use mci_midpoint
    use mci_vamp
    use dispatch_mci

    ⟨Standard module head⟩

    ⟨Dispatch mci: test declarations⟩

    contains

    ⟨Dispatch mci: tests⟩

  end module dispatch_mci_util
API: driver for the unit tests below.
⟨Dispatch mci: public test⟩≡
  public :: dispatch_mci_test
⟨Dispatch mci: test driver⟩≡
  subroutine dispatch_mci_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    ⟨Dispatch mci: execute tests⟩
  end subroutine dispatch_mci_test

```

Select type: integrator core

```

⟨Dispatch mci: execute tests⟩≡
  call test (dispatch_mci_1, "dispatch_mci_1", &
    "integration method", &
    u, results)
⟨Dispatch mci: test declarations⟩≡
  public :: dispatch_mci_1
⟨Dispatch mci: tests⟩≡
  subroutine dispatch_mci_1 (u)
    integer, intent(in) :: u
    type(var_list_t) :: var_list
    class(mci_t), allocatable :: mci
    type(string_t) :: process_id

    write (u, "(A)")  "* Test output: dispatch_mci_1"
    write (u, "(A)")  "* Purpose: select integration method"

```

```

write (u, "(A)")

call var_list%init_defaults (0)

process_id = "dispatch_mci_1"

write (u, "(A)")  "* Allocate MCI as none_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("integration_method"), &
    var_str ("none"), is_known = .true.)
call dispatch_mci_s (mci, var_list, process_id)
select type (mci)
type is (mci_none_t)
    call mci%write (u)
end select

call mci%final ()
deallocate (mci)

write (u, "(A)")
write (u, "(A)")  "* Allocate MCI as midpoint_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call dispatch_mci_s (mci, var_list, process_id)
select type (mci)
type is (mci_midpoint_t)
    call mci%write (u)
end select

call mci%final ()
deallocate (mci)

write (u, "(A)")
write (u, "(A)")  "* Allocate MCI as vamp_t"
write (u, "(A)")

call var_list%set_string (&
    var_str ("integration_method"), &
    var_str ("vamp"), is_known = .true.)
call var_list%set_int (var_str ("threshold_calls"), &
    1, is_known = .true.)
call var_list%set_int (var_str ("min_calls_per_channel"), &
    2, is_known = .true.)
call var_list%set_int (var_str ("min_calls_per_bin"), &
    3, is_known = .true.)
call var_list%set_int (var_str ("min_bins"), &
    4, is_known = .true.)
call var_list%set_int (var_str ("max_bins"), &
    5, is_known = .true.)

```

```

call var_list%set_log (var_str ("?stratified"), &
    .false., is_known = .true.)
call var_list%set_log (var_str ("?use_vamp_equivalences"), &
    .false., is_known = .true.)
call var_list%set_real (var_str ("channel_weights_power"), &
    4._default, is_known = .true.)
call var_list%set_log (&
    var_str ("?vamp_history_global_verbose"), &
    .true., is_known = .true.)
call var_list%set_log (&
    var_str ("?vamp_history_channels"), &
    .true., is_known = .true.)
call var_list%set_log (&
    var_str ("?vamp_history_channels_verbose"), &
    .true., is_known = .true.)
call var_list%set_log (var_str ("?stratified"), &
    .false., is_known = .true.)

call dispatch_mci_s (mci, var_list, process_id)
select type (mci)
type is (mci_vamp_t)
    call mci%write (u)
    call mci%write_history_parameters (u)
end select

call mci%final ()
deallocate (mci)

write (u, "(A)")
write (u, "(A)")  "* Allocate MCI as vamp_t, allow for negative weights"
write (u, "(A)")

call var_list%set_string (&
    var_str ("integration_method"), &
    var_str ("vamp"), is_known = .true.)
call var_list%set_log (var_str ("?negative_weights"), &
    .true., is_known = .true.)

call dispatch_mci_s (mci, var_list, process_id)
select type (mci)
type is (mci_vamp_t)
    call mci%write (u)
    call mci%write_history_parameters (u)
end select

call mci%final ()
deallocate (mci)

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_mci_1"

end subroutine dispatch_mci_1

```


Chapter 22

Parton shower and interface to PYTHIA6

This is the code for the WHIZARD QCD parton shower for final state radiation (FSR) and initial state radiation (ISR) as well as the interface to the PYTHIA module for showering and hadronization.

22.1 Basics of the shower

```
<shower_base.f90>≡  
  <File header>  
  
  module shower_base  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use constants  
    use diagnostics  
    use format_utils, only: write_separator  
    use lorentz  
    use particles  
    use os_interface  
    use rng_base  
    use physics_defs  
    use sm_physics, only: running_as_lam  
    use particles  
    use variables  
    use model_data  
    use pdf  
    use tauola_interface  
  
    <Standard module head>  
  
    <Shower base: public>  
  
    <Shower base: parameters>
```

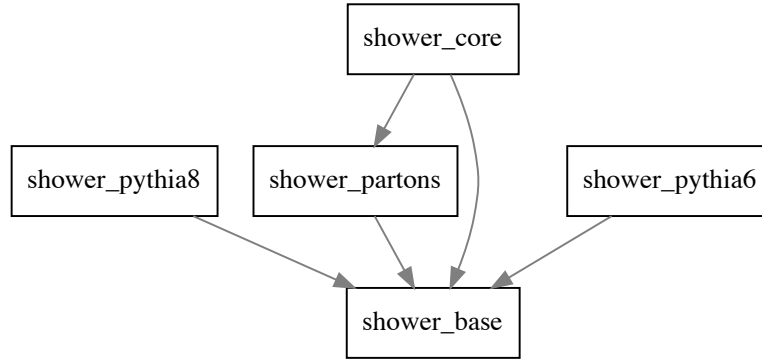


Figure 22.1: Module dependencies in `src/shower`.

⟨Shower base: types⟩

⟨Shower base: interfaces⟩

`contains`

⟨Shower base: procedures⟩

`end module shower_base`

22.1.1 Shower implementations

⟨Shower base: public⟩≡

`public :: PS_WHIZARD, PS_PYTHIA6, PS_PYTHIA8, PS_UNDEFINED`

⟨Shower base: parameters⟩≡

`integer, parameter :: PS_UNDEFINED = 0`

`integer, parameter :: PS_WHIZARD = 1`

`integer, parameter :: PS_PYTHIA6 = 2`

`integer, parameter :: PS_PYTHIA8 = 3`

A dictionary

⟨Shower base: public⟩+≡

`public :: shower_method_of_string`

⟨Shower base: procedures⟩≡

`elemental function shower_method_of_string (string) result (i)`

`integer :: i`

`type(string_t), intent(in) :: string`

`select case (char(string))`

`case ("WHIZARD")`

`i = PS_WHIZARD`

`case ("PYTHIA6")`

```

        i = PS_PYTHIA6
    case ("PYTHIA8")
        i = PS_PYTHIA8
    case default
        i = PS_UNDEFINED
    end select
end function shower_method_of_string

```

```

<Shower base: public>+≡
    public :: shower_method_to_string

<Shower base: procedures>+≡
    elemental function shower_method_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
        select case (i)
            case (PS_WHIZARD)
                string = "WHIZARD"
            case (PS_PYTHIA6)
                string = "PYTHIA6"
            case (PS_PYTHIA8)
                string = "PYTHIA8"
            case default
                string = "UNDEFINED"
        end select
    end function shower_method_to_string

```

22.1.2 Shower settings

These the general shower settings, the settings and parameters for the matching are defined in the corresponding matching modules. The width and the cutoff of the Gaussian primordial k_t distribution, PARP(91) and PARP(93), in GeV, are called `isr_primordial_kt_width` and `isr_primordial_kt_cutoff` in WHIZARD. The parameter MSTJ(45) gives the maximum number of flavors in gluon decay to quarks, and is here called `max_n_flavors`.

The two parameters `isr_alphas_running` and `[fsr_alphas_running` decide whether to use constant or running α_s in the form of the function $D_{\alpha_s}(t)$ for the FSR and ISR (MSTJ(44), MSTP(64)), respectively. The next parameter, `fixed_alpha_s` is the parameter PARU(111), which sets the value for constant α_s , and the flag whether to use P_t -ordered ISR is `isr_pt_ordered`. From the entry `min_voirtuality` on, parameters have meanings both for the PYTHIA and WHIZARD parton shower(s), where PYTHIA values are denoted at the end of the line.

```

<Shower base: public>+≡
    public :: shower_settings_t

<Shower base: types>≡
    type :: shower_settings_t
        logical :: active = .false.
        logical :: isr_active = .false.
        logical :: fsr_active = .false.
        logical :: muli_active = .false.

```

```

logical :: hadronization_active = .false.
logical :: tau_dec = .false.
logical :: verbose = .false.
integer :: method = PS_UNDEFINED
logical :: hadron_collision = .false.
logical :: mlm_matching = .false.
logical :: ckkw_matching = .false.
logical :: powheg_matching = .false.
type(string_t) :: pythia6_pygive
type(string_t) :: pythia8_config
type(string_t) :: pythia8_config_file
real(default) :: min_virtuality = 1._default ! PARJ(82)^2
real(default) :: fsr_lambda = 0.29_default ! PARP(72)
real(default) :: isr_lambda = 0.29_default ! PARP(61)
integer :: max_n_flavors = 5 ! MSTJ(45)
logical :: isr_alphas_running = .true. ! MSTP(64)
logical :: fsr_alphas_running = .true. ! MSTJ(44)
real(default) :: fixed_alpha_s = 0.2_default ! PARU(111)
logical :: alpha_s_fudged = .true.
logical :: isr_pt_ordered = .false.
logical :: isr_angular_ordered = .true. ! MSTP(62)
real(default) :: isr_primordial_kt_width = 1.5_default ! PARP(91)
real(default) :: isr_primordial_kt_cutoff = 5._default ! PARP(93)
real(default) :: isr_z_cutoff = 0.999_default ! 1-PARP(66)
real(default) :: isr_minenergy = 2._default ! PARP(65)
real(default) :: isr_tscalefactor = 1._default
logical :: isr_only_onshell_emitted_partons = .true. ! MSTP(63)
contains
  <Shower base: shower settings: TBP>
end type shower_settings_t

```

Read in the shower settings (and flags whether matching and hadronization are switched on).

```

<Shower base: shower settings: TBP>≡
  procedure :: init => shower_settings_init

<Shower base: procedures>+≡
  subroutine shower_settings_init (settings, var_list)
    class(shower_settings_t), intent(out) :: settings
    type(var_list_t), intent(in) :: var_list

    settings%fsr_active = &
      var_list%get_lval (var_str ("?ps_fsr_active"))
    settings%isr_active = &
      var_list%get_lval (var_str ("?ps_isr_active"))
    settings%tau_dec = &
      var_list%get_lval (var_str ("?ps_taudec_active"))
    settings%multi_active = &
      var_list%get_lval (var_str ("?multi_active"))
    settings%hadronization_active = &
      var_list%get_lval (var_str ("?hadronization_active"))
    settings%mlm_matching = &
      var_list%get_lval (var_str ("?mlm_matching"))
    settings%ckkw_matching = &

```

```

        var_list%get_lval (var_str ("?ckkw_matching"))
settings%powheg_matching = &
        var_list%get_lval (var_str ("?powheg_matching"))
settings%method = shower_method_of_string ( &
        var_list%get_sval (var_str ("$shower_method")))
settings%active = settings%isr_active .or. &
        settings%fsr_active .or. &
        settings%powheg_matching .or. &
        settings%mulit_active .or. &
        settings%hadronization_active
if (.not. settings%active) return
settings%verbose = &
        var_list%get_lval (var_str ("?shower_verbose"))
settings%pythia6_pygive = &
        var_list%get_sval (var_str ("ps_PYTHIA_PYGIVE"))
settings%pythia8_config = &
        var_list%get_sval (var_str ("ps_PYTHIA8_config"))
settings%pythia8_config_file = &
        var_list%get_sval (var_str ("ps_PYTHIA8_config_file"))
settings%min_virtuality = &
        (var_list%get_rval (var_str ("ps_mass_cutoff"))**2)
settings%fsr_lambda = &
        var_list%get_rval (var_str ("ps_fsr_lambda"))
settings%isr_lambda = &
        var_list%get_rval (var_str ("ps_isr_lambda"))
settings%max_n_flavors = &
        var_list%get_ival (var_str ("ps_max_n_flavors"))
settings%isr_alphas_running = &
        var_list%get_lval (var_str ("?ps_isr_alphas_running"))
settings%fsr_alphas_running = &
        var_list%get_lval (var_str ("?ps_fsr_alphas_running"))
settings%fixed_alpha_s = &
        var_list%get_rval (var_str ("ps_fixed_alphas"))
settings%isr_pt_ordered = &
        var_list%get_lval (var_str ("?ps_isr_pt_ordered"))
settings%isr_angular_ordered = &
        var_list%get_lval (var_str ("?ps_isr_angular_ordered"))
settings%isr_primordial_kt_width = &
        var_list%get_rval (var_str ("ps_isr_primordial_kt_width"))
settings%isr_primordial_kt_cutoff = &
        var_list%get_rval (var_str ("ps_isr_primordial_kt_cutoff"))
settings%isr_z_cutoff = &
        var_list%get_rval (var_str ("ps_isr_z_cutoff"))
settings%isr_minenergy = &
        var_list%get_rval (var_str ("ps_isr_minenergy"))
settings%isr_tscalefactor = &
        var_list%get_rval (var_str ("ps_isr_tscalefactor"))
settings%isr_only_onshell_emitted_partons = &
        var_list%get_lval (&
        var_str ("?ps_isr_only_onshell_emitted_partons"))
end subroutine shower_settings_init

```

(Shower base: shower settings: TBP)+≡
 procedure :: write => shower_settings_write

(Shower base: procedures) +=

```

subroutine shower_settings_write (settings, unit)
  class(shower_settings_t), intent(in) :: settings
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)") "Shower settings:"
  call write_separator (u)
  write (u, "(1x,A)") "Master switches:"
  write (u, "(3x,A,1x,L1)") &
    "ps_isr_active           = ", settings%isr_active
  write (u, "(3x,A,1x,L1)") &
    "ps_fsr_active           = ", settings%fsr_active
  write (u, "(3x,A,1x,L1)") &
    "ps_tau_dec              = ", settings%tau_dec
  write (u, "(3x,A,1x,L1)") &
    "multi_active            = ", settings%multi_active
  write (u, "(3x,A,1x,L1)") &
    "hadronization_active    = ", settings%hadronization_active
  write (u, "(1x,A)") "General settings:"
  if (settings%isr_active .or. settings%fsr_active) then
    write (u, "(3x,A)") &
      "method                  = " // &
      char (shower_method_to_string (settings%method))
    write (u, "(3x,A,1x,L1)") &
      "shower_verbose          = ", settings%verbose
    write (u, "(3x,A,ES19.12)") &
      "ps_mass_cutoff          = ", &
      sqrt (abs (settings%min_virtuality))
    write (u, "(3x,A,1x,I1)") &
      "ps_max_n_flavors        = ", settings%max_n_flavors
  else
    write (u, "(3x,A)") " [ISR and FSR off]"
  end if
  if (settings%isr_active) then
    write (u, "(1x,A)") "ISR settings:"
    write (u, "(3x,A,1x,L1)") &
      "ps_isr_pt_ordered       = ", settings%isr_pt_ordered
    write (u, "(3x,A,ES19.12)") &
      "ps_isr_lambda           = ", settings%isr_lambda
    write (u, "(3x,A,1x,L1)") &
      "ps_isr_alphas_running    = ", settings%isr_alphas_running
    write (u, "(3x,A,ES19.12)") &
      "ps_isr_primordial_kt_width = ", settings%isr_primordial_kt_width
    write (u, "(3x,A,ES19.12)") &
      "ps_isr_primordial_kt_cutoff = ", &
      settings%isr_primordial_kt_cutoff
    write (u, "(3x,A,ES19.12)") &
      "ps_isr_z_cutoff          = ", settings%isr_z_cutoff
    write (u, "(3x,A,ES19.12)") &
      "ps_isr_minenergy         = ", settings%isr_minenergy
    write (u, "(3x,A,ES19.12)") &
      "ps_isr_tscalefactor      = ", settings%isr_tscalefactor
  else if (settings%fsr_active) then

```

```

        write (u, "(3x,A)" " [ISR off]"
    end if
    if (settings%fsr_active) then
        write (u, "(1x,A)" "FSR settings:"
        write (u, "(3x,A,ES19.12)" &
            "ps_fsr_lambda                = ", settings%fsr_lambda
        write (u, "(3x,A,1x,L1)" &
            "ps_fsr_alphas_running        = ", settings%fsr_alphas_running
    else if (settings%isr_active) then
        write (u, "(3x,A)" " [FSR off]"
    end if
    write (u, "(1x,A)" "Matching Settings:"
    write (u, "(3x,A,1x,L1)" &
        "mlm_matching                    = ", settings%mlm_matching
    write (u, "(3x,A,1x,L1)" &
        "ckkw_matching                    = ", settings%ckkw_matching
    write (u, "(1x,A)" "PYTHIA6 specific settings:"
    write (u, "(3x,A,A,A)" &
        "ps_PYTHIA_PYGIVE                = '", &
        char(settings%pythia6_pygive), "'"
    write (u, "(1x,A)" "PYTHIA8 specific settings:"
    write (u, "(3x,A,A,A)" &
        "ps_PYTHIA8_config                = '", &
        char (settings%pythia8_config), "'"
    write (u, "(3x,A,A,A)" &
        "ps_PYTHIA8_config_file           = '", &
        char (settings%pythia8_config_file), "'"
end subroutine shower_settings_write

```

22.1.3 Abstract Shower Type

Any parton shower implementation will use random numbers to generate emissions.

```

<Shower base: public>+≡
    public :: shower_base_t

<Shower base: types>+≡
    type, abstract :: shower_base_t
        class(rng_t), allocatable :: rng
        type(string_t) :: name
        type(pdf_data_t) :: pdf_data
        type(shower_settings_t) :: settings
        type(taudec_settings_t) :: taudec_settings
        type(os_data_t) :: os_data
        real(default) :: fac_scale
        real(default) :: alpha_s
    contains
        <Shower base: shower base: TBP>
    end type shower_base_t

<Shower base: shower base: TBP>≡
    procedure :: write_msg => shower_base_write_msg

```



```

<Shower base: procedures>+≡
  subroutine shower_base_write_msg (shower)
    class(shower_base_t), intent(inout) :: shower
    call msg_message ("Shower: Using " // char(shower%name) // " shower")
  end subroutine shower_base_write_msg

```

```

<Shower base: shower base: TBP>+≡
  procedure :: import_rng => shower_base_import_rng

```

```

<Shower base: procedures>+≡
  pure subroutine shower_base_import_rng (shower, rng)
    class(shower_base_t), intent(inout) :: shower
    class(rng_t), intent(inout), allocatable :: rng
    call move_alloc (from = rng, to = shower%rng)
  end subroutine shower_base_import_rng

```

Shower implementations need to know the overall settings as well as pdf_data_t if ISR needs to be simulated. In order to use external files or tools we need access to os_data.

```

<Shower base: shower base: TBP>+≡
  procedure (shower_base_init), deferred :: init

```

```

<Shower base: interfaces>≡
  abstract interface
    subroutine shower_base_init (shower, settings, taudec_settings, pdf_data, os_data)
      import
      class(shower_base_t), intent(out) :: shower
      type(shower_settings_t), intent(in) :: settings
      type(taudec_settings_t), intent(in) :: taudec_settings
      type(pdf_data_t), intent(in) :: pdf_data
      type(os_data_t), intent(in) :: os_data
    end subroutine shower_base_init
  end interface

```

Prepare a new event.

Set event parameters: fac_scale, alpha_s

```

<Shower base: shower base: TBP>+≡
  procedure :: prepare_new_event => shower_base_prepare_new_event

```

```

<Shower base: procedures>+≡
  subroutine shower_base_prepare_new_event (shower, fac_scale, alpha_s)
    class(shower_base_t), intent(inout) :: shower
    real(default), intent(in) :: fac_scale, alpha_s
    shower%fac_scale = fac_scale
    shower%alpha_s = alpha_s
  end subroutine shower_base_prepare_new_event

```

```

<Shower base: shower base: TBP>+≡
  procedure (shower_base_import_particle_set), deferred :: import_particle_set

```

```

<Shower base: interfaces>+≡
  abstract interface
    subroutine shower_base_import_particle_set &
      (shower, particle_set)
    import
      class(shower_base_t), target, intent(inout) :: shower
      type(particle_set_t), intent(in) :: particle_set
    end subroutine shower_base_import_particle_set
  end interface

<Shower base: shower base: TBP>+≡
  procedure (shower_base_generate_emissions), deferred :: generate_emissions

<Shower base: interfaces>+≡
  abstract interface
    subroutine shower_base_generate_emissions &
      (shower, valid, number_of_emissions)
    import
      class(shower_base_t), intent(inout), target :: shower
      logical, intent(out) :: valid
      integer, optional, intent(in) :: number_of_emissions
    end subroutine shower_base_generate_emissions
  end interface

<Shower base: shower base: TBP>+≡
  procedure (shower_base_make_particle_set), deferred :: make_particle_set

<Shower base: interfaces>+≡
  abstract interface
    subroutine shower_base_make_particle_set &
      (shower, particle_set, model, model_hadrons)
    import
      class(shower_base_t), intent(in) :: shower
      type(particle_set_t), intent(inout) :: particle_set
      class(model_data_t), intent(in), target :: model
      class(model_data_t), intent(in), target :: model_hadrons
    end subroutine shower_base_make_particle_set
  end interface

<Shower base: shower base: TBP>+≡
  procedure (shower_base_get_final_colored_ME_momenta), deferred :: &
    get_final_colored_ME_momenta

<Shower base: interfaces>+≡
  abstract interface
    subroutine shower_base_get_final_colored_ME_momenta &
      (shower, momenta)
    import
      class(shower_base_t), intent(in) :: shower
      type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
    end subroutine shower_base_get_final_colored_ME_momenta
  end interface

```

22.1.4 Additional parameters

These parameters are the cut-off scale t_{cut} , given in GeV^2 (PARJ(82)), the cut-off scale for the P_t^2 -ordered shower in GeV^2 , and the two shower parameters PARP(72) and PARP(61), respectively.

(Shower base: parameters)+≡

```
real(default), public :: D_min_scale = 0.5_default
```

Treating either u and d , or all quarks except t as massless:

(Shower base: parameters)+≡

```
logical, public :: treat_light_quarks_massless = .true.
```

```
logical, public :: treat_duscb_quarks_massless = .false.
```

Temporary parameters for the P_t -ordered shower:

(Shower base: parameters)+≡

```
real(default), public :: scalefactor1 = 0.02_default
```

```
real(default), public :: scalefactor2 = 0.02_default
```

(Shower base: public)+≡

```
public :: D_alpha_s_isr
```

```
public :: D_alpha_s_fsr
```

(Shower base: procedures)+≡

```
function D_alpha_s_isr (tin, settings) result (alpha_s)
  real(default), intent(in) :: tin
  type(shower_settings_t), intent(in) :: settings
  real(default) :: min_virtuality, d_constalpha_s, d_lambda_isr
  integer :: d_nf
  real(default) :: t
  real(default) :: alpha_s
  min_virtuality = settings%min_virtuality
  d_lambda_isr = settings%isr_lambda
  d_constalpha_s = settings%fixed_alpha_s
  d_nf = settings%max_n_flavors
  if (settings%alpha_s_fudged) then
    t = max (max (0.1_default * min_virtuality, &
                  1.1_default * d_lambda_isr**2), abs(tin))
  else
    t = abs(tin)
  end if
  if (settings%isr_alphas_running) then
    alpha_s = running_as_lam (number_of_flavors(t, d_nf, min_virtuality), &
                              sqrt(t), d_lambda_isr, 0)
  else
    alpha_s = d_constalpha_s
  end if
end function D_alpha_s_isr
```

```
function D_alpha_s_fsr (tin, settings) result (alpha_s)
  real(default), intent(in) :: tin
  type(shower_settings_t), intent(in) :: settings
  real(default) :: min_virtuality, d_lambda_fsr, d_constalpha_s
  integer :: d_nf
  real(default) :: t
  real(default) :: alpha_s
  min_virtuality = settings%min_virtuality
```

```

d_lambda_fsr = settings%fsr_lambda
d_constalpha_s = settings%fixed_alpha_s
d_nf = settings%max_n_flavors
if (settings%alpha_s_fudged) then
    t = max (max (0.1_default * min_virtuality, &
                  1.1_default * d_lambda_fsr**2), abs(tin))
else
    t = abs(tin)
end if
if (settings%fsr_alphas_running) then
    alpha_s = running_as_lam (number_of_flavors (t, d_nf, min_virtuality), &
                              sqrt(t), d_lambda_fsr, 0)
else
    alpha_s = d_constalpha_s
end if
end function D_alpha_s_fsr

```

Mass and mass squared selection functions. All masses are in GeV. Light quarks are assumed to be ordered, $m_1 < m_2 < m_3 \dots$, and they get current masses, not elementary ones. Mesons and baryons other than proton and neutron are needed as beam-remnants. Particles with PDG number zero are taken massless, as well as proper beam remnants and any other particles.

```

(Shower base: public)+≡
    public :: mass_type
    public :: mass_squared_type

(Shower base: procedures)+≡
    elemental function mass_type (type, m2_default) result (mass)
        integer, intent(in) :: type
        real(default), intent(in) :: m2_default
        real(default) :: mass
        mass = sqrt (mass_squared_type (type, m2_default))
    end function mass_type

    elemental function mass_squared_type (type, m2_default) result (mass2)
        integer, intent(in) :: type
        real(default), intent(in) :: m2_default
        real(default) :: mass2
        select case (abs (type))
            !!! case (1,2)
            !!!     if (treat_light_quarks_massless .or. &
            !!!         treat_duscb_quarks_massless) then
            !!!         mass2 = zero
            !!!     else
            !!!         mass2 = 0.330_default**2
            !!!     end if
            !!! case (3)
            !!!     if (treat_duscb_quarks_massless) then
            !!!         mass2 = zero
            !!!     else
            !!!         mass2 = 0.500_default**2
            !!!     end if
            !!! case (4)
            !!!     if (treat_duscb_quarks_massless) then

```

```

!!!      mass2 = zero
!!!      else
!!!      mass2 = 1.500_default**2
!!!      end if
!!!      case (5)
!!!      if (treat_duscb_quarks_massless) then
!!!      mass2 = zero
!!!      else
!!!      mass2 = 4.800_default**2
!!!      end if
!!!      case (GLUON)
!!!      mass2 = zero
case (NEUTRON)
    mass2 = 0.939565_default**2
case (PROTON)
    mass2 = 0.93827_default**2
case (DPLUS)
    mass2 = 1.86960_default**2
case (D0)
    mass2 = 1.86483_default**2
case (B0)
    mass2 = 5.27950_default**2
case (BPLUS)
    mass2 = 5.27917_default**2
case (DELTAPLUSPLUS)
    mass2 = 1.232_default**2
case (SIGMA0)
    mass2 = 1.192642_default**2
case (SIGMAPLUS)
    mass2 = 1.18937_default**2
case (SIGMACPLUS)
    mass2 = 2.4529_default**2
case (SIGMACPLUSPLUS)
    mass2 = 2.45402_default**2
case (SIGMAB0)
    mass2 = 5.8152_default**2
case (SIGMABPLUS)
    mass2 = 5.8078_default**2
case (BEAM_REMNANT)
    mass2 = zero !!! don't know how to handle the beamremnant
case default
    mass2 = m2_default
end select
end function mass_squared_type

```

The number of flavors active at a certain scale (virtuality) t .

(Shower base: public)+≡

```
public :: number_of_flavors
```

(Shower base: procedures)+≡

```

elemental function number_of_flavors (t, d_nf, min_virtuality) result (nr)
    real(default), intent(in) :: t, min_virtuality
    integer, intent(in) :: d_nf
    real(default) :: nr

```

```

integer :: i
nr = 0
if (t < min_virtuality) return ! arbitrary cut off
! TODO: do i = 1, min (max (3, d_nf), 6)
do i = 1, min (3, d_nf)
!!! to do: take heavier quarks(-> cuts on allowed costheta in g->qq)
!!!      into account
      if ((four * mass_squared_type (i, zero) + min_virtuality) < t ) then
        nr = i
      else
        exit
      end if
end do
end function number_of_flavors

```

22.1.5 Unit tests

Test module, followed by the corresponding implementation module.

```

<shower_base_ut.f90>≡
  <File header>

  module shower_base_ut
    use unit_tests
    use shower_base_utl

    <Standard module head>

    <Shower base: public test>

    contains

    <Shower base: test driver>

  end module shower_base_ut

<shower_base_uti.f90>≡
  <File header>

  module shower_base_uti

    <Use kinds>
    <Use strings>
    use format_utils, only: write_separator
    use variables
    use shower_base

    <Standard module head>

    <Shower base: test declarations>

    contains

    <Shower base: tests>

```

```
end module shower_base_util
```

API: driver for the unit tests below.

```
<Shower base: public test>≡
  public :: shower_base_test

<Shower base: test driver>≡
  subroutine shower_base_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
  <Shower base: execute tests>
  end subroutine shower_base_test
```

Shower settings

This test dispatches an `shower_settings` object, which is used to steer the initial and final state showers.

```
<Shower base: execute tests>≡
  call test (shower_base_1, "shower_base_1", &
    "Shower settings", &
    u, results)

<Shower base: test declarations>≡
  public :: shower_base_1

<Shower base: tests>≡
  subroutine shower_base_1 (u)
    integer, intent(in) :: u
    type(var_list_t) :: var_list
    type(shower_settings_t) :: shower_settings

    write (u, "(A)")  "* Test output: shower_base_1"
    write (u, "(A)")  "* Purpose: setting ISR/FSR shower"
    write (u, "(A)")

    write (u, "(A)")  "* Default settings"
    write (u, "(A)")

    call var_list%init_defaults (0)
    call var_list%set_log (var_str ("?alphas_is_fixed"), &
      .true., is_known = .true.)
    call shower_settings%init (var_list)
    call write_separator (u)
    call shower_settings%write (u)
    call write_separator (u)

    write (u, "(A)")
    write (u, "(A)")  "* Switch on ISR/FSR showers, hadronization"
    write (u, "(A)")  "      and MLM matching"
    write (u, "(A)")

    call var_list%set_string (var_str ("$shower_method"), &
```

```

        var_str ("PYTHIA6"), is_known = .true.)
call var_list%set_log (var_str ("?ps_fsr_active"), &
    .true., is_known = .true.)
call var_list%set_log (var_str ("?ps_isr_active"), &
    .true., is_known = .true.)
call var_list%set_log (var_str ("?hadronization_active"), &
    .true., is_known = .true.)
call var_list%set_log (var_str ("?mlm_matching"), &
    .true., is_known = .true.)
call var_list%set_int &
    (var_str ("ps_max_n_flavors"), 4, is_known = .true.)
call var_list%set_real &
    (var_str ("ps_isr_z_cutoff"), 0.1234_default, &
    is_known=.true.)
call var_list%set_real (&
    var_str ("mlm_etamax"), 3.456_default, is_known=.true.)
call var_list%set_string (&
    var_str ("ps_PYTHIA_PYGIVE"), var_str ("abcdefgh"), is_known=.true.)
call shower_settings%init (var_list)
call write_separator (u)
call shower_settings%write (u)
call write_separator (u)

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: shower_base_1"

end subroutine shower_base_1

```

22.2 Parton module for the shower

```

(shower_partons.f90)≡
  {File header}

  module shower_partons

    {Use kinds with double}
    {Use debug}
    use io_units
    use constants
    use system_defs, only: TAB
    use diagnostics
    use physics_defs
    use lorentz
    use sm_physics
    use particles
    use flavors
    use colors
    use subevents
    use model_data
    use shower_base

```



```

    use rng_base

    <Standard module head>

    <Shower partons: public>

    <Shower partons: types>

contains

    <Shower partons: procedures>

end module shower_partons

```

22.2.1 The basic type defintions

The type `parton_t` defines a parton for the shower. The `x` value of the parton is only needed for spacelike showers. The pointer `initial` is only needed for partons in initial showers, it points to the hadron the parton is coming from. An auxiliary value for the P_t -ordered ISR is `aux_pt`. Then, there are two auxiliary entries for the clustering of CKKW pseudo weights and CKKW matching, `ckkwlabel` and `ckkwscale`. In order to make shower settings available to all operations on the shower partons, we endow the `parton_t` type with a pointer to `shower_settings_t`.

```

<Shower partons: public>≡
    public :: parton_t

<Shower partons: types>≡
    type :: parton_t
        integer :: nr = 0
        integer :: type = 0
        type(shower_settings_t), pointer :: settings => null()
        type(vector4_t) :: momentum = vector4_null
        real(default) :: t = zero
        real(default) :: mass2 = zero
        real(default) :: scale = zero
        real(default) :: z = zero
        real(default) :: costheta = zero
        real(default) :: x = zero
        logical :: simulated = .false.
        logical :: belongstoFSR = .true.
        logical :: belongstointeraction = .false.
        type(parton_t), pointer :: parent => null ()
        type(parton_t), pointer :: child1 => null ()
        type(parton_t), pointer :: child2 => null ()
        type(parton_t), pointer :: initial => null ()
        integer :: c1 = 0, c2 = 0
        integer :: aux_pt = 0
        integer :: ckkwlabel = 0
        real(default) :: ckkwscale = zero
        integer :: ckkwtype = -1
        integer :: interactionnr = 0
contains

```

```

    <Shower partons: parton: TBP>
end type parton_t

```

```

<Shower partons: public>+≡
    public :: parton_pointer_t

<Shower partons: types>+≡
    type :: parton_pointer_t
        type(parton_t), pointer :: p => null ()
end type parton_pointer_t

```

22.2.2 Routines

```

<Shower partons: parton: TBP>≡
    procedure :: to_particle => parton_to_particle

<Shower partons: procedures>≡
    function parton_to_particle (parton, model, from_hard_int) result (particle)
        type(particle_t) :: particle
        class(parton_t), intent(in) :: parton
        class(model_data_t), pointer, intent(in) :: model
        logical, intent(in), optional :: from_hard_int
        integer :: col, anti_col
        call parton%to_color (col, anti_col, from_hard_int)
        call particle%init (parton%to_status (from_hard_int), parton%type, &
            model, col, anti_col, parton%momentum)
    end function parton_to_particle

<Shower partons: public>+≡
    public :: parton_of_particle

<Shower partons: procedures>+≡
    ! pure
    function parton_of_particle (particle, nr) result (parton)
        type(parton_t) :: parton
        type(particle_t), intent(in) :: particle
        integer, intent(in) :: nr
        integer, dimension(2) :: col_array
        parton%nr = nr
        parton%momentum = particle%p
        parton%t = particle%p2
        parton%type = particle%flv%get_pdg ()
        col_array = particle%get_color ()
        parton%c1 = col_array (1)
        parton%c2 = col_array (2)
        parton%interactionnr = 1
        parton%mass2 = particle%flv%get_mass () ** 2
    end function parton_of_particle

<Shower partons: parton: TBP>+≡
    procedure :: to_status => parton_to_status

```

<Shower partons: procedures>+≡

```

pure function parton_to_status (parton, from_hard_int) result (status)
  integer :: status
  class(parton_t), intent(in) :: parton
  logical, intent(in), optional :: from_hard_int
  logical :: fhi
  fhi = .false.; if (present (from_hard_int)) fhi = from_hard_int
  if (fhi .or. parton%is_colored ()) then
    if (associated (parton%initial) .and. .not. parton%belongstoFSR) then
      status = PRT_INCOMING
    else
      status = PRT_OUTGOING
    end if
  else
    status = PRT_BEAM_REMNANT
  end if
end function parton_to_status

```

<Shower partons: parton: TBP>+≡

```

procedure :: to_color => parton_to_color

```

<Shower partons: procedures>+≡

```

pure subroutine parton_to_color (parton, c1, c2, from_hard_int)
  class(parton_t), intent(in) :: parton
  integer, intent(out) :: c1, c2
  logical, intent(in), optional :: from_hard_int
  logical :: fhi
  fhi = .false.; if (present (from_hard_int)) fhi = from_hard_int
  c1 = 0
  c2 = 0
  if (parton%is_colored ()) then
    if (fhi) then
      if (parton%c1 /= 0) c1 = parton%c1
      if (parton%c2 /= 0) c2 = parton%c2
    else
      if (parton%c1 /= 0) c1 = 500 + parton%c1
      if (parton%c2 /= 0) c2 = 500 + parton%c2
    end if
  end if
end subroutine parton_to_color

```

<Shower partons: public>+≡

```

public :: parton_copy

```

<Shower partons: procedures>+≡

```

subroutine parton_copy (prt1, prt2)
  type(parton_t), intent(in) :: prt1
  type(parton_t), intent(out) :: prt2
  if (associated (prt1%settings)) prt2%settings => prt1%settings
  prt2%nr = prt1%nr
  prt2%type = prt1%type
  prt2%momentum = prt1%momentum
  prt2%t = prt1%t
  prt2%mass2 = prt1%mass2

```

```

prt2%scale = prt1%scale
prt2%z = prt1%z
prt2%costheta = prt1%costheta
prt2%x = prt1%x
prt2%simulated = prt1%simulated
prt2%belongstoFSR = prt1%belongstoFSR
prt2%belongstointeraction = prt1%belongstointeraction
prt2%interactionnr = prt1%interactionnr
if (associated (prt1%parent)) prt2%parent => prt1%parent
if (associated (prt1%child1)) prt2%child1 => prt1%child1
if (associated (prt1%child2)) prt2%child2 => prt1%child2
if (associated (prt1%initial)) prt2%initial => prt1%initial
prt2%c1 = prt1%c1
prt2%c2 = prt1%c2
prt2%aux_pt = prt1%aux_pt
end subroutine parton_copy

```

This returns the angle between the daughters assuming them to be massless.

```

(Shower partons: parton: TBP)+≡
  procedure :: get_costheta => parton_get_costheta

(Shower partons: procedures)+≡
  elemental function parton_get_costheta (prt) result (costheta)
    class(parton_t), intent(in) :: prt
    real(default) :: costheta
    real(default) :: denom
    denom = two * prt%z * (one - prt%z) * prt%momentum%p(0)**2
    if (denom > eps0) then
      costheta = one - prt%t / denom
    else
      costheta = - one
    end if
  end function parton_get_costheta

```

The same for massive daughters.

```

(Shower partons: parton: TBP)+≡
  procedure :: get_costheta_mass => parton_get_costheta_mass

(Shower partons: procedures)+≡
  elemental function parton_get_costheta_mass (prt) result (costheta)
    class(parton_t), intent(in) :: prt
    real(default) :: costheta, sqrt12
    if (prt%is_branched ()) then
      if (prt%child1%simulated .and. &
          prt%child2%simulated) then
        sqrt12 = sqrt (max (zero, (prt%z)**2 * prt%momentum%p(0)**2 &
                               - prt%child1%t)) * &
                   sqrt (max (zero, (one - prt%z)**2 * prt%momentum%p(0)**2 &
                               - prt%child2%t))
      end if
      if (sqrt12 > eps0) then
        costheta = (prt%t - prt%child1%t - prt%child2%t - &
                    two * prt%z * (one - prt%z) * prt%momentum%p(0)**2) / &
                    (- two * sqrt12)
      end if
    end if
    return
  end function parton_get_costheta_mass

```

```

        end if
    end if
end if
    costheta = prt%get_costheta ()
end function parton_get_costheta_mass

```

This function returns the angle between the momentum vectors of the parton and first daughter. This is only used for debugging.

```

<Shower partons: parton: TBP>+=
    procedure :: get_costheta_motherfirst => parton_get_costheta_motherfirst

<Shower partons: procedures>+=
    elemental function parton_get_costheta_motherfirst (prt) result (costheta)
        class(parton_t), intent(in) :: prt
        real(default) :: costheta
        if (prt%is_branched ()) then
            if ((prt%child1%simulated .or. &
                prt%child1%is_final () .or. &
                prt%child1%is_branched ()) .and. &
                (prt%child2%simulated .or. &
                prt%child2%is_final () .or. &
                prt%child2%is_branched ())) then
                costheta = enclosed_angle_ct (prt%momentum, prt%child1%momentum)
            return
        end if
    end if
    costheta = - two
end function parton_get_costheta_motherfirst

```

Get the parton velocities.

```

<Shower partons: parton: TBP>+=
    procedure :: get_beta => parton_get_beta

<Shower partons: procedures>+=
    pure function get_beta (t,E) result (beta)
        real(default), intent(in) :: t,E
        real(default) :: beta
        beta = sqrt (max (tiny_07, one - t /(E**2)))
    end function get_beta

    elemental function parton_get_beta (prt) result (beta)
        class(parton_t), intent(in) :: prt
        real(default) :: beta
        beta = sqrt (max (tiny_07, one - prt%t / prt%momentum%p(0)**2))
    end function parton_get_beta

```

Write routine.

```

<Shower partons: parton: TBP>+=
    procedure :: write => parton_write

<Shower partons: procedures>+=
    subroutine parton_write (prt, unit)
        class(parton_t), intent(in) :: prt
        integer, intent(in), optional :: unit
    end subroutine parton_write

```

```

integer :: u
u = given_output_unit (unit); if (u < 0) return

write (u, "(1x,7A)") "Shower parton <nr>", TAB, "<type>", TAB // TAB, &
    "<parent>", TAB, "<mom(0:3)>"
write (u, "(2x,I5,3A)", advance = "no") prt%nr, TAB, TAB, TAB
if (prt%is_final ()) then
    write (u, "(1x,I5,1x,A)", advance = "no") prt%type, TAB // TAB
else
    write (u, "(' ',I5,']',A)", advance = "no") prt%type, TAB // TAB
end if
if (associated (prt%parent)) then
    write (u, "(I5,A)", advance = "no") prt%parent%nr, TAB // TAB
else
    write (u, "(5x,2A)", advance = "no") TAB, TAB
end if
write (u, "(4(ES12.5,A))") prt%momentum%p(0), TAB, &
    prt%momentum%p(1), TAB, &
    prt%momentum%p(2), TAB, &
    prt%momentum%p(3)
write (u, "(1x,9A)") "<p4square>", TAB // TAB, "<t>", TAB // TAB, &
    "<scale>", TAB // TAB, "<c1>", TAB, "<c2>", TAB, "<mass2>"
write (u, "(1x,3(ES12.5,A))", advance = "no") &
    prt%momentum ** 2, TAB // TAB, prt%t, TAB, prt%scale, TAB, prt%mass2
write (u, "(2(I4,A))") prt%c1, TAB, prt%c2, TAB
if (prt%is_branched ()) then
    if (prt%belongstoFSR) then
        write (u, "(1x,9A)") "costheta(prt)", TAB, &
            "costheta_correct(prt)", TAB, &
            "prt%costheta", TAB, "prt%z", TAB, &
            "costheta_motherfirst(prt)"
        write (u, "(1X,5(ES12.5,A))") &
            prt%get_costheta (), TAB, &
            prt%get_costheta_mass (), TAB // TAB, &
            prt%costheta, TAB, prt%z, TAB, &
            prt%get_costheta_motherfirst (), TAB
    else
        write (u, "(1x,9A)") "prt%z", TAB, "prt%x", TAB, &
            "costheta_correct(prt)", TAB, &
            "prt%costheta", TAB, &
            "costheta_motherfirst(prt)"
        write (u, "(1X,5(ES12.5,A))") &
            prt%z, TAB, prt%x, TAB, &
            prt%get_costheta_mass (), TAB, &
            prt%costheta, TAB, &
            prt%get_costheta_motherfirst (), TAB
    end if
else
    if (prt%belongstoFSR) then
        write (u, "(1X,A)") "not branched."
    else
        write (u, "(1X,A,ES12.5)") "not branched. x = ", prt%x
    end if
end if
end if

```

```

write (u, "(A)", advance = "no") " Parton"
if (prt%belongstoFSR) then
  write (u, "(A)", advance = "no") " is FSR,"
else
  if (associated (prt%initial)) then
    write (u, "(A,I1)", advance = "no") " from hadron,", prt%initial%nr
  else
    write (u, "(A)", advance = "no") ""
  end if
end if
if (prt%is_final ()) then
  write (u, "(A)", advance = "no") " is final,"
else
  write (u, "(A)", advance = "no") ""
end if
if (prt%simulated) then
  write (u, "(A)", advance = "no") " is simulated,"
else
  write (u, "(A)", advance = "no") ""
end if
if (associated (prt%child1) .and. associated (prt%child2)) then
  write (u, "(A,2(I5),A)", advance = "no") &
    " has children: ", prt%child1%nr, prt%child2%nr, ", "
else if (associated (prt%child1)) then
  write (u, "(A,1(I5),A)", advance = "no") &
    " has one child: ", prt%child1%nr, ", "
end if
if (prt%belongstointeraction) then
  write (u, "(A,I2)") " belongs to interaction ", &
    prt%interactionnr
else
  write (u, "(A,I2)") " does not belong to interaction ", &
    prt%interactionnr
end if
write (u, "(A)") TAB
end subroutine parton_write

```

<Shower partons: parton: TBP>+≡

```
procedure :: is_final => parton_is_final
```

<Shower partons: procedures>+≡

```

elemental function parton_is_final (prt) result (is_final)
  class(parton_t), intent(in) :: prt
  logical :: is_final
  is_final = .false.
  if (prt%belongstoFSR) then
    is_final = .not. associated (prt%child1) .and. &
      (.not. prt%belongstointeraction .or. &
        (prt%belongstointeraction .and. prt%simulated))
  end if
end function parton_is_final

```

<Shower partons: parton: TBP>+≡

```
procedure :: is_branched => parton_is_branched
```

```

<Shower partons: procedures>+≡
    elemental function parton_is_branched (prt) result (is_branched)
        class(parton_t), intent(in) :: prt
        logical :: is_branched
        is_branched = associated (prt%child1) .and. associated (prt%child2)
    end function parton_is_branched

<Shower partons: parton: TBP>+≡
    procedure :: set_simulated => parton_set_simulated

<Shower partons: procedures>+≡
    pure subroutine parton_set_simulated (prt, sim)
        class(parton_t), intent(inout) :: prt
        logical, intent(in), optional :: sim
        if (present (sim)) then
            prt%simulated = sim
        else
            prt%simulated = .true.
        end if
    end subroutine parton_set_simulated

<Shower partons: public>+≡
    public :: parton_set_parent

<Shower partons: procedures>+≡
    subroutine parton_set_parent (prt, parent)
        type(parton_t), intent(inout) :: prt
        type(parton_t), intent(in) , target :: parent
        prt%parent => parent
    end subroutine parton_set_parent

<Shower partons: public>+≡
    public :: parton_get_parent

<Shower partons: procedures>+≡
    function parton_get_parent (prt) result (parent)
        type(parton_t), intent(in) :: prt
        type(parton_t), pointer :: parent
        parent => prt%parent
    end function parton_get_parent

<Shower partons: public>+≡
    public :: parton_set_initial

<Shower partons: procedures>+≡
    subroutine parton_set_initial (prt, initial)
        type(parton_t), intent(inout) :: prt
        type(parton_t), intent(in) , target :: initial
        prt%initial => initial
    end subroutine parton_set_initial

<Shower partons: public>+≡
    public :: parton_get_initial

```



```

<Shower partons: procedures>+≡
function parton_get_initial (prt) result (initial)
    type(parton_t), intent(in) :: prt
    type(parton_t), pointer :: initial
    initial => prt%initial
end function parton_get_initial

```

```

<Shower partons: public>+≡
public :: parton_set_child

```

```

<Shower partons: procedures>+≡
subroutine parton_set_child (prt, child, i)
    type(parton_t), intent(inout) :: prt
    type(parton_t), intent(in), target :: child
    integer, intent(in) :: i
    if (i == 1) then
        prt%child1 => child
    else
        prt%child2 => child
    end if
end subroutine parton_set_child

```

```

<Shower partons: public>+≡
public :: parton_get_child

```

```

<Shower partons: procedures>+≡
function parton_get_child (prt, i) result (child)
    type(parton_t), pointer :: child
    type(parton_t), intent(in) :: prt
    integer, intent(in) :: i
    child => null ()
    if (i == 1) then
        child => prt%child1
    else
        child => prt%child2
    end if
end function parton_get_child

```

```

<Shower partons: parton: TBP>+≡
procedure :: is_quark => parton_is_quark

```

```

<Shower partons: procedures>+≡
elemental function parton_is_quark (prt) result (is_quark)
    class(parton_t), intent(in) :: prt
    logical :: is_quark
    is_quark = abs (prt%type) <= 6 .and. prt%type /= 0
end function parton_is_quark

```

```

<Shower partons: parton: TBP>+≡
procedure :: is_squark => parton_is_squark

```

```

<Shower partons: procedures>+=
  elemental function parton_is_squark (prt) result (is_squark)
    class(parton_t), intent(in) :: prt
    logical :: is_squark
    is_squark = ((abs(prt%type) >= 1000001) .and. (abs(prt%type) <= 1000006)) &
      .or. ((abs(prt%type) >= 2000001) .and. (abs(prt%type) <= 2000006))
  end function parton_is_squark

```

9 can be used for gluons in codes for glueballs

```

<Shower partons: parton: TBP>+=
  procedure :: is_gluon => parton_is_gluon

```

```

<Shower partons: procedures>+=
  elemental function parton_is_gluon (prt) result (is_gluon)
    class(parton_t), intent(in) :: prt
    logical :: is_gluon
    is_gluon = prt%type == GLUON .or. prt%type == 9
  end function parton_is_gluon

```

```

<Shower partons: parton: TBP>+=
  procedure :: is_gluino => parton_is_gluino

```

```

<Shower partons: procedures>+=
  elemental function parton_is_gluino (prt) result (is_gluino)
    class(parton_t), intent(in) :: prt
    logical :: is_gluino
    is_gluino = prt%type == 1000021
  end function parton_is_gluino

```

```

<Shower partons: parton: TBP>+=
  procedure :: is_proton => parton_is_proton

```

```

<Shower partons: procedures>+=
  elemental function parton_is_proton (prt) result (is_hadron)
    class(parton_t), intent(in) :: prt
    logical :: is_hadron
    is_hadron = abs (prt%type) == PROTON
  end function parton_is_proton

```

TODO: SUSY partons.

```

<Shower partons: parton: TBP>+=
  procedure :: is_colored => parton_is_colored

```

```

<Shower partons: procedures>+=
  pure function parton_is_colored (parton) result (is_colored)
    logical :: is_colored
    class(parton_t), intent(in) :: parton
    is_colored = parton_is_quark (parton) .or. parton_is_gluon (parton)
  end function parton_is_colored

```

```

<Shower partons: parton: TBP>+=
  procedure :: mass => parton_mass

```

```

<Shower partons: procedures>+≡
  elemental function parton_mass (prt) result (mass)
    class(parton_t), intent(in) :: prt
    real(default) :: mass
    mass = mass_type (prt%type, prt%mass2)
  end function parton_mass

<Shower partons: parton: TBP>+≡
  procedure :: mass_squared => parton_mass_squared

<Shower partons: procedures>+≡
  elemental function parton_mass_squared (prt) result (mass_squared)
    class(parton_t), intent(in) :: prt
    real(default) :: mass_squared
    mass_squared = mass_squared_type (prt%type, prt%mass2)
  end function parton_mass_squared

<Shower partons: parton: TBP>+≡
  procedure :: momentum_to_pythia6 => parton_momentum_to_pythia6

<Shower partons: procedures>+≡
  pure function parton_momentum_to_pythia6 (prt) result (p)
    real(double), dimension(1:5) :: p
    class(parton_t), intent(in) :: prt
    real(default) :: mass
    !!! gfortran 5.1 complains about 'ELEMENTAL procedure pointer
    !!! component 'mass' is not allowed as an actual argument'
    !!! p = prt%momentum%to_pythia6 (prt%mass ())
    mass = prt%mass ()
    p = prt%momentum%to_pythia6 (mass)
  end function parton_momentum_to_pythia6

<Shower partons: public>+≡
  public :: P_prt_to_child1

<Shower partons: procedures>+≡
  function P_prt_to_child1 (prt) result (retvalue)
    type(parton_t), intent(in) :: prt
    real(default) :: retvalue
    retvalue = zero
    if (prt%is_gluon ()) then
      if (prt%child1%is_quark ()) then
        retvalue = P_gqq (prt%z)
      else if (prt%child1%is_gluon ()) then
        retvalue = P_ggg (prt%z) + P_ggg (one - prt%z)
      end if
    else if (prt%is_quark ()) then
      if (prt%child1%is_quark ()) then
        retvalue = P_qqq (prt%z)
      else if (prt%child1%is_gluon ()) then
        retvalue = P_qqg (one - prt%z)
      end if
    end if
  end function P_prt_to_child1

```

This function returns whether the kinematics of the branching of parton prt into its daughters are allowed or not.

<Shower partons: public>+≡

public :: thetabar

<Shower partons: procedures>+≡

```
function thetabar (prt, recoiler, isr_ang, E3out) result (retvalue)
  type(parton_t), intent(inout) :: prt
  type(parton_t), intent(in) :: recoiler
  real(default), intent(out), optional :: E3out
  logical, intent(in) :: isr_ang
  logical :: retvalue
  real(default) :: ctheta, cthetachild1
  real(default) p1, p4, p3, E3, shat

  shat = (prt%child1%momentum + recoiler%momentum)**2
  E3 = 0.5_default * (shat / prt%z - recoiler%t + prt%child1%t - &
    prt%child2%mass_squared ()) / sqrt(shat)
  if (present (E3out)) then
    E3out = E3
  end if
  !!! absolute values of momenta in a 3 -> 1 + 4 branching
  p3 = sqrt (E3**2 - prt%t)
  p1 = sqrt (prt%child1%momentum%p(0)**2 - prt%child1%t)
  p4 = sqrt (max (zero, (E3 - prt%child1%momentum%p(0))**2 &
    - prt%child2%t))
  if (p3 > zero) then
    retvalue = ((p1 + p4 >= p3) .and. (p3 >= abs(p1 - p4)) )
    if (retvalue .and. isr_ang) then
      !!! check angular ordering
      if (associated (prt%child1)) then
        if (associated (prt%child1%child2)) then
          ctheta = (E3**2 - p1**2 - p4**2 + prt%t) / (two * p1 * p4)
          cthetachild1 = (prt%child1%momentum%p(0)**2 - &
            space_part (prt%child1%child1%momentum)**2 &
            - space_part (prt%child1%child2%momentum)**2 + prt%child1%t) &
            / (two * space_part (prt%child1%child1%momentum)**1 * &
            space_part (prt%child1%child2%momentum)**1)
          retvalue = (ctheta > cthetachild1)
        end if
      end if
    end if
  else
    retvalue = .false.
  end if
end function thetabar
```

<Shower partons: public>+≡

public :: parton_apply_cstheta

<Shower partons: procedures>+≡

```
recursive subroutine parton_apply_cstheta (prt, rng)
  type(parton_t), intent(inout) :: prt
  class(rng_t), intent(inout), allocatable :: rng
```

```

if (debug2_active (D_SHOWER)) then
  print *, "D: parton_apply_cstheta for parton " , prt%nr
  print *, 'prt%momentum%p = ', prt%momentum%p
  if (debug_on) call msg_debug2 (D_SHOWER, "prt%type", prt%type)
end if
prt%z = 0.5_default * (one + prt%get_beta () * prt%costheta)
if (associated (prt%child1) .and. associated (prt%child2)) then
  if (prt%child1%simulated .and. prt%child2%simulated) then
    prt%z = 0.5_default * (one + (prt%child1%t - prt%child2%t) / &
      prt%t + prt%get_beta () * prt%costheta * &
      sqrt((prt%t - prt%child1%t - prt%child2%t)**2 - &
        4 * prt%child1%t * prt%child2%t) / prt%t)
  if (prt%type /= INTERNAL) then
    prt%child1%momentum%p(0) = prt%z * prt%momentum%p(0)
    prt%child2%momentum%p(0) = (one - prt%z) * prt%momentum%p(0)
  end if
  call prt%generate_ps (rng)
  call parton_apply_cstheta (prt%child1, rng)
  call parton_apply_cstheta (prt%child2, rng)
end if
end if
end subroutine parton_apply_cstheta

```

<Shower partons: public>+≡
 public :: parton_apply_lorentztrafo

<Shower partons: procedures>+≡
 subroutine parton_apply_lorentztrafo (prt, L)
 type(parton_t), intent(inout) :: prt
 type(lorentz_transformation_t), intent(in) :: L
 prt%momentum = L * prt%momentum
end subroutine parton_apply_lorentztrafo

<Shower partons: public>+≡
 public :: parton_apply_lorentztrafo_recursive

<Shower partons: procedures>+≡
 recursive subroutine parton_apply_lorentztrafo_recursive (prt, L)
 type(parton_t), intent(inout) :: prt
 type(lorentz_transformation_t), intent(in) :: L
 if (prt%type /= PROTON .and. prt%type /= BEAM_REMNANT) then
 !!! don't boost hadrons and beam-remnants
 call parton_apply_lorentztrafo (prt, L)
 end if
 if (associated (prt%child1) .and. associated (prt%child2)) then
 if ((space_part_norm (prt%child1%momentum) < eps0) .and. &
 (space_part_norm (prt%child2%momentum) < eps0) .and. &
 (.not. prt%child1%belongstointeraction) .and. &
 (.not. prt%child2%belongstointeraction)) then
 !!! don't boost unevolved timelike partons
 else
 call parton_apply_lorentztrafo_recursive (prt%child1, L)
 call parton_apply_lorentztrafo_recursive (prt%child2, L)
 end if
 end if

```

else
  if (associated (prt%child1)) then
    call parton_apply_lorentztrafo_recursive (prt%child1, L)
  end if
  if (associated (prt%child2)) then
    call parton_apply_lorentztrafo_recursive (prt%child2, L)
  end if
end if
end if
end subroutine parton_apply_lorentztrafo_recursive

```

This takes the three-momentum of a parton and generates three-momenta of its children given their energy and virtuality

<Shower partons: parton: TBP>+≡

```

  procedure :: generate_ps => parton_generate_ps

```

<Shower partons: procedures>+≡

```

subroutine parton_generate_ps (prt, rng)
  class(parton_t), intent(inout) :: prt
  class(rng_t), intent(inout), allocatable :: rng
  real(default), dimension(1:3, 1:3) :: directions
  integer i,j
  real(default) :: scproduct, pabs, plabs, p2abs, x, ptabs, phi
  real(default), dimension(1:3) :: momentum
  type(vector3_t) :: pchild1_direction
  type(lorentz_transformation_t) :: L, rotation
  if (debug2_active (D_SHOWER)) print *, "D: parton_generate_ps for parton " , prt%nr
  if (debug_active (D_SHOWER)) then
    if (.not. (associated (prt%child1) .and. associated (prt%child2))) then
      call msg_fatal ("no children for generate_ps")
    end if
  end if
  !!! test if parton is a virtual parton from the imagined parton shower history
  if (prt%type == INTERNAL) then
    L = inverse (boost (prt%momentum, sqrt(prt%t)))
    !!! boost to restframe of mother
    call parton_apply_lorentztrafo (prt, L)
    call parton_apply_lorentztrafo (prt%child1, L)
    call parton_apply_lorentztrafo (prt%child2, L)
    !!! Store child1's momenta
    pchild1_direction = direction (space_part (prt%child1%momentum))
    !!! Redistribute energy
    prt%child1%momentum%p(0) = (prt%momentum%p(0)**2 - &
      prt%child2%t + prt%child1%t) / (two * prt%momentum%p(0))
    prt%child2%momentum%p(0) = prt%momentum%p(0) - &
      prt%child1%momentum%p(0)

    ! rescale momenta and set momenta to be along z-axis
    prt%child1%momentum = vector4_moving (prt%child1%momentum%p(0), &
      vector3_canonical(3) * &
      sqrt(prt%child1%momentum%p(0)**2 - prt%child1%t))
    prt%child2%momentum = vector4_moving (prt%child2%momentum%p(0), &
      - vector3_canonical(3) * &
      sqrt(prt%child2%momentum%p(0)**2 - prt%child2%t))
  end if
end subroutine parton_generate_ps

```

```

!!! rotate so that total momentum is along former total momentum
rotation = rotation_to_2nd (space_part (prt%child1%momentum), &
    pchild1_direction)
call parton_apply_lorentztrafo (prt%child1, rotation)
call parton_apply_lorentztrafo (prt%child2, rotation)

L = inverse (L)          !!! inverse of the boost to restframe of mother
call parton_apply_lorentztrafo (prt, L)
call parton_apply_lorentztrafo (prt%child1, L)
call parton_apply_lorentztrafo (prt%child2, L)
else
!!! directions(1,:) -> direction of the parent parton
if (space_part_norm (prt%momentum) < eps0) return
directions(1,1:3) = prt%momentum%p(1:3) / space_part_norm (prt%momentum)
!!! directions(2,:) and directions(3,:) -> two random directions
!!! perpendicular to the direction of the parent parton
do j = 2, 3
    call rng%generate (directions(j,:))
end do
do i = 2, 3
    scproduct = zero
    do j = 1, i - 1
        scproduct = directions(i,1) * directions(j,1) + &
            directions(i,2) * directions(j,2) + &
            directions(i,3) * directions(j,3)
        directions(i,1) = directions(i,1) - directions(j,1) * scproduct
        directions(i,2) = directions(i,2) - directions(j,2) * scproduct
        directions(i,3) = directions(i,3) - directions(j,3) * scproduct
    end do
    scproduct = directions(i,1)**2 + directions(i,2)**2 + &
        directions(i,3)**2
    do j = 1, 3
        directions(i,j) = directions(i,j) / sqrt(scproduct)
    end do
end do
<Enforce right-handed system for directions>

pabs = space_part_norm (prt%momentum)
if ((prt%child1%momentum%p(0)**2 - prt%child1%t < 0) .or. &
    (prt%child2%momentum%p(0)**2 - prt%child2%t < 0)) then
    if (debug_on) call msg_debug(D_SHOWER, "generate_ps error at E^2 < t")
    return
end if
p1abs = sqrt (prt%child1%momentum%p(0)**2 - prt%child1%t)
p2abs = sqrt (prt%child2%momentum%p(0)**2 - prt%child2%t)
x = (pabs**2 + p1abs**2 - p2abs**2) / (two * pabs)
if (pabs > p1abs + p2abs .or. &
    pabs < abs(p1abs - p2abs)) then
    if (debug_active (D_SHOWER)) then
        print *, "D: parton_generate_ps Dreiecksungleichung error &
            &for parton ", prt%nr, " ", &
            space_part_norm (prt%momentum), " ", p1abs, " ", p2abs
        call prt%write ()
        call prt%child1%write ()
    end if
end if

```

```

        call prt%child2%write ()
    end if
    return
end if
!!! Due to numerical problems transverse momentum could be imaginary ->
!!!     set transverse momentum to zero
ptabs = sqrt (max (plabs * plabs - x * x, zero))
call rng%generate (phi)
phi = twopi * phi
do i = 1, 3
    momentum(i) = x * directions(1,i) + ptabs * &
        (cos(phi) * directions(2,i) + sin(phi) * directions(3,i))
end do
prt%child1%momentum%p(1:3) = momentum(1:3)
do i = 1, 3
    momentum(i) = (space_part_norm (prt%momentum) - x) * directions(1,i) - &
        ptabs * (cos(phi) * directions(2,i) + sin(phi) * directions(3,i))
end do
prt%child2%momentum%p(1:3) = momentum(1:3)
end if
end subroutine parton_generate_ps

```

(Enforce right-handed system for directions)≡

```

if ((directions(1,1) * (directions(2,2) * directions(3,3) - &
    directions(2,3) * directions(3,2)) + &
    directions(1,2) * (directions(2,3) * directions(3,1) - &
    directions(2,1) * directions(3,3)) + &
    directions(1,3) * (directions(2,1) * directions(3,2) - &
    directions(2,2) * directions(3,1))) < 0) then
    directions(3,:) = - directions(3,:)
end if

```

This routine is similar to `parton_generate_ps`, but now for the ISR. It takes the three-momentum of a parton's first child as fixed and generates the two remaining three-momenta.

(Shower partons: parton: TBP)+≡

```

procedure :: generate_ps_ini => parton_generate_ps_ini

```

(Shower partons: procedures)+≡

```

subroutine parton_generate_ps_ini (prt, rng)
    class(parton_t), intent(inout) :: prt
    class(rng_t), intent(inout), allocatable :: rng
    real(default), dimension(1:3, 1:3) :: directions
    integer :: i,j
    real(default) :: scproduct, pabs, plabs, p2abs, x, ptabs, phi
    real(default), dimension(1:3) :: momentum
    if (debug_active (D_SHOWER)) print *, "D: parton_generate_ps_ini: for parton " , prt%nr
    if (debug_active (D_SHOWER)) then
        if (.not. (associated (prt%child1) .and. associated (prt%child2))) then
            call msg_fatal ("no children for generate_ps")
        end if
    end if
end if

if (.not. prt%is_proton()) then

```



```

!!! generate ps for normal partons
do i = 1, 3
    directions(1,i) = prt%child1%momentum%p(i) / &
        space_part_norm(prt%child1%momentum)
end do
do j = 2, 3
    call rng%generate (directions(j,:))
end do
do i = 2, 3
    scproduct = zero
    do j = 1, i - 1
        scproduct = directions(i,1) * directions(j,1) + &
            directions(i,2) * directions(j,2) + &
            directions(i,3) * directions(j,3)
        directions(i,1) = directions(i,1) - directions(j,1) * scproduct
        directions(i,2) = directions(i,2) - directions(j,2) * scproduct
        directions(i,3) = directions(i,3) - directions(j,3) * scproduct
    end do
    scproduct = directions(i,1)**2 + directions(i,2)**2 + &
        directions(i,3)**2
    do j = 1, 3
        directions(i,j) = directions(i,j) / sqrt(scproduct)
    end do
end do
<Enforce right-handed system for directions>

pabs = space_part_norm (prt%child1%momentum)
p1abs = sqrt (prt%momentum%p(0)**2 - prt%t)
p2abs = sqrt (max(zero, prt%child2%momentum%p(0)**2 - &
    prt%child2%t))

x = (pabs**2 + p1abs**2 - p2abs**2) / (two * pabs)
if (debug_active (D_SHOWER)) then
    if (pabs > p1abs + p2abs .or. pabs < abs(p1abs - p2abs)) then
        print *, "error at generate_ps, Dreiecksungleichung for parton ", &
            prt%nr, " ", pabs," ",p1abs," ",p2abs
        call prt%write ()
        call prt%child1%write ()
        call prt%child2%write ()
        call msg_fatal ("parton_generate_ps_ini: Dreiecksungleichung")
    end if
end if
if (debug_active (D_SHOWER)) print *, "D: parton_generate_ps_ini: x = ", x
ptabs = sqrt (p1abs * p1abs - x**2)
call rng%generate (phi)
phi = twopi * phi
do i = 1,3
    momentum(i) = x * directions(1,i) + ptabs * (cos(phi) * &
        directions(2,i) + sin(phi) * directions(3,i))
end do
prt%momentum%p(1:3) = momentum
do i = 1, 3
    momentum(i) = (x - pabs) * directions(1,i) + ptabs * (cos(phi) * &
        directions(2,i) + sin(phi) * directions(3,i))

```

```

        end do
        prt%child2%momentum%p(1:3) = momentum(1:3)
    else
        !!! for first partons just set beam remnants momentum
        prt%child2%momentum = prt%momentum - prt%child1%momentum
    end if
end subroutine parton_generate_ps_ini

```

22.2.3 The analytic FSR

```

<Shower partons: parton: TBP>+=
    procedure :: next_t_ana => parton_next_t_ana

<Shower partons: procedures>+=
    subroutine parton_next_t_ana (prt, rng)
        class(parton_t), intent(inout) :: prt
        class(rng_t), intent(inout), allocatable :: rng
        integer :: gtoqq
        real(default) :: integral, random
        if (signal_is_pending ()) return
        if (debug_on) call msg_debug (D_SHOWER, "next_t_ana")
        ! check if branchings are possible at all
        if (min (prt%t, prt%momentum%p(0)**2) < &
            prt%mass_squared () + prt%settings%min_virtuality) then
            prt%t = prt%mass_squared ()
            call prt%set_simulated ()
            return
        end if
        integral = zero
        call rng%generate (random)
        do
            call parton_simulate_stept (prt, rng, integral, random, gtoqq, .false.)
            if (prt%simulated) then
                if (prt%is_gluon ()) then
                    !!! Abusing the x-variable to store the information to which
                    !!! quark flavor the gluon branches (if any)
                    prt%x = one * gtoqq + 0.1_default
                    !!! x = gtoqq + 0.1 -> int(x) will be the quark flavor or
                    !!! zero for g -> gg
                end if
                exit
            end if
        end do
    end subroutine parton_next_t_ana

```

The shower is actually sensitive to how close we go to the one here.

```

<Shower partons: procedures>+=
    function cmax (prt, tt) result (cmaxx)
        type(parton_t), intent(in) :: prt
        real(default), intent(in), optional :: tt
        real(default) :: t, cost, cmaxx, radicand
        t = prt%t; if (present (tt)) t = tt

```

```

if (associated (prt%parent)) then
  cost = prt%parent%get_costheta ()
  radicand = max(zero, one - &
    t / (prt%get_beta () * prt%momentum%p(0))**2 * &
    (one + cost) / (one - cost))
  if (debug_on) call msg_debug2 (D_SHOWER, "cmax: sqrt (radicand)", sqrt (radicand))
  cmaxx = min (0.99999_default, sqrt (radicand))
else
  cmaxx = 0.99999_default
end if
end function cmax

```

Simulation routine. The variable `lookatsister` takes constraints from the sister parton into account, if not given it is assumed `.true.`. `a` and `x` are three-dimensional arrays for values used for the integration.

```

<Shower partons: public>+=
  public :: parton_simulate_stept

<Shower partons: procedures>+=
  subroutine parton_simulate_stept &
    (prt, rng, integral, random, gtoqq, lookatsister)
    type(parton_t), intent(inout) :: prt
    class(rng_t), intent(inout), allocatable :: rng
    real(default), intent(inout) :: integral
    real(default), intent(inout) :: random
    integer, intent(out) :: gtoqq
    logical, intent(in), optional :: lookatsister

    type(parton_t), pointer :: sister
    real(default) :: tstep, tmin, oldt
    real(default) :: c, cstep
    real(default), dimension(3) :: z, P
    real(default) :: to_integral
    real(default) :: a11,a12,a13,a21,a22,a23
    real(default) :: cmax_t
    real(default) :: temprand
    real(default), dimension(3) :: a, x

    ! higher values -> faster but coarser
    real(default), parameter :: tstepfactor = 0.02_default
    real(default), parameter :: tstepmin = 0.5_default
    real(default), parameter :: cstepfactor = 0.8_default
    real(default), parameter :: cstepmin = 0.03_default

    if (signal_is_pending ()) return
    if (debug_on) call msg_debug (D_SHOWER, "parton_simulate_stept")
    gtoqq = 111 ! illegal value
    call prt%set_simulated (.false.)

    <Set sister if lookatsister is true or not given>

    tmin = prt%settings%min_virtuality + prt%mass_squared ()
    if (prt%is_quark ()) then
      to_integral = three * pi * log(one / random)

```

```

else if (prt%is_gluon ()) then
    to_integral = four *pi * log(one / random)
else
    prt%t = prt%mass_squared ()
    call prt%set_simulated ()
    return
end if

if (associated (sister)) then
    if (sqrt(prt%t) > sqrt(prt%parent%t) - &
        sqrt(sister%mass_squared ())) then
        prt%t = (sqrt (prt%parent%t) - sqrt (sister%mass_squared ()))**2
    end if
end if

if (prt%t > prt%momentum%p(0)**2) then
    prt%t = prt%momentum%p(0)**2
end if

if (prt%t <= tmin) then
    prt%t = prt%mass_squared ()
    call prt%set_simulated ()
    return
end if

! simulate the branchings between prt%t and prt%t - tstep
tstep = max(tstepfactor * (prt%t - 0.9_default * tmin), tstepmin)
cmax_t = cmax(prt)
c = - cmax_t ! take highest t -> minimal constraint
cstep = max(cstepfactor * (one - abs(c)), cstepmin)
! get values at border of "previous" bin -> to be used in first bin
z(3) = 0.5_default + 0.5_default * get_beta (prt%t - &
    0.5_default * tstep, prt%momentum%p(0)) * c
if (prt%is_gluon ()) then
    P(3) = P_ggg (z(3)) + P_gqq (z(3)) * number_of_flavors &
        (prt%t, prt%settings%max_n_flavors, prt%settings%min_virtuality)
else
    P(3) = P_qqg (z(3))
end if
a(3) = D_alpha_s_fsr (z(3) * (one - z(3)) * prt%t, &
    prt%settings) * P(3) / (prt%t - 0.5_default * tstep)

do while (c < cmax_t .and. (integral < to_integral))
    if (signal_is_pending ()) return
    cmax_t = cmax (prt)
    cstep = max (cstepfactor * (one - abs(c)**2), cstepmin)
    if (c + cstep > cmax_t) then
        cstep = cmax_t - c
    end if
    if (cstep < 1E-9_default) then
        !!! reject too small bins
        exit
    end if
    z(1) = z(3)
    z(2) = 0.5_default + 0.5_default * get_beta &

```

```

        (prt%t - 0.5_default * tstep, prt%momentum%p(0)) * &
        (c + 0.5_default * cstep)
z(3) = 0.5_default + 0.5_default * get_beta &
        (prt%t - 0.5_default * tstep, prt%momentum%p(0)) * (c + cstep)
P(1) = P(3)
if (prt%is_gluon ()) then
    P(2) = P_ggg(z(2)) + P_gqq(z(2)) * number_of_flavors &
        (prt%t, prt%settings%max_n_flavors, prt%settings%min_virtuality)
    P(3) = P_ggg(z(3)) + P_gqq(z(3)) * number_of_flavors &
        (prt%t, prt%settings%max_n_flavors, prt%settings%min_virtuality)
else
    P(2) = P_qqg(z(2))
    P(3) = P_qqg(z(3))
end if
! get values at borders of the integral and in the middle
a(1) = a(3)
a(2) = D_alpha_s_fsr (z(2) * (one - z(2)) * prt%t, &
    prt%settings) * P(2) / &
    (prt%t - 0.5_default * tstep)
a(3) = D_alpha_s_fsr (z(3) * (one - z(3)) * prt%t, &
    prt%settings) * P(3) / &
    (prt%t - 0.5_default * tstep)

!!! a little tricky:
!!! fit x(1) + x(2)/(1 + c) + x(3)/(1 - c) to these values
a11 = (one+c+0.5_default*cstep) * (one-c-0.5_default*cstep) - &
    (one-c) * (one+c+0.5_default*cstep)
a12 = (one-c-0.5_default*cstep) - (one+c+0.5_default*cstep) * &
    (one-c) / (one+c)
a13 = a(2) * (one+c+0.5_default*cstep) * (one-c-0.5_default*cstep) - &
    a(1) * (one-c) * (one+c+0.5_default*cstep)
a21 = (one+c+cstep) * (one-c-cstep) - (one+c+cstep) * (one-c)
a22 = (one-c-cstep) - (one+c+cstep) * (one-c) / (one+c)
a23 = a(3) * (one+c+cstep) * (one-c-cstep) - &
    a(1) * (one-c) * (one+c+cstep)

x(2) = (a23 - a21 * a13 / a11) / (a22 - a12 * a21 / a11)
x(1) = (a13 - a12 * x(2)) / a11
x(3) = a(1) * (one - c) - x(1) * (one - c) - x(2) * (one - c) / (one + c)

integral = integral + tstep * (x(1) * cstep + x(2) * &
    log((one + c + cstep) / (one + c)) - x(3) * &
    log((one - c - cstep) / (one - c)))

if (integral > to_integral) then
    oldt = prt%t
    call rng%generate (temprand)
    prt%t = prt%t - temprand * tstep
    call rng%generate (temprand)
    prt%costheta = c + (0.5_default - temprand) * cstep
    call prt%set_simulated ()

    if (prt%t < prt%settings%min_virtuality + prt%mass_squared ()) then
        prt%t = prt%mass_squared ()
    end if
end if

```

```

end if
if (abs(prt%costheta) > cmax_t) then
! reject branching due to violation of costheta-limits
call rng%generate (random)
if (prt%is_quark ()) then
to_integral = three * pi * log(one / random)
else if (prt%is_gluon ()) then
to_integral = four * pi * log(one / random)
end if
integral = zero
prt%t = oldt
call prt%set_simulated (.false.)
end if
if (prt%is_gluon ()) then
! decide between g->gg and g->qqbar splitting
z(1) = 0.5_default + 0.5_default * prt%costheta
call rng%generate (temprand)
if (P_ggg(z(1)) > temprand * (P_ggg (z(1)) + P_gqq (z(1)) * &
number_of_flavors(prt%t, prt%settings%max_n_flavors, &
prt%settings%min_virtuality))) then
gtoqq = 0
else
call rng%generate (temprand)
gtoqq = 1 + int (temprand * number_of_flavors &
(prt%t, prt%settings%max_n_flavors, &
prt%settings%min_virtuality))
end if
end if
else
c = c + cstep
end if
cmax_t = cmax (prt)
end do
if (integral <= to_integral) then
prt%t = prt%t - tstep
if (prt%t < prt%settings%min_virtuality + prt%mass_squared ()) then
prt%t = prt%mass_squared ()
call prt%set_simulated ()
end if
end if
end if
end subroutine parton_simulate_step

```

(Set sister if lookatsister is true or not given)≡

```

sister => null()
SET_SISTER: do
if (present (lookatsister)) then
if (.not. lookatsister) then
exit SET_SISTER
end if
end if
if (prt%nr == prt%parent%child1%nr) then
sister => prt%parent%child2
else
sister => prt%parent%child1

```

```

        end if
        exit SET_SISTER
    end do SET_SISTER

```

From the whole ISR algorithm all functionality has been moved to `shower_core.f90`. Only `maxzz` remains here, because more than one module needs to access it.

```

<Shower partons: public>+≡
    public :: maxzz

<Shower partons: procedures>+≡
    function maxzz (shat, s, maxz_isr, minenergy_timelike) result (maxz)
        real(default), intent(in) :: shat, s, minenergy_timelike, maxz_isr
        real(default) :: maxz
        maxz = min (maxz_isr, one - (two * minenergy_timelike * sqrt(shat)) / s)
    end function maxzz

```

22.3 Main shower module

```

<shower_core.f90>≡
    <File header>

    module shower_core

        <Use kinds with double>
        <Use strings>
        <Use debug>
        use io_units
        use constants
        use format_utils, only: write_separator
        use numeric_utils
        use diagnostics
        use physics_defs
        use os_interface
        use lorentz
        use sm_physics
        use particles
        use model_data
        use flavors
        use colors
        use subevents
        use pdf
        use rng_base
        use shower_base
        use shower_partons
        use muli, only: muli_t
        use hep_common
        use tauola_interface

        <Standard module head>

        <Shower core: public>

        <Shower core: parameters>

```

```

    <Shower core: types>

    <Shower core: interfaces>

    contains

    <Shower core: procedures>

    end module shower_core

    <Shower core: public>≡
        public :: shower_interaction_t

    <Shower core: types>≡
        type :: shower_interaction_t
            type(parton_pointer_t), dimension(:), allocatable :: partons
        end type shower_interaction_t

        type :: shower_interaction_pointer_t
            type(shower_interaction_t), pointer :: i => null ()
        end type shower_interaction_pointer_t

```

The WHIZARD internal shower. Flags distinguish between analytic and k_T -ordered showers.

```

    <Shower core: public>+≡
        public :: shower_t

    <Shower core: types>+≡
        type, extends (shower_base_t) :: shower_t
            type(shower_interaction_pointer_t), dimension(:), allocatable :: &
                interactions
            type(parton_pointer_t), dimension(:), allocatable :: partons
            type(muli_t) :: mi
            integer :: next_free_nr
            integer :: next_color_nr
            logical :: valid
        contains
            <Shower core: shower: TBP>
        end type shower_t

    <Shower core: shower: TBP>≡
        procedure :: init => shower_init

    <Shower core: procedures>≡
        subroutine shower_init (shower, settings, taudec_settings, pdf_data, os_data)
            class(shower_t), intent(out) :: shower
            type(shower_settings_t), intent(in) :: settings
            type(taudec_settings_t), intent(in) :: taudec_settings
            type(pdf_data_t), intent(in) :: pdf_data
            type(os_data_t), intent(in) :: os_data
            if (debug_on) call msg_debug (D_SHOWER, "shower_init")
            shower%settings = settings
            shower%taudec_settings = taudec_settings
            shower%os_data = os_data
        end subroutine shower_init

```



```

    call shower%pdf_data%init (pdf_data)
    shower%name = "WHIZARD internal"
    call shower%write_msg ()
end subroutine shower_init

```

<Shower core: shower: TBP>+≡

```

    procedure :: prepare_new_event => shower_prepare_new_event

```

<Shower core: procedures>+≡

```

subroutine shower_prepare_new_event (shower, fac_scale, alpha_s)
    class(shower_t), intent(inout) :: shower
    real(default), intent(in) :: fac_scale, alpha_s
    call shower%cleanup ()
    shower%next_free_nr = 1
    shower%next_color_nr = 1
    if (debug_active (D_SHOWER)) then
        if (allocated (shower%interactions)) then
            call msg_bug ("Shower: creating new shower while old one " // &
                "is still associated (interactions)")
        end if
        if (allocated (shower%partons)) then
            call msg_bug ("Shower: creating new shower while old one " // &
                "is still associated (partons)")
        end if
    end if
    treat_light_quarks_massless = .true.
    treat_duscb_quarks_massless = .false.
    shower%valid = .true.
end subroutine shower_prepare_new_event

```

It would be better to have the muli type outside of the shower.

<Shower core: shower: TBP>+≡

```

    procedure :: activate_multiple_interactions => shower_activate_multiple_interactions

```

<Shower core: procedures>+≡

```

subroutine shower_activate_multiple_interactions (shower)
    class(shower_t), intent(inout) :: shower
    if (shower%mi%is_initialized ()) then
        call shower%mi%restart ()
    else
        call shower%mi%initialize (&
            GeV2_scale_cutoff=shower%settings%min_virtuality, &
            GeV2_s=shower_interaction_get_s &
            (shower%interactions(1)%i), &
            muli_dir=char(shower%os_data%whizard_mulpith))
    end if
    call shower%mi%apply_initial_interaction ( &
        GeV2_s=shower_interaction_get_s(shower%interactions(1)%i), &
        x1=shower%interactions(1)%i%partons(1)%p%parent%x, &
        x2=shower%interactions(1)%i%partons(2)%p%parent%x, &
        pdg_f1=shower%interactions(1)%i%partons(1)%p%parent%type, &
        pdg_f2=shower%interactions(1)%i%partons(2)%p%parent%type, &
        n1=shower%interactions(1)%i%partons(1)%p%parent%nr, &
        n2=shower%interactions(1)%i%partons(2)%p%parent%nr)

```

```

end subroutine shower_activate_multiple_interactions

<Shower core: shower: TBP>+≡
  procedure :: import_particle_set => shower_import_particle_set
<Shower core: procedures>+≡
  subroutine shower_import_particle_set (shower, particle_set)
    class(shower_t), target, intent(inout) :: shower
    type(particle_set_t), intent(in) :: particle_set
    !integer, dimension(:), allocatable :: connections
    type(parton_t), dimension(:), allocatable, target, save :: partons, hadrons
    type(parton_pointer_t), dimension(:), allocatable :: &
      parton_pointers
    integer :: n_beam, n_in, n_out, n_tot
    integer :: i, j, nr, max_color_nr
    if (debug_on) call msg_debug (D_SHOWER, 'shower_import_particle_set')
    call count_and_allocate ()
    call setup_hadrons_from_particle_set ()
    call setup_partons_from_particle_set ()
    call shower%update_max_color_nr (1 + max_color_nr)
    call shower%add_interaction_2ton (parton_pointers)
    if (shower%settings%multi_active) then
      call shower%activate_multiple_interactions ()
    end if
    if (debug_on) call msg_debug2 (D_SHOWER, 'shower%write() after shower_import_particle_set')
    if (debug2_active (D_SHOWER)) then
      call shower%write ()
    end if
  contains
  <Shower core: shower import particle set: procedures>
end subroutine shower_import_particle_set

<Shower core: shower import particle set: procedures>≡
  subroutine count_and_allocate ()
    max_color_nr = 0
    n_beam = particle_set%get_n_beam ()
    n_in = particle_set%get_n_in ()
    n_out = particle_set%get_n_out ()
    n_tot = particle_set%get_n_tot ()
    if (allocated (partons)) deallocate (partons)
    allocate (partons (n_in + n_out))
    allocate (parton_pointers (n_in+n_out))
  end subroutine count_and_allocate

<Shower core: shower import particle set: procedures>+≡
  subroutine setup_hadrons_from_particle_set ()
    j = 0
    !!! !!! !!! Workaround for Portland 16.1 compiler bug
    !!! if (n_beam > 0 .and. all (particle_set%prt(1:2)%flv%get_pdg_abs () > TAU)) then
    if (n_beam > 0 .and. particle_set%prt(1)%flv%get_pdg_abs () > TAU .and. &
      particle_set%prt(2)%flv%get_pdg_abs () > TAU) then
      if (debug_on) call msg_debug (D_SHOWER, 'Copy hadrons from particle_set to hadrons')
      if (.not. allocated (hadrons)) allocate (hadrons (1:2))

```

```

do i = 1, n_tot
  if (particle_set%prt(i)%status == PRT_BEAM) then
    j = j + 1
    nr = shower%get_next_free_nr ()
    hadrons(j) = parton_of_particle (particle_set%prt(i), nr)
    hadrons(j)%settings => shower%settings
    max_color_nr = max (max_color_nr, abs(hadrons(j)%c1), &
                        abs(hadrons(j)%c2))
  end if
end do
end if
end subroutine setup_hadrons_from_particle_set

```

(Shower core: shower import particle set: procedures)+≡

```

subroutine setup_partons_from_particle_set ()
  integer, dimension(1) :: parent
  j = 0
  if (debug_on) call msg_debug (D_SHOWER, "Copy partons from particle_set to partons")
  do i = 1, n_tot
    if (particle_set%prt(i)%get_status () == PRT_INCOMING .or. &
        particle_set%prt(i)%get_status () == PRT_OUTGOING) then
      j = j + 1
      nr = shower%get_next_free_nr ()
      partons(j) = parton_of_particle (particle_set%prt(i), nr)
      partons(j)%settings => shower%settings
      parton_pointers(j)%p => partons(j)
      max_color_nr = max (max_color_nr, abs (partons(j)%c1), &
                          abs (partons(j)%c2))
      if (particle_set%prt(i)%get_status () == PRT_INCOMING .and. &
          particle_set%prt(i)%get_n_parents () == 1 .and. &
          allocated (hadrons)) then
        parent = particle_set%prt(i)%get_parents ()
        partons(j)%initial => hadrons (parent(1))
        partons(j)%x = space_part_norm (partons(j)%momentum) / &
                      space_part_norm (partons(j)%initial%momentum)
      end if
    end if
  end do
end subroutine setup_partons_from_particle_set

```

(Shower core: shower: TBP)+≡

```

procedure :: generate_emissions => shower_generate_emissions

```

(Shower core: procedures)+≡

```

subroutine shower_generate_emissions &
  (shower, valid, number_of_emissions)
  class(shower_t), intent(inout), target :: shower
  logical, intent(out) :: valid
  integer, optional, intent(in) :: number_of_emissions

  type(parton_t), dimension(:), allocatable, target :: partons
  type(parton_pointer_t), dimension(:), allocatable :: &
    parton_pointers
  real(default) :: mi_scale, ps_scale, shat, phi

```

```

type(parton_pointer_t) :: temppp
integer :: i, j, k
integer :: n_int, max_color_nr
integer, dimension(2,4) :: color_corr
if (debug_on) call msg_debug (D_SHOWER, "shower_generate_emissions")
if (shower%settings%isr_active) then
  if (debug_on) call msg_debug (D_SHOWER, "Generate ISR with FSR")
  i = 0
  BRANCHINGS: do
    i = i + 1
    if (signal_is_pending ()) return
    if (shower%settings%multi_active) then
      call shower%mi%generate_gev2_pt2 &
        (shower%get_ISR_scale (), mi_scale)
    else
      mi_scale = 0.0
    end if

    !!! Shower: debugging
    !!! shower%generate_next_isr_branching returns a pointer to
    !!! the parton with the next ISR-branching, this parton's
    !!! scale is the scale of the next branching
    ! temppp=shower%generate_next_isr_branching_veto ()
    temppp = shower%generate_next_isr_branching ()

    if (.not. associated (temppp%p) .and. &
        mi_scale < shower%settings%min_virtuality) then
      exit BRANCHINGS
    end if
    !!! check if branching or interaction occurs next
    if (associated (temppp%p)) then
      ps_scale = abs(temppp%p%t)
    else
      ps_scale = 0._default
    end if
    if (mi_scale > ps_scale) then
      !!! discard branching evolution lower than mi_scale
      call shower%set_max_ISR_scale (mi_scale)
      if (associated (temppp%p)) &
        call temppp%p%set_simulated (.false.)

      !!! execute new interaction
      deallocate (partons)
      deallocate (parton_pointers)
      allocate (partons(1:4))
      allocate (parton_pointers(1:4))
      do j = 1, 4
        partons(j)%nr = shower%get_next_free_nr ()
        partons(j)%belongstointeraction = .true.
        parton_pointers(j)%p => partons(j)
      end do
      call shower%mi%generate_partons (partons(1)%nr, partons(2)%nr, &
        partons(1)%x, partons(2)%x, &
        partons(1)%type, partons(2)%type, &

```

```

        partons(3)%type, partons(4)%type)
!!! calculate momenta
shat = partons(1)%x *partons(2)%x * &
        shower_interaction_get_s (shower%interactions(1)%i)
partons(1)%momentum = [0.5_default * sqrt(shat), &
        zero, zero, 0.5_default*sqrt(shat)]
partons(2)%momentum = [0.5_default * sqrt(shat), &
        zero, zero, -0.5_default*sqrt(shat)]
call parton_set_initial (partons(1), &
        shower%interactions(1)%i%partons(1)%p%initial)
call parton_set_initial (partons(2), &
        shower%interactions(1)%i%partons(2)%p%initial)
partons(1)%belongstoFSR = .false.
partons(2)%belongstoFSR = .false.
!!! calculate color connection
call shower%mi%get_color_correlations &
        (shower%get_next_color_nr (), &
        max_color_nr,color_corr)
call shower%update_max_color_nr (max_color_nr)

partons(1)%c1 = color_corr(1,1)
partons(1)%c2 = color_corr(2,1)
partons(2)%c1 = color_corr(1,2)
partons(2)%c2 = color_corr(2,2)
partons(3)%c1 = color_corr(1,3)
partons(3)%c2 = color_corr(2,3)
partons(4)%c1 = color_corr(1,4)
partons(4)%c2 = color_corr(2,4)

call shower%rng%generate (phi)
phi = 2 * pi * phi
partons(3)%momentum = [0.5_default*sqrt(shat), &
        sqrt(mi_scale)*cos(phi), &
        sqrt(mi_scale)*sin(phi), &
        sqrt(0.25_default*shat - mi_scale)]
partons(4)%momentum = [ 0.5_default*sqrt(shat), &
        -sqrt(mi_scale)*cos(phi), &
        -sqrt(mi_scale)*sin(phi), &
        -sqrt(0.25_default*shat - mi_scale)]
partons(3)%belongstoFSR = .true.
partons(4)%belongstoFSR = .true.

call shower%add_interaction_2ton (parton_pointers)
n_int = size (shower%interactions)
do k = 1, 2
call shower%mi%replace_parton &
        (shower%interactions(n_int)%i%partons(k)%p%initial%nr, &
        shower%interactions(n_int)%i%partons(k)%p%nr, &
        shower%interactions(n_int)%i%partons(k)%p%parent%nr, &
        shower%interactions(n_int)%i%partons(k)%p%type, &
        shower%interactions(n_int)%i%partons(k)%p%x, &
        mi_scale)
end do
else

```

```

        !!! execute the next branching 'found' in the previous step
        call shower%execute_next_isr_branching (temppp)
        if (shower%settings%multi_active) then
            call shower%mi%replace_parton (temppp%p%initial%nr, &
                temppp%p%child1%nr, temppp%p%nr, &
                temppp%p%type, temppp%p%x, ps_scale)
        end if

    end if
end do BRANCHINGS

    call shower%generate_fsr_for_isr_partons ()
else
    if (signal_is_pending ()) return
    if (debug_on) call msg_debug (D_SHOWER, "Generate FSR without ISR")
    call shower%simulate_no_isr_shower ()
end if

!!! some bookkeeping, needed after the shower is done
call shower%boost_to_labframe ()
call shower%generate_primordial_kt ()
call shower%update_beamremnants ()

if (shower%settings%fsr_active) then
    do i = 1, size (shower%interactions)
        if (signal_is_pending ()) return
        call shower%interaction_generate_fsr_2ton &
            (shower%interactions(i)%i)
    end do
else
    call shower%simulate_no_fsr_shower ()
end if

if (debug_on) call msg_debug (D_SHOWER, "Shower finished:")
if (debug_active (D_SHOWER)) call shower%write ()

valid = shower%valid
!!! clean-up multi: we should finalize the multi pdf sets
!!!      when _all_ runs are done. Not after every event if possible
! call shower%mi%finalize()
end subroutine shower_generate_emissions

```

<Shower core: shower: TBP>+≡

```

    procedure :: make_particle_set => shower_make_particle_set

```

<Shower core: procedures>+≡

```

    subroutine shower_make_particle_set &
        (shower, particle_set, model, model_hadrons)
    class(shower_t), intent(in) :: shower
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    class(model_data_t), intent(in), target :: model_hadrons
    call shower%combine_with_particle_set (particle_set, model, &
        model_hadrons)
    if (shower%settings%hadronization_active) then

```

```

        call shower%converttopythia ()
    end if
end subroutine shower_make_particle_set

```

The parameters of the shower module:

```

<Shower core: parameters>≡
    real(default), save :: alphaspdfmax = 12._default

```

In this routine, y and y_{\min} are the jet measures, w and w_{\max} are weights, s is the kinematic energy squared of the interaction. The flag `isr_is_possible_and_allowed` checks whether the initial parton is set, lepton-hadron collisions are not implemented (yet).

As a workaround: as WHIZARD can treat partons as massless, there might be partons with $E < m$: if such a parton is found, quarks will be treated massless.

```

<Shower core: shower: TBP>+≡
    procedure :: add_interaction_2ton => shower_add_interaction_2ton

<Shower core: procedures>+≡
    subroutine shower_add_interaction_2ton (shower, partons)
        class(shower_t), intent(inout) :: shower
        type(parton_pointer_t), intent(in), dimension(:), allocatable :: partons
        !type(ckkw_pseudo_shower_weights_t), intent(in) :: ckkw_pseudo_weights

        integer :: n_partons, n_out
        integer :: i, j, imin, jmin
        real(default) :: y, ymin
        !real(default) :: w, wmax
        !real(default) :: random, sum
        type(parton_pointer_t), dimension(:), allocatable :: new_partons
        type(parton_t), pointer :: prt
        integer :: n_int
        type(shower_interaction_pointer_t), dimension(:), allocatable :: temp
        type(vector4_t) :: prtmomentum, childmomentum
        logical :: isr_is_possible_and_allowed
        type(lorentz_transformation_t) :: L

        if (signal_is_pending ()) return
        if (debug_on) call msg_debug (D_SHOWER, "Add interaction2toN")
        n_partons = size (partons)
        n_out = n_partons - 2
        if (n_out < 2) then
            call msg_bug &
                ("Shower core: trying to add a 2-> (something<2) interaction")
        end if

        isr_is_possible_and_allowed = (associated (partons(1)%p%initial) &
            .and. associated (partons(2)%p%initial)) .and. &
            shower%settings%isr_active
        if (debug_on) call msg_debug (D_SHOWER, "isr_is_possible_and_allowed", &
            isr_is_possible_and_allowed)

        if (associated (partons(1)%p%initial) .and. &

```

```

        partons(1)%p%is_quark ()) then
    if (partons(1)%p%momentum%p(0) < &
        two * partons(1)%p%mass()) then
        if (abs(partons(1)%p%type) < 2) then
            treat_light_quarks_massless = .true.
        else
            treat_duscb_quarks_massless = .true.
        end if
    end if
end if
if (associated (partons(2)%p%initial) .and. &
    partons(2)%p%is_quark ()) then
    if (partons(2)%p%momentum%p(0) < &
        two * partons(2)%p%mass()) then
        if (abs(partons(2)%p%type) < 2) then
            treat_light_quarks_massless = .true.
        else
            treat_duscb_quarks_massless = .true.
        end if
    end if
end if

<Add a new interaction to shower%interactions>

if (associated (shower%interactions(n_int)%i%partons(1)%p%initial)) &
    call shower%interactions(n_int)%i%partons(1)%p%initial%set_simulated ()
if (associated (shower%interactions(n_int)%i%partons(2)%p%initial)) &
    call shower%interactions(n_int)%i%partons(2)%p%initial%set_simulated ()
if (isr_is_possible_and_allowed) then
    !!! boost to the CMFrame of the incoming partons
    L = boost (-(shower%interactions(n_int)%i%partons(1)%p%momentum + &
        shower%interactions(n_int)%i%partons(2)%p%momentum), &
        (shower%interactions(n_int)%i%partons(1)%p%momentum + &
        shower%interactions(n_int)%i%partons(2)%p%momentum)**1 )
    do i = 1, n_partons
        call parton_apply_lorentztrafo &
            (shower%interactions(n_int)%i%partons(i)%p, L)
    end do
end if
do i = 1, size (partons)
    if (signal_is_pending ()) return
    !!! partons are marked as belonging to the hard interaction
    shower%interactions(n_int)%i%partons(i)%p%belongstointeraction &
        = .true.
    shower%interactions(n_int)%i%partons(i)%p%belongstoFSR = i > 2
    shower%interactions(n_int)%i%partons(i)%p%interactionnr = n_int
    !!! include a 2^(i - 1) number as a label for the ckkw clustering
    shower%interactions(n_int)%i%partons(i)%p%ckkwlabel = 2**(i - 1)
end do

<Add partons from shower%interactions to shower%partons>

if (isr_is_possible_and_allowed) then
    if (shower%settings%isr_pt_ordered) then

```



```

        call shower_prepare_for_simulate_isr_pt &
            (shower, shower%interactions(size (shower%interactions))%i)
    else
        call shower_prepare_for_simulate_isr_ana_test &
            (shower, shower%interactions(n_int)%i%partons(1)%p, &
            shower%interactions(n_int)%i%partons(2)%p)
    end if
end if

!!! generate pseudo parton shower history and add all partons to
!!! shower%partons-array
!!! TODO initial -> initial + final branchings ??
allocate (new_partons(1:(n_partons - 2)))
do i = 1, size (new_partons)
    nullify (new_partons(i)%p)
end do
do i = 1, size (new_partons)
    new_partons(i)%p => shower%interactions(n_int)%i%partons(i + 2)%p
end do
imin = 0
jmin = 0

! TODO: (bcn 2015-04-24) make this a clustering step of the matching
! if (allocated (ckkw_pseudo_weights%weights)) then
!     !<Perform clustering using the CKKW weights>>
! else
!     <Perform clustering in the usual way>
! end if

!!! set the FSR starting scale for all partons
do i = 1, size (new_partons)
    !!! the imaginary mother is the only parton remaining in new_partons
    if (.not. associated (new_partons(i)%p)) cycle
    call set_starting_scale (new_partons(i)%p, &
        get_starting_scale (new_partons(i)%p))
    exit
end do

contains

<Procedures of shower.add.interaction.2ton>
end subroutine shower_add_interaction_2ton

<Add a new interaction to shower%interactions>≡
if (allocated (shower%interactions)) then
    n_int = size (shower%interactions) + 1
else
    n_int = 1
end if
allocate (temp (1:n_int))
do i = 1, n_int - 1
    allocate (temp(i)%i)
    temp(i)%i = shower%interactions(i)%i
end do

```

```

allocate (temp(n_int)%i)
allocate (temp(n_int)%i%partons(1:n_partons))
do i = 1, n_partons
    allocate (temp(n_int)%i%partons(i)%p)
    call parton_copy (partons(i)%p, temp(n_int)%i%partons(i)%p)
end do
if (allocated (shower%interactions)) deallocate(shower%interactions)
allocate (shower%interactions(1:n_int))
do i = 1, n_int
    shower%interactions(i)%i => temp(i)%i
end do
deallocate (temp)

<Add partons from shower%interactions to shower%partons>≡
if (allocated (shower%partons)) then
    allocate (new_partons(1:size(shower%partons) + &
        size(shower%interactions(n_int)%i%partons)))
    do i = 1, size (shower%partons)
        new_partons(i)%p => shower%partons(i)%p
    end do
    do i = 1, size (shower%interactions(n_int)%i%partons)
        new_partons(size(shower%partons) + i)%p => &
            shower%interactions(n_int)%i%partons(i)%p
    end do
    deallocate (shower%partons)
else
    allocate (new_partons(1:size(shower%interactions(n_int)%i%partons)))
    do i = 1, size (partons)
        new_partons(i)%p => shower%interactions(n_int)%i%partons(i)%p
    end do
end if
allocate (shower%partons(1:size (new_partons)))
do i = 1, size (new_partons)
    shower%partons(i)%p => new_partons(i)%p
end do
deallocate (new_partons)

<Perform clustering using the CKKW weights>≡
CKKW_CLUSTERING: do
    !!! search for the combination with the highest weight
    wmax = zero
    CKKW_OUTER: do i = 1, size (new_partons)
        CKKW_INNER: do j = i + 1, size (new_partons)
            if (.not. associated (new_partons(i)%p)) cycle
            if (.not. associated (new_partons(j)%p)) cycle
            w = ckkw_pseudo_weights%weights(new_partons(i)%p%ckkwlabel + &
                new_partons(j)%p%ckkwlabel)
            if (w > wmax .or. vanishes(wmax)) then
                wmax = w
                imin = i
                jmin = j
            end if
        end do CKKW_INNER
    end do CKKW_OUTER
    if (wmax > zero) then

```

```

call shower%add_parent (new_partons(imin)%p)
call parton_set_child (new_partons(imin)%p%parent, &
    new_partons(jmin)%p, 2)
call parton_set_parent (new_partons(jmin)%p, &
    new_partons(imin)%p%parent)
prt => new_partons(imin)%p%parent
prt%nr = shower_get_next_free_nr (shower)
prt%type = INTERNAL

prt%momentum = new_partons(imin)%p%momentum + &
    new_partons(jmin)%p%momentum
prt%t = prt%momentum**2

!!! auxilliary values for the ckkw matching
!!! for now, randomly choose the type of the intermediate
prt%ckkwlabel = new_partons(imin)%p%ckkwlabel + &
    new_partons(jmin)%p%ckkwlabel
sum = zero
call shower%rng%generate (random)
CKKW_TYPE: do i = 0, 4
    if (sum + &
        ckkw_pseudo_weights%weights_by_type(prt%ckkwlabel, i) > &
        random * ckkw_pseudo_weights%weights(prt%ckkwlabel) ) then
        prt%ckkwtype = i
        exit ckkw_type
    end if
    sum = sum + &
        ckkw_pseudo_weights%weights_by_type(prt%ckkwlabel, i)
end do CKKW_TYPE

!!! TODO -> calculate costheta and store it for
!!!         later use in generate_ps

if (space_part_norm(prt%momentum) > tiny_10) then
    prtmomentum = prt%momentum
    childmomentum = prt%child1%momentum
    prtmomentum = boost (- prt%get_beta() / &
        sqrt (one - &
            (prt%get_beta ())**2), space_part (prt%momentum) / &
            space_part_norm(prt%momentum)) * prtmomentum
    childmomentum = boost (- prt%get_beta () / &
        sqrt(one - &
            (prt%get_beta ())**2), space_part (prt%momentum) / &
            space_part_norm(prt%momentum)) * childmomentum
    prt%costheta = enclosed_angle_ct(prtmomentum, childmomentum)
else
    prt%costheta = - one
end if

prt%belongstointeraction = .true.
prt%belongstoFSR = &
    new_partons(imin)%p%belongstoFSR .and. &
    new_partons(jmin)%p%belongstoFSR

```

```

        nullify (new_partons(imin)%p)
        nullify (new_partons(jmin)%p)
        new_partons(imin)%p => prt
    else
        exit CKKW_CLUSTERING
    end if
end do CKKW_CLUSTERING
(Perform clustering in the usual way)≡
CLUSTERING: do
    !!! search for the partons to be clustered together
    ymin = zero
    OUTER: do i = 1, size (new_partons)
        INNER: do j = i + 1, size (new_partons)
            !!! calculate the jet measure
            if (.not.associated (new_partons(i)%p)) cycle INNER
            if (.not.associated (new_partons(j)%p)) cycle INNER
            !if (.not. shower_clustering_allowed &
                !(shower, new_partons, i,j)) &
                !cycle inner
            !!! Durham jet-measure ! don't care about constants
            y = min (new_partons(i)%p%momentum%p(0), &
                new_partons(j)%p%momentum%p(0)) * &
                (one - enclosed_angle_ct &
                (new_partons(i)%p%momentum, &
                new_partons(j)%p%momentum))
            if (y < ymin .or. vanishes(ymin)) then
                ymin = y
                imin = i
                jmin = j
            end if
        end do INNER
    end do OUTER
    if (ymin > zero) then
        call shower%add_parent (new_partons(imin)%p)
        call parton_set_child &
            (new_partons(imin)%p%parent, new_partons(jmin)%p, 2)
        call parton_set_parent &
            (new_partons(jmin)%p, new_partons(imin)%p%parent)
        prt => new_partons(imin)%p%parent
        prt%nr = shower_get_next_free_nr (shower)
        prt%type = INTERNAL

        prt%momentum = new_partons(imin)%p%momentum + &
            new_partons(jmin)%p%momentum
        prt%t = prt%momentum**2
        !!! TODO -> calculate costheta and store it for
        !!!         later use in generate_ps

        if (space_part_norm(prt%momentum) > tiny_10) then
            prtmomentum = prt%momentum
            childmomentum = prt%child1%momentum
            prtmomentum = boost (- prt%get_beta () / sqrt(one - &
                (prt%get_beta ()**2), space_part(prt%momentum) / &
                space_part_norm(prt%momentum)) * prtmomentum

```

```

        childmomentum = boost (- prt%get_beta() / &
                               sqrt(one - &
                                   (prt%get_beta ())*2), space_part(prt%momentum) / &
                               space_part_norm(prt%momentum)) * childmomentum
        prt%costheta = enclosed_angle_ct (prtmomentum, childmomentum)
    else
        prt%costheta = - one
    end if

    prt%belongstointeraction = .true.
    nullify (new_partons(imin)%p)
    nullify (new_partons(jmin)%p)
    new_partons(imin)%p => prt
else
    exit CLUSTERING
end if
end do CLUSTERING

<Procedures of shower.add.interaction.2ton>≡
recursive subroutine transfer_pointers (destiny, start, prt)
    type(parton_pointer_t), dimension(:), allocatable :: destiny
    integer, intent(inout) :: start
    type(parton_t), pointer :: prt
    destiny(start)%p => prt
    start = start + 1
    if (associated (prt%child1)) then
        call transfer_pointers (destiny, start, prt%child1)
    end if
    if (associated (prt%child2)) then
        call transfer_pointers (destiny, start, prt%child2)
    end if
end subroutine transfer_pointers

<Procedures of shower.add.interaction.2ton>+≡
recursive function get_starting_scale (prt) result (scale)
    type(parton_t), pointer :: prt
    real(default) :: scale
    scale = huge (scale)
    if (associated (prt%child1) .and. associated (prt%child2)) then
        scale = min(scale, prt%t)
    end if
    if (associated (prt%child1)) then
        scale = min (scale, get_starting_scale (prt%child1))
    end if
    if (associated (prt%child2)) then
        scale = min (scale, get_starting_scale (prt%child2))
    end if
end function get_starting_scale

<Procedures of shower.add.interaction.2ton>+≡
recursive subroutine set_starting_scale (prt, scale)
    type(parton_t), pointer :: prt
    real(default) :: scale
    if (prt%type /= INTERNAL) then

```

```

    if (scale > prt%settings%min_virtuality + prt%mass_squared ()) then
        prt%t = scale
    else
        prt%t = prt%mass_squared ()
        call prt%set_simulated ()
    end if
end if
if (associated (prt%child1)) then
    call set_starting_scale (prt%child1, scale)
end if
if (associated (prt%child2)) then
    call set_starting_scale (prt%child2, scale)
end if
end subroutine set_starting_scale

```

(Shower core: shower: TBP)+≡

```

    procedure :: simulate_no_isr_shower => shower_simulate_no_isr_shower

```

(Shower core: procedures)+≡

```

subroutine shower_simulate_no_isr_shower (shower)
    class(shower_t), intent(inout) :: shower
    integer :: i, j
    type(parton_t), pointer :: prt
    if (debug_on) call msg_debug (D_SHOWER, "shower_simulate_no_isr_shower")
    do i = 1, size (shower%interactions)
        do j = 1, 2
            prt => shower%interactions(i)%i%partons(j)%p
            if (associated (prt%initial)) then
                !!! for virtuality ordered: remove unneeded partons
                if (associated (prt%parent)) then
                    if (.not. prt%parent%is_proton ()) then
                        if (associated (prt%parent%parent)) then
                            if (.not. prt%parent%is_proton ()) then
                                call shower_remove_parton_from_partons &
                                    (shower, prt%parent%parent)
                            end if
                        end if
                    end if
                    call shower_remove_parton_from_partons &
                        (shower, prt%parent)
                end if
            end if
            call parton_set_parent (prt, prt%initial)
            call parton_set_child (prt%initial, prt, 1)
            if (associated (prt%initial%child2)) then
                call shower_remove_parton_from_partons &
                    (shower, prt%initial%child2)
                deallocate (prt%initial%child2)
            end if
            call shower%add_child (prt%initial, 2)
        end if
    end do
end do
end subroutine shower_simulate_no_isr_shower

```

```

<Shower core: shower: TBP>+=
  procedure :: simulate_no_fsr_shower => shower_simulate_no_fsr_shower

<Shower core: procedures>+=
  subroutine shower_simulate_no_fsr_shower (shower)
    class(shower_t), intent(inout) :: shower
    integer :: i, j
    type(parton_t), pointer :: prt
    do i = 1, size (shower%interactions)
      do j = 3, size (shower%interactions(i)%i%partons)
        prt => shower%interactions(i)%i%partons(j)%p
        call prt%set_simulated ()
        prt%scale = zero
        prt%t = prt%mass_squared ()
      end do
    end do
  end subroutine shower_simulate_no_fsr_shower

<Shower core: procedures>+=
  subroutine swap_pointers (prtp1, prtp2)
    type(parton_pointer_t), intent(inout) :: prtp1, prtp2
    type(parton_pointer_t) :: prtptemp
    prtptemp%p => prtp1%p
    prtp1%p => prtp2%p
    prtp2%p => prtptemp%p
  end subroutine swap_pointers

```

This removes emitted timelike partons.

```

<Shower core: procedures>+=
  recursive subroutine shower_remove_parton_from_partons (shower, prt)
    type(shower_t), intent(inout) :: shower
    type(parton_t), pointer :: prt
    integer :: i
    if (.not. prt%belongstoFSR .and. associated (prt%child2)) then
      call shower_remove_parton_from_partons_recursive (shower, prt%child2)
    end if
    do i = 1, size (shower%partons)
      if (associated (shower%partons(i)%p, prt)) then
        shower%partons(i)%p => null()
        ! TODO: (bcn 2015-05-05) memory leak here? no deallocation?
        exit
      end if
      if (debug_active (D_SHOWER)) then
        if (i == size (shower%partons)) then
          call msg_bug ("shower_remove_parton_from_partons: parton&
            &to be removed not found")
        end if
      end if
    end do
  end subroutine shower_remove_parton_from_partons

```

This removes the parton `prt` and all its children.

```

<Shower core: procedures>+=

```

```

recursive subroutine shower_remove_parton_from_partons_recursive (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), pointer :: prt
  if (associated (prt%child1)) then
    call shower_remove_parton_from_partons_recursive (shower, prt%child1)
    deallocate (prt%child1)
  end if
  if (associated (prt%child2)) then
    call shower_remove_parton_from_partons_recursive (shower, prt%child2)
    deallocate (prt%child2)
  end if
  call shower_remove_parton_from_partons (shower, prt)
end subroutine shower_remove_parton_from_partons_recursive

```

<Shower core: shower: TBP>+≡

```

  procedure :: sort_partons => shower_sort_partons

```

<Shower core: procedures>+≡

```

subroutine shower_sort_partons (shower)
  class(shower_t), intent(inout) :: shower
  integer :: i, j, maxsort, size_partons
  logical :: changed
  if (debug_on) call msg_debug2 (D_SHOWER, "shower_sort_partons")
  if (.not. allocated (shower%partons)) return
  size_partons = size (shower%partons)
  maxsort = 0
  do i = 1, size_partons
    if (associated (shower%partons(i)%p)) maxsort = i
  end do
  if (signal_is_pending ()) return
  size_partons = size (shower%partons)
  if (size_partons <= 1) return
  do i = 1, maxsort
    if (.not. associated (shower%partons(i)%p)) cycle
    if (.not. shower%settings%isr_pt_ordered) then
      !!! set unsimulated ISR partons to be "typeless" to prevent
      !!! influences from "wrong" masses
      if (.not. shower%partons(i)%p%belongstoFSR .and. &
        .not. shower%partons(i)%p%simulated .and. &
        .not. shower%partons(i)%p%belongstointeraction) then
        shower%partons(i)%p%type = 0
      end if
    end if
  end do
  if (signal_is_pending ()) return
  !!! Just a Bubblesort
  !!! Different algorithms needed for t-ordered and pt^2-ordered shower
  !!! Pt-ordered:
  if (shower%settings%isr_pt_ordered) then
    OUTERDO_PT: do i = 1, maxsort - 1
      changed = .false.
      INNERDO_PT: do j = 1, maxsort - i
        if (.not. associated (shower%partons(j + 1)%p)) cycle
        if (.not. associated (shower%partons(j)%p)) then

```



```

        !!! change if j + 1 ist assoaciated and j is not
        call swap_pointers (shower%partons(j), shower%partons(j + 1))
        changed = .true.
    else if (shower%partons(j)%p%scale < &
            shower%partons(j + 1)%p%scale) then
        call swap_pointers (shower%partons(j), shower%partons(j + 1))
        changed = .true.
    else if (nearly_equal(shower%partons(j)%p%scale, &
            shower%partons(j + 1)%p%scale)) then
        if (shower%partons(j)%p%nr > shower%partons(j + 1)%p%nr) then
            call swap_pointers (shower%partons(j), shower%partons(j + 1))
            changed = .true.
        end if
    end if
end do INNERDO_PT
if (.not. changed) exit OUTERDO_PT
end do outerdo_pt
!!! |t|-ordered
else
    OUTERDO_T: do i = 1, maxsort - 1
        changed = .false.
        INNERDO_T: do j = 1, maxsort - i
            if (.not. associated (shower%partons(j + 1)%p)) cycle
            if (.not. associated (shower%partons(j)%p)) then
                !!! change if j+1 is associated and j isn't
                call swap_pointers (shower%partons(j), shower%partons(j + 1))
                changed = .true.
            else if (.not. shower%partons(j)%p%belongstointeraction .and. &
                    shower%partons(j + 1)%p%belongstointeraction) then
                !!! move partons belonging to the interaction to the front
                call swap_pointers (shower%partons(j), shower%partons(j + 1))
                changed = .true.
            else if (.not. shower%partons(j)%p%belongstointeraction .and. &
                    .not. shower%partons(j + 1)%p%belongstointeraction ) then
                if (abs (shower%partons(j)%p%t) - &
                    shower%partons(j)%p%mass_squared () < &
                    abs(shower%partons(j + 1)%p%t) - &
                    shower%partons(j + 1)%p%mass_squared ()) then
                    call swap_pointers (shower%partons(j), shower%partons(j + 1))
                    changed = .true.
                else
                    if (nearly_equal(abs (shower%partons(j)%p%t) - &
                        shower%partons(j)%p%mass_squared (), &
                        abs(shower%partons(j + 1)%p%t) - &
                        shower%partons(j + 1)%p%mass_squared ())) then
                        if (shower%partons(j)%p%nr > &
                            shower%partons(j + 1)%p%nr) then
                            call swap_pointers (shower%partons(j), &
                                shower%partons(j + 1))
                            changed = .true.
                        end if
                    end if
                end if
            end if
        end do INNERDO_T
    end do OUTERDO_T
end if
end if
end if

```

```

        end do INNERDO_T
        if (.not. changed) exit OUTERDO_T
    end do OUTERDO_T
end if
end subroutine shower_sort_partons

```

Deallocate the interaction pointers.

```

<Shower core: shower: TBP>+≡
    procedure :: cleanup => shower_cleanup

<Shower core: procedures>+≡
    subroutine shower_cleanup (shower)
        class(shower_t), intent(inout) :: shower
        integer :: i
        if (allocated (shower%interactions)) then
            do i = 1, size (shower%interactions)
                if (allocated (shower%interactions(i)%i%partons)) &
                    deallocate (shower%interactions(i)%i%partons)
                deallocate (shower%interactions(i)%i)
            end do
            deallocate (shower%interactions)
        end if
        if (allocated (shower%partons)) deallocate (shower%partons)
    end subroutine shower_cleanup

```

Bookkeeping functions.

```

<Shower core: shower: TBP>+≡
    procedure :: get_next_free_nr => shower_get_next_free_nr

<Shower core: procedures>+≡
    function shower_get_next_free_nr (shower) result (next_number)
        class(shower_t), intent(inout) :: shower
        integer :: next_number
        next_number = shower%next_free_nr
        shower%next_free_nr = shower%next_free_nr + 1
    end function shower_get_next_free_nr

<Shower core: shower: TBP>+≡
    procedure :: update_max_color_nr => shower_update_max_color_nr

<Shower core: procedures>+≡
    pure subroutine shower_update_max_color_nr (shower, index)
        class(shower_t), intent(inout) :: shower
        integer, intent(in) :: index
        if (index > shower%next_color_nr) then
            shower%next_color_nr = index
        end if
    end subroutine shower_update_max_color_nr

<Shower core: shower: TBP>+≡
    procedure :: get_next_color_nr => shower_get_next_color_nr

```

<Shower core: procedures>+≡

```
function shower_get_next_color_nr (shower) result (next_color)
  class(shower_t), intent(inout) :: shower
  integer :: next_color
  next_color = shower%next_color_nr
  shower%next_color_nr = shower%next_color_nr + 1
end function shower_get_next_color_nr
```

<Shower core: procedures>+≡

```
subroutine shower_enlarge_partons_array (shower, custom_length)
  type(shower_t), intent(inout) :: shower
  integer, intent(in), optional :: custom_length
  integer :: i, length, oldlength
  type(parton_pointer_t), dimension(:), allocatable :: tmp_partons
  if (debug_on) call msg_debug (D_SHOWER, "shower_enlarge_partons_array")
  if (present(custom_length)) then
    length = custom_length
  else
    length = 10
  end if
  if (debug_active (D_SHOWER)) then
    if (length < 1) then
      call msg_bug ("Shower: no parton_pointers added in shower%partons")
    end if
  end if
  if (allocated (shower%partons)) then
    oldlength = size (shower%partons)
    allocate (tmp_partons(1:oldlength))
    do i = 1, oldlength
      tmp_partons(i)%p => shower%partons(i)%p
    end do
    deallocate (shower%partons)
  else
    oldlength = 0
  end if
  allocate (shower%partons(1:oldlength + length))
  do i = 1, oldlength
    shower%partons(i)%p => tmp_partons(i)%p
  end do
  do i = oldlength + 1, oldlength + length
    shower%partons(i)%p => null()
  end do
end subroutine shower_enlarge_partons_array
```

<Shower core: shower: TBP>+≡

```
procedure :: add_child => shower_add_child
```

<Shower core: procedures>+≡

```
subroutine shower_add_child (shower, prt, child)
  class(shower_t), intent(inout) :: shower
  type(parton_t), pointer :: prt
  integer, intent(in) :: child
  integer :: i, lastfree
  type(parton_pointer_t) :: newprt
```

```

if (child /= 1 .and. child /= 2) then
    call msg_bug ("Shower: Adding child in nonexisting place")
end if
allocate (newprt%p)
newprt%p%nr = shower%get_next_free_nr ()
!!! add new parton as child
if (child == 1) then
    prt%child1 => newprt%p
else
    prt%child2 => newprt%p
end if
newprt%p%parent => prt
if (associated (prt%settings)) then
    newprt%p%settings => prt%settings
end if
newprt%p%interactionnr = prt%interactionnr
!!! add new parton to shower%partons list
if (associated (shower%partons (size(shower%partons))%p)) then
    call shower_enlarge_partons_array (shower)
end if
!!! find last free pointer and let it point to the new parton
lastfree = 0
do i = size (shower%partons), 1, -1
    if (.not. associated (shower%partons(i)%p)) then
        lastfree = i
    end if
end do
if (lastfree == 0) then
    call msg_bug ("Shower: no free pointers found")
end if
shower%partons(lastfree)%p => newprt%p
end subroutine shower_add_child

```

<Shower core: shower: TBP>+≡

```

procedure :: add_parent => shower_add_parent

```

<Shower core: procedures>+≡

```

subroutine shower_add_parent (shower, prt)
    class(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout), target :: prt
    integer :: i, lastfree
    type(parton_pointer_t) :: newprt
    if (debug_on) call msg_debug2 (D_SHOWER, "shower_add_parent: for parton nr", prt%nr)
    allocate (newprt%p)
    newprt%p%nr = shower%get_next_free_nr ()
    !!! add new parton as parent
    newprt%p%child1 => prt
    prt%parent => newprt%p
    if (associated (prt%settings)) then
        newprt%p%settings => prt%settings
    end if
    newprt%p%interactionnr = prt%interactionnr
    !!! add new parton to shower%partons list
    if (.not. allocated (shower%partons) .or. &

```

```

        associated (shower%partons(size(shower%partons))%p)) then
        call shower_enlarge_partons_array (shower)
    end if
    !!! find last free pointer and let it point to the new parton
    lastfree = 0
    do i = size(shower%partons), 1, -1
        if (.not. associated (shower%partons(i)%p)) then
            lastfree = i
        end if
    end do
    if (debug_active (D_SHOWER)) then
        if (lastfree == 0) then
            call msg_bug ("Shower: no free pointers found")
        end if
    end if
    shower%partons(lastfree)%p => newprt%p
end subroutine shower_add_parent

```

For debugging:

```

<Shower core: procedures>+≡
pure function shower_get_total_momentum (shower) result (mom)
    type(shower_t), intent(in) :: shower
    type(vector4_t) :: mom
    integer :: i
    if (.not. allocated (shower%partons)) return
    mom = vector4_null
    do i = 1, size (shower%partons)
        if (.not. associated (shower%partons(i)%p)) cycle
        if (shower%partons(i)%p%is_final ()) then
            mom = mom + shower%partons(i)%p%momentum
        end if
    end do
end function shower_get_total_momentum

```

Count the number of partons by going through `shower%partons` whereby you can require a minimum energy `mine` and specify whether to `include_remnants`, which is done if not given.

```

<Shower core: shower: TBP>+≡
procedure :: get_nr_of_partons => shower_get_nr_of_partons

<Shower core: procedures>+≡
function shower_get_nr_of_partons (shower, mine, &
    include_remnants, no_hard_prts, only_colored) result (nr)
    class(shower_t), intent(in) :: shower
    real(default), intent(in), optional :: mine
    logical, intent(in), optional :: include_remnants, no_hard_prts, &
        only_colored
    logical :: no_hard, only_col, include_rem
    integer :: nr, i
    nr = 0
    no_hard = .false.; if (present (no_hard_prts)) &
        no_hard = no_hard_prts
    only_col = .false.; if (present (only_colored)) &

```

```

        only_col = only_colored
include_rem = .true.; if (present (include_remnants)) &
    include_rem = include_remnants
do i = 1, size (shower%partons)
    if (.not. associated (shower%partons(i)%p)) cycle
    associate (prt => shower%partons(i)%p)
        if (.not. prt%is_final ()) cycle
        if (present (only_colored)) then
            if (only_col) then
                if (.not. prt%is_colored ()) cycle
            else
                if (prt%is_colored ()) cycle
            end if
        end if
        if (no_hard) then
            if (shower%partons(i)%p%belongstointeraction) cycle
        end if
        if (.not. include_rem) then
            if (prt%type == BEAM_REMNANT) cycle
        end if
        if (present(mine)) then
            if (prt%momentum%p(0) < mine) cycle
        end if
        nr = nr + 1
    end associate
end do
end function shower_get_nr_of_partons

```

(Shower core: procedures)+≡

```

function shower_get_nr_of_final_colored_ME_partons (shower) result (nr)
    type(shower_t), intent(in) :: shower
    integer :: nr
    integer :: i, j
    type(parton_t), pointer :: prt
    nr = 0
do i = 1, size (shower%interactions)
    do j = 1, size (shower%interactions(i)%i%partons)
        prt => shower%interactions(i)%i%partons(j)%p
        if (.not. associated (prt)) cycle
        if (.not. prt%is_colored ()) cycle
        if (prt%belongstointeraction .and. prt%belongstoFSR .and. &
            (prt%type /= INTERNAL)) then
            nr = nr +1
        end if
    end do
end do
end function shower_get_nr_of_final_colored_ME_partons

```

(Shower core: shower: TBP)+≡

```

procedure :: get_final_colored_ME_momenta => &
    shower_get_final_colored_ME_momenta

```

(Shower core: procedures)+≡

```

subroutine shower_get_final_colored_ME_momenta (shower, momenta)

```

```

class(shower_t), intent(in) :: shower
type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
type(parton_pointer_t), dimension(:), allocatable :: partons
integer :: i, j, index, s
type(parton_t), pointer :: prt
s = shower_get_nr_of_final_colored_ME_partons (shower)
if (s == 0) return
allocate (partons(1:s))
allocate (momenta(1:s))
index = 0
do i = 1, size (shower%interactions)
  do j = 1, size (shower%interactions(i)%i%partons)
    prt => shower%interactions(i)%i%partons(j)%p
    if (.not. associated (prt)) cycle
    if (.not. prt%is_colored ()) cycle
    if (prt%belongstointeraction .and. prt%belongstoFSR .and. &
        (prt%type /= INTERNAL)) then
      index = index + 1
      partons(index)%p => prt
    end if
  end do
end do
do i = 1, s ! pointers forbid array notation
  momenta(i) = partons(i)%p%momentum
end do
end subroutine shower_get_final_colored_ME_momenta

```

(Shower core: procedures)+≡

```

recursive function interaction_fsr_is_finished_for_parton &
  (prt) result (finished)
type(parton_t), intent(in) :: prt
logical :: finished
if (prt%belongstoFSR) then
  !!! FSR partons
  if (associated (prt%child1)) then
    finished = interaction_fsr_is_finished_for_parton (prt%child1) &
      .and. interaction_fsr_is_finished_for_parton (prt%child2)
  else
    finished = prt%t <= prt%mass_squared ()
  end if
else
  !!! search for emitted timelike partons in ISR shower
  if (.not. associated (prt%initial)) then
    !!! no initial -> no ISR
    finished = .true.
  else if (.not. associated (prt%parent)) then
    finished = .false.
  else
    if (.not. prt%parent%is_proton ()) then
      if (associated (prt%child2)) then
        finished = interaction_fsr_is_finished_for_parton (prt%parent) .and. &
          interaction_fsr_is_finished_for_parton (prt%child2)
      else
        finished = interaction_fsr_is_finished_for_parton (prt%parent)
      end if
    end if
  end if
end if
end function

```

```

        end if
    else
        if (associated (prt%child2)) then
            finished = interaction_fsr_is_finished_for_parton (prt%child2)
        else
            !!! only second partons can come here -> if that happens FSR
            !!!     evolution is not existing
            finished = .true.
        end if
    end if
end if
end if
end if
end function interaction_fsr_is_finished_for_parton

```

<Shower core: procedures>+≡

```

function interaction_fsr_is_finished (interaction) result (finished)
    type(shower_interaction_t), intent(in) :: interaction
    logical :: finished
    integer :: i
    finished = .true.
    if (.not. allocated (interaction%partons)) return
    do i = 1, size (interaction%partons)
        if (.not. interaction_fsr_is_finished_for_parton &
            (interaction%partons(i)%p)) then
            finished = .false.
            exit
        end if
    end do
end function interaction_fsr_is_finished

```

<Shower core: public>+≡

```

public :: shower_interaction_get_s

```

<Shower core: procedures>+≡

```

function shower_interaction_get_s (interaction) result (s)
    type(shower_interaction_t), intent(in) :: interaction
    real(default) :: s
    s = (interaction%partons(1)%p%initial%momentum + &
        interaction%partons(2)%p%initial%momentum)**2
end function shower_interaction_get_s

```

<Shower core: procedures>+≡

```

function shower_fsr_is_finished (shower) result (finished)
    type(shower_t), intent(in) :: shower
    logical :: finished
    integer :: i
    finished = .true.
    if (.not. allocated (shower%interactions)) return
    do i = 1, size(shower%interactions)
        if (.not. interaction_fsr_is_finished (shower%interactions(i)%i)) then
            finished = .false.
            exit
        end if
    end if
end function shower_fsr_is_finished

```



```

end do
end function shower_fsr_is_finished

```

(Shower core: procedures)+≡

```

function shower_isr_is_finished (shower) result (finished)
  type(shower_t), intent(in) :: shower
  logical :: finished
  integer :: i
  type(parton_t), pointer :: prt
  finished = .true.
  if (.not.allocated (shower%partons)) return
  do i = 1, size (shower%partons)
    if (.not. associated (shower%partons(i)%p)) cycle
    prt => shower%partons(i)%p
    if (shower%settings%isr_pt_ordered) then
      if (.not. prt%belongstoFSR .and. .not. prt%simulated &
        .and. prt%scale > zero) then
        finished = .false.
        exit
      end if
    else
      if (.not. prt%belongstoFSR .and. .not. prt%simulated &
        .and. prt%t < zero) then
        finished = .false.
        exit
      end if
    end if
  end do
end function shower_isr_is_finished

```

(Shower core: procedures)+≡

```

subroutine interaction_find_partons_nearest_to_hadron &
  (interaction, prt1, prt2, isr_pt_ordered)
  type(shower_interaction_t), intent(in) :: interaction
  type(parton_t), pointer :: prt1, prt2
  logical, intent(in) :: isr_pt_ordered
  prt1 => null ()
  prt2 => null ()
  prt1 => interaction%partons(1)%p
  do
    if (associated (prt1%parent)) then
      if (prt1%parent%is_proton ()) then
        exit
      else if ((.not. isr_pt_ordered .and. .not. prt1%parent%simulated) &
        .or. (isr_pt_ordered .and. .not. prt1%simulated)) then
        exit
      else
        prt1 => prt1%parent
      end if
    else
      exit
    end if
  end do

```

```

prt2 => interaction%partons(2)%p
do
  if (associated (prt2%parent)) then
    if (prt2%parent%is_proton ()) then
      exit
    else if ((.not. isr_pt_ordered .and. .not. prt2%parent%simulated) &
      .or. (isr_pt_ordered .and. .not. prt2%simulated)) then
      exit
    else
      prt2 => prt2%parent
    end if
  else
    exit
  end if
end do
end subroutine interaction_find_partons_nearest_to_hadron

```

<Shower core: shower: TBP>+≡

```

procedure :: update_beamremnants => shower_update_beamremnants

```

<Shower core: procedures>+≡

```

subroutine shower_update_beamremnants (shower)
  class(shower_t), intent(inout) :: shower
  type(parton_t), pointer :: hadron, remnant
  integer :: i
  real(default) :: random
  !!! only proton in first interaction !!!
  !!! currently only first beam-remnant will be updated
  do i = 1,2
    if (associated (shower%interactions(1)%i%partons(i)%p%initial)) then
      hadron => shower%interactions(1)%i%partons(i)%p%initial
    else
      cycle
    end if
    remnant => hadron%child2
    if (associated (remnant)) then
      remnant%momentum = hadron%momentum - hadron%child1%momentum
    end if
    !!! generate flavor of the beam-remnant if beam was proton
    if (abs (hadron%type) == PROTON .and. associated (hadron%child1)) then
      if (hadron%child1%is_quark ()) then
        !!! decide if valence (u,d) or sea quark (s,c,b)
        if ((abs (hadron%child1%type) <= 2) .and. &
          (hadron%type * hadron%child1%type > zero)) then
          !!! valence quark
          if (abs (hadron%child1%type) == 1) then
            !!! if d then remaining diquark is uu_1
            remnant%type = sign (UU1, hadron%type)
          else
            call shower%rng%generate (random)
            !!! if u then remaining diquark is ud_0 or ud_1
            if (random < 0.75_default) then
              remnant%type = sign (UD0, hadron%type)
            else

```

```

        remnant%type = sign (UD1, hadron%type)
    end if
    end if
    remnant%c1 = hadron%child1%c2
    remnant%c2 = hadron%child1%c1
else if ((hadron%type * hadron%child1%type) < zero) then
    !!! antiquark
    if (.not. associated (remnant%child1)) then
        call shower%add_child (remnant, 1)
    end if
    if (.not. associated (remnant%child2)) then
        call shower%add_child (remnant, 2)
    end if
    call shower%rng%generate (random)
    if (random < 0.6666_default) then
        !!! 2/3 into udq + u
        if (abs (hadron%child1%type) == 1) then
            remnant%child1%type = sign (NEUTRON, hadron%type)
        else if (abs (hadron%child1%type) == 2) then
            remnant%child1%type = sign (PROTON, hadron%type)
        else if (abs (hadron%child1%type) == 3) then
            remnant%child1%type = sign (SIGMA0, hadron%type)
        else if (abs (hadron%child1%type) == 4) then
            remnant%child1%type = sign (SIGMACPLUS, hadron%type)
        else if (abs (hadron%child1%type) == 5) then
            remnant%child1%type = sign (SIGMAB0, hadron%type)
        end if
        remnant%child2%type = sign (2, hadron%type)
    else
        !!! 1/3 into uuq + d
        if (abs (hadron%child1%type) == 1) then
            remnant%child1%type = sign (PROTON, hadron%type)
        else if (abs (hadron%child1%type) == 2) then
            remnant%child1%type = sign (DELTAPLUSPLUS, hadron%type)
        else if (abs (hadron%child1%type) == 3) then
            remnant%child1%type = sign (SIGMAPLUS, hadron%type)
        else if (abs (hadron%child1%type) == 4) then
            remnant%child1%type = sign (SIGMACPLUSPLUS, hadron%type)
        else if (abs (hadron%child1%type) == 5) then
            remnant%child1%type = sign (SIGMABPLUS, hadron%type)
        end if
        remnant%child2%type = sign (1, hadron%type)
    end if
    remnant%c1 = hadron%child1%c2
    remnant%c2 = hadron%child1%c1
    remnant%child1%c1 = 0
    remnant%child1%c2 = 0
    remnant%child2%c1 = remnant%c1
    remnant%child2%c2 = remnant%c2
else
    !!! sea quark
    if (.not. associated (remnant%child1)) then
        call shower%add_child (remnant, 1)
    end if

```

```

if (.not. associated (remnant%child2)) then
  call shower%add_child (remnant, 2)
end if
call shower%rng%generate (random)
if (random < 0.5_default) then
  !!! 1/2 into usbar + ud_0
  if (abs (hadron%child1%type) == 3) then
    remnant%child1%type = sign (KPLUS, hadron%type)
  else if (abs (hadron%child1%type) == 4) then
    remnant%child1%type = sign (D0, hadron%type)
  else if (abs (hadron%child1%type) == 5) then
    remnant%child1%type = sign (BPLUS, hadron%type)
  end if
  remnant%child2%type = sign (UD0, hadron%type)
else if (random < 0.6666_default) then
  !!! 1/6 into usbar + ud_1
  if (abs (hadron%child1%type) == 3) then
    remnant%child1%type = sign (KPLUS, hadron%type)
  else if (abs (hadron%child1%type) == 4) then
    remnant%child1%type = sign (D0, hadron%type)
  else if (abs (hadron%child1%type) == 5) then
    remnant%child1%type = sign (BPLUS, hadron%type)
  end if
  remnant%child2%type = sign (UD1, hadron%type)
else
  !!! 1/3 into dsbar + uu_1
  if (abs (hadron%child1%type) == 3) then
    remnant%child1%type = sign (K0, hadron%type)
  else if (abs (hadron%child1%type) == 4) then
    remnant%child1%type = sign (DPLUS, hadron%type)
  else if (abs (hadron%child1%type) == 5) then
    remnant%child1%type = sign (B0, hadron%type)
  end if
  remnant%child2%type = sign (UU1, hadron%type)
end if
remnant%c1 = hadron%child1%c2
remnant%c2 = hadron%child1%c1
remnant%child1%c1 = 0
remnant%child1%c2 = 0
remnant%child2%c1 = remnant%c1
remnant%child2%c2 = remnant%c2
end if
else if (hadron%child1%is_gluon ()) then
  if (.not.associated (remnant%child1)) then
    call shower%add_child (remnant, 1)
  end if
  if (.not.associated (remnant%child2)) then
    call shower%add_child (remnant, 2)
  end if
  call shower%rng%generate (random)
  if (random < 0.5_default) then
    !!! 1/2 into u + ud_0
    remnant%child1%type = sign (2, hadron%type)
    remnant%child2%type = sign (UD0, hadron%type)
  end if
end if

```

```

else if (random < 0.6666_default) then
  !!! 1/6 into u + ud_1
  remnant%child1%type = sign (2, hadron%type)
  remnant%child2%type = sign (UD1, hadron%type)
else
  !!! 1/3 into d + uu_1
  remnant%child1%type = sign (1, hadron%type)
  remnant%child2%type = sign (UU1, hadron%type)
end if
remnant%c1 = hadron%child1%c2
remnant%c2 = hadron%child1%c1
if (hadron%type > 0) then
  remnant%child1%c1 = remnant%c1
  remnant%child2%c2 = remnant%c2
else
  remnant%child1%c2 = remnant%c2
  remnant%child2%c1 = remnant%c1
end if
end if
remnant%initial => hadron
if (associated (remnant%child1)) then
  remnant%child1%initial => hadron
  remnant%child2%initial => hadron
  !!! don't care about on-shellness for now
  remnant%child1%momentum = 0.5_default * remnant%momentum
  remnant%child2%momentum = 0.5_default * remnant%momentum
  !!! but care about on-shellness for baryons
  if (mod (remnant%child1%type, 100) >= 10) then
    !!! check if the third quark is set -> meson or baryon
    remnant%child1%t = remnant%child1%mass_squared ()
    remnant%child1%momentum = [remnant%child1%momentum%p(0), &
      (remnant%child1%momentum%p(1:3) / &
        remnant%child1%momentum%p(1:3)**1) * &
      sqrt (remnant%child1%momentum%p(0)**2 - remnant%child1%t)]
    remnant%child2%momentum = remnant%momentum &
      - remnant%child1%momentum
  end if
end if
end if
end do
end subroutine shower_update_beamremnants

```

(Shower core: procedures)+≡

```

subroutine interaction_apply_lorentztrafo (interaction, L)
  type(shower_interaction_t), intent(inout) :: interaction
  type(lorentz_transformation_t), intent(in) :: L
  type(parton_t), pointer :: prt
  integer :: i
  !!! ISR part
  do i = 1,2
    prt => interaction%partons(i)%p
    !!! loop over ancestors
    MOTHERS: do
      !!! boost parton

```

```

    call parton_apply_lorentztrafo (prt, L)
    if (associated (prt%child2)) then
        !!! boost emitted timelike parton (and daughters)
        call parton_apply_lorentztrafo_recursive (prt%child2, L)
    end if
    if (associated (prt%parent)) then
        if (.not. prt%parent%is_proton ()) then
            prt => prt%parent
        else
            exit
        end if
    else
        exit
    end if
end do MOTHERS
end do
!!! FSR part
if (associated (interaction%partons(3)%p%parent)) then
    !!! pseudo Parton-Shower histora has been generated -> find
    !!! mother and go on from there recursively
    prt => interaction%partons(3)%p
    do while (associated (prt%parent))
        prt => prt%parent
    end do
    call parton_apply_lorentztrafo_recursive (prt, L)
else
    do i = 3, size (interaction%partons)
        call parton_apply_lorentztrafo (interaction%partons(i)%p, L)
    end do
end if
end subroutine interaction_apply_lorentztrafo

```

(Shower core: procedures)+≡

```

subroutine shower_apply_lorentztrafo (shower, L)
    type(shower_t), intent(inout) :: shower
    type(lorentz_transformation_t), intent(in) :: L
    integer :: i
    do i = 1, size (shower%interactions)
        call interaction_apply_lorentztrafo (shower%interactions(i)%i, L)
    end do
end subroutine shower_apply_lorentztrafo

```

This boosts partons belonging to the interaction to the center-of-mass frame of its partons nearest to the hadron.

(Shower core: procedures)+≡

```

subroutine interaction_boost_to_CMframe (interaction, isr_pt_ordered)
    type(shower_interaction_t), intent(inout) :: interaction
    logical, intent(in) :: isr_pt_ordered
    type(vector4_t) :: beta
    type(parton_t), pointer :: prt1, prt2
    call interaction_find_partons_nearest_to_hadron &
        (interaction, prt1, prt2, isr_pt_ordered)
    beta = prt1%momentum + prt2%momentum

```

```

    beta = beta / beta%p(0)
    if (debug_active (D_SHOWER)) then
        if (beta**2 > one) then
            call msg_error ("Shower: boost to CM frame: beta > 1")
            return
        end if
    end if
    if (space_part(beta)**2 > tiny_13) then
        call interaction_apply_lorentztrafo (interaction, &
            boost(space_part(beta)**1 / &
                sqrt (one - space_part(beta)**2), -direction(beta)))
    end if
end subroutine interaction_boost_to_CMframe

```

This boosts every interaction to the center-of-mass-frame of its partons nearest to the hadron.

```

<Shower core: shower: TBP>+≡
    procedure :: boost_to_CMframe => shower_boost_to_CMframe

<Shower core: procedures>+≡
    subroutine shower_boost_to_CMframe (shower)
        class(shower_t), intent(inout) :: shower
        integer :: i
        do i = 1, size (shower%interactions)
            call interaction_boost_to_CMframe &
                (shower%interactions(i)%i, shower%settings%isr_pt_ordered)
        end do
        ! TODO: (bcn 2015-03-23) this shouldnt be here !
        call shower%update_beamremnants ()
    end subroutine shower_boost_to_CMframe

```

This boost all partons so that initial partons have their assigned x -value.

```

<Shower core: shower: TBP>+≡
    procedure :: boost_to_labframe => shower_boost_to_labframe

<Shower core: procedures>+≡
    subroutine shower_boost_to_labframe (shower)
        class(shower_t), intent(inout) :: shower
        integer :: i
        do i = 1, size (shower%interactions)
            call interaction_boost_to_labframe &
                (shower%interactions(i)%i, shower%settings%isr_pt_ordered)
        end do
    end subroutine shower_boost_to_labframe

```

This boosts all partons so that initial partons have their assigned x -value.

```

<Shower core: procedures>+≡
    subroutine interaction_boost_to_labframe (interaction, isr_pt_ordered)
        type(shower_interaction_t), intent(inout) :: interaction
        logical, intent(in) :: isr_pt_ordered
        type(parton_t), pointer :: prt1, prt2
        type(vector3_t) :: beta
        call interaction_find_partons_nearest_to_hadron &

```

```

        (interaction, prt1, prt2, isr_pt_ordered)
    if (.not. associated (prt1%initial) .or. .not. &
        associated (prt2%initial)) then
        return
    end if
    !!! transform partons to overall labframe.
    beta = vector3_canonical(3) * &
        ((prt1%x * prt2%momentum%p(0) - &
          prt2%x * prt1%momentum%p(0)) / &
         (prt1%x * prt2%momentum%p(3) - &
          prt2%x * prt1%momentum%p(3)))
    if (beta**1 > tiny_10) &
        call interaction_apply_lorentztrafo (interaction, &
            boost (beta**1 / sqrt(one - beta**2), -direction(beta)))
    end subroutine interaction_boost_to_labframe

```

Only rotate to z if initial hadrons are given (and they are assumed to be aligned along the z-axis).

```

<Shower core: procedures>+=
subroutine interaction_rotate_to_z (interaction, isr_pt_ordered)
    type(shower_interaction_t), intent(inout) :: interaction
    logical, intent(in) :: isr_pt_ordered
    type(parton_t), pointer :: prt1, prt2
    call interaction_find_partons_nearest_to_hadron &
        (interaction, prt1, prt2, isr_pt_ordered)
    if (associated (prt1%initial)) then
        call interaction_apply_lorentztrafo (interaction, &
            rotation_to_2nd (space_part (prt1%momentum), &
                vector3_canonical(3) * sign (one, &
                    prt1%initial%momentum%p(3)))
        end if
    end subroutine interaction_rotate_to_z

```

Rotate initial partons to lie along $\pm z$ axis.

```

<Shower core: shower: TBP>+=
procedure :: rotate_to_z => shower_rotate_to_z

<Shower core: procedures>+=
subroutine shower_rotate_to_z (shower)
    class(shower_t), intent(inout) :: shower
    integer :: i
    do i = 1, size (shower%interactions)
        call interaction_rotate_to_z &
            (shower%interactions(i)%i, shower%settings%isr_pt_ordered)
    end do
    ! TODO: (bcn 2015-03-23) this shouldnt be here !
    call shower%update_beamremnants ()
end subroutine shower_rotate_to_z

```

Return if there are no initials, electron-hadron collision not implemented.

```

<Shower core: procedures>+=
subroutine interaction_generate_primordial_kt &
    (interaction, primordial_kt_width, primordial_kt_cutoff, rng)

```



```

type(shower_interaction_t), intent(inout) :: interaction
real(default), intent(in) :: primordial_kt_width, primordial_kt_cutoff
class(rng_t), intent(inout), allocatable :: rng
type(parton_t), pointer :: had1, had2
type(vector4_t) :: momenta(2)
type(vector3_t) :: beta
real(default) :: pt (2), phi(2)
real(default) :: shat
real(default) :: btheta, bphi
integer :: i
if (vanishes (primordial_kt_width)) return
if (.not. associated (interaction%partons(1)%p%initial) .or. &
    .not. associated (interaction%partons(2)%p%initial)) then
    return
end if
had1 => interaction%partons(1)%p%initial
had2 => interaction%partons(2)%p%initial
!!! copy momenta and energy
momenta(1) = had1%child1%momentum
momenta(2) = had2%child1%momentum
GENERATE_PT_PHI: do i = 1, 2
    !!! generate transverse momentum and phi
    GENERATE_PT: do
        call rng%generate (pt (i))
        pt(i) = primordial_kt_width * sqrt(-log(pt(i)))
        if (pt(i) < primordial_kt_cutoff) exit
    end do GENERATE_PT
    call rng%generate (phi (i))
    phi(i) = twopi * phi(i)
end do GENERATE_PT_PHI
!!! adjust momenta
shat = (momenta(1) + momenta(2))**2
momenta(1) = [momenta(1)%p(0), &
    pt(1) * cos(phi(1)), &
    pt(1) * sin(phi(1)), &
    momenta(1)%p(3)]
momenta(2) = [momenta(2)%p(0), &
    pt(2) * cos(phi(2)), &
    pt(2) * sin(phi(2)), &
    momenta(2)%p(3)]
beta = [momenta(1)%p(1) + momenta(2)%p(1), &
    momenta(1)%p(2) + momenta(2)%p(2), zero] / sqrt(shat)
momenta(1) = boost (beta**1 / sqrt(one - beta**2), -direction(beta)) &
    * momenta(1)
bphi = azimuthal_angle (momenta(1))
btheta = polar_angle (momenta(1))
call interaction_apply_lorentztrafo (interaction, &
    rotation (cos(bphi), sin(bphi), 3) * rotation(cos(btheta), &
    sin(btheta), 2) * rotation(cos(-bphi), sin(-bphi), 3))
call interaction_apply_lorentztrafo (interaction, &
    boost (beta**1 / sqrt(one - beta**2), -direction(beta)))
end subroutine interaction_generate_primordial_kt

```

(Shower core: shower: TBP)+≡

```

procedure :: generate_primordial_kt => shower_generate_primordial_kt
<Shower core: procedures>+=
subroutine shower_generate_primordial_kt (shower)
class(shower_t), intent(inout) :: shower
integer :: i
do i = 1, size (shower%interactions)
call interaction_generate_primordial_kt (shower%interactions(i)%i, &
shower%settings%isr_primordial_kt_width, &
shower%settings%isr_primordial_kt_cutoff, shower%rng)
end do
! TODO: (bcn 2015-03-23) this shouldnt be here !
call shower%update_beamremnants ()
end subroutine shower_generate_primordial_kt

```

Output.

```

<Shower core: procedures>+=
subroutine interaction_write (interaction, unit)
type(shower_interaction_t), intent(in) :: interaction
integer, intent(in), optional :: unit
integer :: i, u
u = given_output_unit (unit); if (u < 0) return
if (associated (interaction%partons(1)%p)) then
if (associated (interaction%partons(1)%p%initial)) &
call interaction%partons(1)%p%initial%write (u)
end if
if (associated (interaction%partons(2)%p)) then
if (associated (interaction%partons(2)%p%initial)) &
call interaction%partons(2)%p%initial%write (u)
end if
if (allocated (interaction%partons)) then
do i = 1, size (interaction%partons)
call interaction%partons(i)%p%write (u)
end do
end if
write (u, "(A)")
end subroutine interaction_write

```

```

<Shower core: shower: TBP>+=
procedure :: write => shower_write

```

```

<Shower core: procedures>+=
subroutine shower_write (shower, unit)
class(shower_t), intent(in) :: shower
integer, intent(in), optional :: unit
integer :: i, u
u = given_output_unit (unit); if (u < 0) return
write (u, "(1x,A)") "-----"
write (u, "(1x,A)") "WHIZARD internal parton shower"
write (u, "(1x,A)") "-----"
call shower%pdf_data%write (u)
if (size (shower%interactions) > 0) then
write (u, "(3x,A)") "Interactions: "
do i = 1, size (shower%interactions)

```

```

        write (u, "(4x,A,I0)") "Interaction number ", i
        if (.not. associated (shower%interactions(i)%i)) then
            call msg_fatal ("Shower: missing interaction in shower")
        end if
        call interaction_write (shower%interactions(i)%i, u)
    end do
else
    write (u, "(3x,A)") "[no interactions in shower]"
end if
write (u, "(A)")
if (allocated (shower%partons)) then
    write (u, "(5x,A)") "Partons:"
    do i = 1, size (shower%partons)
        if (associated (shower%partons(i)%p)) then
            call shower%partons(i)%p%write (u)
            if (i < size (shower%partons)) then
                if (associated (shower%partons(i + 1)%p)) then
                    if (shower%partons(i)%p%belongstointeraction .and. &
                        .not. shower%partons(i + 1)%p%belongstointeraction) then
                        call write_separator (u)
                    end if
                end if
            end if
        end if
    end do
else
    write (u, "(5x,A)") "[no partons in shower]"
end if
write (u, "(4x,A)") "Total Momentum: "
call vector4_write (shower_get_total_momentum (shower))
write (u, "(1x,A,L1)") "ISR finished: ", shower_isr_is_finished (shower)
write (u, "(1x,A,L1)") "FSR finished: ", shower_fsr_is_finished (shower)
end subroutine shower_write

```

We combine the `particle_set` from the hard interaction with the partons of the shower. For simplicity, we do not maintain the mother-daughter-relations of the shower. Hadronic `beam_remnants` of the old `particle_set` are removed as they are provided, including proper flavor information, by the ISR shower.

(Shower core: shower: TBP)+≡

```

    procedure :: combine_with_particle_set => shower_combine_with_particle_set

```

(Shower core: procedures)+≡

```

    subroutine shower_combine_with_particle_set (shower, particle_set, &
        model_in, model_hadrons)
        class(shower_t), intent(in) :: shower
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model_in
        class(model_data_t), intent(in), target :: model_hadrons
        type(particle_t), dimension(:), allocatable :: particles
        integer, dimension(:), allocatable :: hard_colored_ids, &
            shower_partons_ids, incoming_ids, outgoing_ids
        class(model_data_t), pointer :: model
        logical, dimension(:), allocatable :: hard_colored_mask
        integer :: n_shower_partons, n_remnants, i, j
    end subroutine

```

```

integer :: n_in, n_out, n_beam, n_tot_old
if (signal_is_pending ()) return
if (debug_on) call msg_debug (D_SHOWER, "shower_combine_with_particle_set")
if (debug_on) call msg_debug (D_SHOWER, "Particle set before replacing")
if (debug_active (D_SHOWER)) &
    call particle_set%write (summary=.true., compressed=.true.)

n_shower_partons = shower%get_nr_of_partons (only_colored = &
    .true., no_hard_prts = .true.)
n_remnants = shower%get_nr_of_partons (only_colored = .false., &
    no_hard_prts = .true.)
if (n_shower_partons + n_remnants > 0) then
    call particle_set%without_hadronic_remnants &
        (particles, n_tot_old, n_shower_partons + n_remnants)
    call count_and_allocate ()
    call replace_outgoings ()
    call set_hard_colored_as_resonant_parents_for_shower ()
    call add_to_pset (n_tot_old, .true.)
    call add_to_pset (n_tot_old + n_remnants, .false.)
    call particle_set%replace (particles)
end if

if (debug_on) call msg_debug (D_SHOWER, 'Particle set after replacing')
if (debug_active (D_SHOWER)) &
    call particle_set%write (summary=.true., compressed=.true.)

contains

<Shower core: shower combine with particle set: procedures>

end subroutine shower_combine_with_particle_set

```

```

<Shower core: shower combine with particle set: procedures>≡
subroutine count_and_allocate ()
    n_beam = particle_set%get_n_beam ()
    n_in = particle_set%get_n_in ()
    n_out = particle_set%get_n_out ()
    allocate (hard_colored_mask (size (particles)))
    hard_colored_mask = (particles%get_status () == PRT_INCOMING .or. &
        particles%get_status () == PRT_OUTGOING) .and. &
        particles%is_colored ()
    allocate (hard_colored_ids (count (hard_colored_mask)))
    hard_colored_ids = pack ([i, i=1, size (particles)], hard_colored_mask)
    allocate (shower_partons_ids (n_shower_partons))
    shower_partons_ids = [(n_tot_old + n_remnants + i, i=1, n_shower_partons)]
    allocate (incoming_ids(n_in))
    incoming_ids = [(n_beam + i, i=1, n_in)]
    allocate (outgoing_ids(n_out))
    outgoing_ids = [(n_tot_old - n_out + i, i=1, n_out)]
    if (debug_active (D_SHOWER)) then
        print *, 'n_remnants = ', n_remnants
        print *, 'n_shower_partons = ', n_shower_partons
        print *, 'n_tot_old = ', n_tot_old
        print *, 'n_beam = ', n_beam
    end if
end subroutine count_and_allocate

```

```

        print *, 'n_in, n_out = ', n_in, n_out
    end if
end subroutine count_and_allocate

```

(Shower core: shower combine with particle set: procedures)+≡

```

subroutine replace_outgoings ()
    do i = 1, size (shower%interactions)
        if (i > 1) then
            call msg_bug ('shower_combine_with_particle_set assumes 1 interaction')
        end if
        associate (interaction => shower%interactions(i)%i)
            do j = 3, size (interaction%partons)
                if (associated (interaction%partons(j)%p)) then
                    call replace_parton_in_particles (j, interaction%partons(j)%p)
                end if
            end do
        end associate
    end do
end subroutine replace_outgoings

```

(Shower core: shower combine with particle set: procedures)+≡

```

subroutine replace_parton_in_particles (j, prt)
    integer, intent(in) :: j
    type(parton_t), intent(in) :: prt
    integer :: idx
    if (j <= 2) then
        idx = n_beam + j
    else
        idx = n_tot_old - n_out - n_in + j
    end if
    call particles(idx)%set_momentum (prt%momentum)
end subroutine replace_parton_in_particles

```

(Shower core: shower combine with particle set: procedures)+≡

```

subroutine set_hard_colored_as_resonant_parents_for_shower ()
    do i = 1, n_tot_old
        if (hard_colored_mask (i)) then
            if (has_splitted (i)) then
                call particles(i)%add_children (shower_partons_ids)
                if (particles(i)%get_status () == PRT_OUTGOING) then
                    call particles(i)%set_status (PRT_RESONANT)
                end if
            end if
        end if
    end do
end subroutine set_hard_colored_as_resonant_parents_for_shower

```

(Shower core: shower combine with particle set: procedures)+≡

```

function has_splitted (i) result (splitted)
    logical :: splitted
    integer, intent(in) :: i
    splitted = .false.

```

```

do j = 1, size (shower%partons)
  if (.not. associated (shower%partons(j)%p)) cycle
  if (particles(i)%flv%get_pdg () == shower%partons(j)%p%type) then
    if (all (nearly_equal (particles(i)%p%p, &
                          shower%partons(j)%p%momentum%p))) then
      splitted = shower%partons(j)%p%is_branched ()
    end if
  end if
end if
end do
end function has_splitted

<Shower core: shower combine with particle set: procedures>+≡
subroutine add_to_pset (offset, remnants)
  integer, intent(in) :: offset
  logical, intent(in) :: remnants
  integer :: i, j
  j = offset
do i = 1, size (shower%partons)
  if (.not. associated (shower%partons(i)%p)) cycle
  associate (prt => shower%partons(i)%p)
    if (.not. prt%is_final () .or. &
        prt%belongstointeraction) cycle
    if (remnants) then
      if (prt%is_colored ()) cycle
    else
      if (.not. (prt%is_colored ())) cycle
    end if
    j = j + 1
    call find_model (model, prt%type, model_in, model_hadrons)
    particles (j) = prt%to_particle (model)
    if (remnants) then
      call particles(j)%set_parents ([prt%initial%nr])
      call particles(prt%initial%nr)%add_child (j)
    else
      call particles(j)%set_parents (hard_colored_ids)
    end if
  end associate
end do
end subroutine add_to_pset

<Shower core: shower: TBP>+≡
procedure :: write_lhef => shower_write_lhef

<Shower core: procedures>+≡
subroutine shower_write_lhef (shower, unit)
  class(shower_t), intent(in) :: shower
  integer, intent(in), optional :: unit
  integer :: u
  integer :: i
  integer :: c1, c2
  u = given_output_unit (unit); if (u < 0) return
  write(u,'(A)') '<LesHouchesEvents version="1.0">'
  write(u,'(A)') '<-- not a complete lhe file - just one event -->'
  write(u,'(A)') '<event>'
  write(u, *) 2 + shower%get_nr_of_partons (), 1, 1.0, 1.0, 1.0, 1.0

```

```

!!! write incoming partons
do i = 1, 2
  if (abs (shower%partons(i)%p%type) < 1000) then
    c1 = 0
    c2 = 0
    if (shower%partons(i)%p%is_colored ()) then
      if (shower%partons(i)%p%c1 /= 0) c1 = 500 + shower%partons(i)%p%c1
      if (shower%partons(i)%p%c2 /= 0) c2 = 500 + shower%partons(i)%p%c2
    end if
    write (u,*) shower%partons(i)%p%type, -1, 0, 0, c1, c2, &
      shower%partons(i)%p%momentum%p(1), &
      shower%partons(i)%p%momentum%p(2), &
      shower%partons(i)%p%momentum%p(3), &
      shower%partons(i)%p%momentum%p(0), &
      shower%partons(i)%p%momentum**2, zero, 9.0
  else
    write (u,*) shower%partons(i)%p%type, -9, 0, 0, 0, 0, &
      shower%partons(i)%p%momentum%p(1), &
      shower%partons(i)%p%momentum%p(2), &
      shower%partons(i)%p%momentum%p(3), &
      shower%partons(i)%p%momentum%p(0), &
      shower%partons(i)%p%momentum**2, zero, 9.0
  end if
end do
!!! write outgoing partons
do i = 3, size (shower%partons)
  if (.not. associated (shower%partons(i)%p)) cycle
  if (.not. shower%partons(i)%p%is_final ()) cycle
  c1 = 0
  c2 = 0
  if (shower%partons(i)%p%is_colored ()) then
    if (shower%partons(i)%p%c1 /= 0) c1 = 500 + shower%partons(i)%p%c1
    if (shower%partons(i)%p%c2 /= 0) c2 = 500 + shower%partons(i)%p%c2
  end if
  write (u,*) shower%partons(i)%p%type, 1, 1, 2, c1, c2, &
    shower%partons(i)%p%momentum%p(1), &
    shower%partons(i)%p%momentum%p(2), &
    shower%partons(i)%p%momentum%p(3), &
    shower%partons(i)%p%momentum%p(0), &
    shower%partons(i)%p%momentum**2, zero, 9.0
end do
write(u,'(A)') '</event>'
write(u,'(A)') '</LesHouchesEvents>'
end subroutine shower_write_lhef

```

(Shower core: procedures)+≡

```

subroutine shower_replace_parent_by_hadron (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), intent(inout), target :: prt
  type(parton_t), pointer :: remnant => null()
  if (associated (prt%parent)) then
    call shower_remove_parton_from_partons (shower, prt%parent)
    deallocate (prt%parent)
  end if

```

```

if (.not. associated (prt%initial%child2)) then
  call shower%add_child (prt%initial, 2)
end if
prt%parent => prt%initial
prt%parent%child1 => prt
! make other child to be a beam-remnant
remnant => prt%initial%child2
remnant%type = BEAM_REMNANT
remnant%momentum = prt%parent%momentum - prt%momentum
remnant%x = one - prt%x
remnant%parent => prt%initial
remnant%t = zero
end subroutine shower_replace_parent_by_hadron

```

(*Shower core: procedures*) +=

```

subroutine shower_get_first_ISR_scale_for_parton (shower, prt, tmax)
  type(shower_t), intent(inout), target :: shower
  type(parton_t), intent(inout), target :: prt
  real(default), intent(in), optional :: tmax
  real(default) :: t, tstep, random, integral, temp1
  real(default) :: temprand
  if (present(tmax)) then
    t = max (max (-shower%settings%isr_tscalefactor * prt%momentum%p(0)**2, &
      -abs(tmax)), prt%t)
  else
    t = max (-shower%settings%isr_tscalefactor * prt%momentum%p(0)**2, prt%t)
  end if
  call shower%rng%generate (random)
  random = -twopi * log(random)
  !!! compare Integral and log(random) instead of random and exp(-Integral)
  integral = zero
  call prt%set_simulated (.false.)
  do
    call shower%rng%generate (temprand)
    tstep = max (abs (0.01_default * t) * temprand, 0.1_default * &
      shower%settings%min_virtuality)
    if (t + 0.5_default * tstep > - shower%settings%min_virtuality) then
      prt%t = prt%mass_squared ()
      call prt%set_simulated ()
      exit
    end if
    prt%t = t + 0.5_default * tstep
    temp1 = integral_over_z_simple (prt, (random - integral) / tstep)
    integral = integral + tstep * temp1
    if (integral > random) then
      prt%t = t + 0.5_default * tstep
      exit
    end if
    t = t + tstep
  end do
  if (prt%t > - shower%settings%min_virtuality) then
    call shower_replace_parent_by_hadron (shower, prt)
  end if
end if

```


contains

```

function integral_over_z_simple (prt, final) result (integral)
  type(parton_t), intent(inout) :: prt
  real(default), intent(in) :: final
  real(default), volatile :: integral

  real(default), parameter :: zstepfactor = one
  real(default), parameter :: zstepmin = 0.0001_default
  real(default) :: z, zstep, minz, maxz
  real(default) :: pdfsum
  integer :: quark, d_nf

  integral = zero
  if (debug2_active (D_SHOWER)) then
    print *, "D: integral_over_z_simple: t = ", prt%t
  end if
  minz = prt%x
  ! maxz = maxx(shat, s, shower%settings%isr_z_cutoff, shower%settings%isr_minenergy)
  maxz = shower%settings%isr_z_cutoff
  z = minz
  d_nf = shower%settings%max_n_flavors
  !!! TODO -> Adapt zstep to structure of divergencies
  if (prt%child1%is_gluon ()) then
    !!! gluon coming from g->gg
    do
      call shower%rng%generate (temprand)
      zstep = max(zstepmin, temprand * zstepfactor * z * (one - z))
      zstep = min(zstep, maxz - z)
      integral = integral + zstep * (D_alpha_s_isr ((one - &
        (z + 0.5_default * zstep)) * abs(prt%t), &
        shower%settings) / (abs(prt%t))) * &
        P_ggg (z + 0.5_default * zstep) * &
        shower%get_pdf (prt%initial%type, &
          prt%x / (z + 0.5_default * zstep), abs(prt%t), GLUON)
      if (integral > final) then
        exit
      end if
      z = z + zstep
      if (z >= maxz) then
        exit
      end if
    end do
    !!! gluon coming from q->qg ! correctly implemented yet?
    if (integral < final) then
      z = minz
      do
        call shower%rng%generate (temprand)
        zstep = max(zstepmin, temprand * zstepfactor * z * (one - z))
        zstep = min(zstep, maxz - z)
        pdfsum = zero
        do quark = -d_nf, d_nf
          if (quark == 0) cycle
          pdfsum = pdfsum + shower%get_pdf (prt%initial%type, &

```

```

        prt%x / (z + 0.5_default * zstep), abs(prt%t), quark)
    end do
    integral = integral + zstep * (D_alpha_s_isr &
        ((z + 0.5_default * zstep) * abs(prt%t), &
        shower%settings) / (abs(prt%t))) * &
        P_qqg (one - (z + 0.5_default * zstep)) * pdfsum
    if (integral > final) then
        exit
    end if
    z = z + zstep
    if (z >= maxz) then
        exit
    end if
end do
end if
else if (prt%child1%is_quark ()) then
    !!! quark coming from q->qg
    do
        call shower%rng%generate(temprand)
        zstep = max(zstepmin, temprand * zstepfactor * z * (one - z))
        zstep = min(zstep, maxz - z)
        integral = integral + zstep * (D_alpha_s_isr ((one - &
            (z + 0.5_default * zstep)) * abs(prt%t), &
            shower%settings) / (abs(prt%t))) * &
            P_qqg (z + 0.5_default * zstep) * &
            shower%get_pdf (prt%initial%type, &
            prt%x / (z + 0.5_default * zstep), abs(prt%t), prt%type)
        if (integral > final) then
            exit
        end if
        z = z + zstep
        if (z >= maxz) then
            exit
        end if
    end do
    !!! quark coming from g->qqbar
    if (integral < final) then
        z = minz
        do
            call shower%rng%generate (temprand)
            zstep = max(zstepmin, temprand * zstepfactor * z*(one - z))
            zstep = min(zstep, maxz - z)
            integral = integral + zstep * (D_alpha_s_isr &
                ((one - (z + 0.5_default * zstep)) * abs(prt%t), &
                shower%settings) / (abs(prt%t))) * &
                P_gqq (z + 0.5_default * zstep) * &
                shower%get_pdf (prt%initial%type, &
                prt%x / (z + 0.5_default * zstep), abs(prt%t), GLUON)
            if (integral > final) then
                exit
            end if
            z = z + zstep
            if (z >= maxz) then
                exit
            end if
        end do
    end if
end if

```

```

        end if
      end do
    end if

    end if
    integral = integral / shower%get_pdf (prt%initial%type, prt%x, &
      abs(prt%t), prt%type)
  end function integral_over_z_simple

end subroutine shower_get_first_ISR_scale_for_parton

```

(Shower core: procedures)+≡

```

subroutine shower_prepare_for_simulate_isr_pt (shower, interaction)
  type(shower_t), intent(inout) :: shower
  type(shower_interaction_t), intent(inout) :: interaction
  real(default) :: s
  s = (interaction%partons(1)%p%momentum + &
    interaction%partons(2)%p%momentum)**2
  interaction%partons(1)%p%scale = shower%settings%isr_tscalefactor * 0.25_default * s
  interaction%partons(2)%p%scale = shower%settings%isr_tscalefactor * 0.25_default * s
end subroutine shower_prepare_for_simulate_isr_pt

```

(Shower core: procedures)+≡

```

subroutine shower_prepare_for_simulate_isr_ana_test (shower, prt1, prt2)
  type(shower_t), intent(inout) :: shower
  type(parton_t), intent(inout), target :: prt1, prt2
  type(parton_t), pointer :: prt, prta, prtb
  real(default) :: scale, factor, E
  integer :: i
  if (.not. associated (prt1%initial) .or. .not. associated (prt2%initial)) then
    return
  end if
  scale = - (prt1%momentum + prt2%momentum) ** 2
  call prt1%set_simulated ()
  call prt2%set_simulated ()
  call shower%add_parent (prt1)
  call shower%add_parent (prt2)
  factor = sqrt (energy (prt1%momentum)**2 - scale) / &
    space_part_norm(prt1%momentum)
  prt1%parent%type = prt1%type
  prt1%parent%z = one
  prt1%parent%momentum = prt1%momentum
  prt1%parent%t = scale
  prt1%parent%x = prt1%x
  prt1%parent%initial => prt1%initial
  prt1%parent%belongstoFSR = .false.
  prt1%parent%c1 = prt1%c1
  prt1%parent%c2 = prt1%c2

  prt2%parent%type= prt2%type
  prt2%parent%z = one
  prt2%parent%momentum = prt2%momentum
  prt2%parent%t = scale

```

```

prt2%parent%x = prt2%x
prt2%parent%initial => prt2%initial
prt2%parent%belongstoFSR = .false.
prt2%parent%c1 = prt2%c1
prt2%parent%c2 = prt2%c2

call shower_get_first_ISR_scale_for_parton (shower, prt1%parent)
call shower_get_first_ISR_scale_for_parton (shower, prt2%parent)

!!! redistribute energy among first partons
prta => prt1%parent
prtb => prt2%parent

E = energy (prt1%momentum + prt2%momentum)
prta%momentum%p(0) = (E**2 - prtb%t + prta%t) / (two * E)
prtb%momentum%p(0) = E - prta%momentum%p(0)

call prt1%parent%set_simulated ()
call prt2%parent%set_simulated ()
!!! rescale momenta
do i = 1, 2
  if (i == 1) then
    prt => prt1%parent
  else
    prt => prt2%parent
  end if
  factor = sqrt (energy (prt%momentum)**2 - prt%t) &
    / space_part_norm (prt%momentum)
  prt%momentum = vector4_moving (energy (prt%momentum), &
    factor * space_part (prt%momentum))
end do

if (prt1%parent%t < zero) then
  call shower%add_parent (prt1%parent)
  prt1%parent%parent%momentum = prt1%parent%momentum
  prt1%parent%parent%t = prt1%parent%t
  prt1%parent%parent%x = prt1%parent%x
  prt1%parent%parent%initial => prt1%parent%initial
  prt1%parent%parent%belongstoFSR = .false.
  call shower%add_child (prt1%parent%parent, 2)
end if

if (prt2%parent%t < zero) then
  call shower%add_parent (prt2%parent)
  prt2%parent%parent%momentum = prt2%parent%momentum
  prt2%parent%parent%t = prt2%parent%t
  prt2%parent%parent%x = prt2%parent%x
  prt2%parent%parent%initial => prt2%parent%initial
  prt2%parent%parent%belongstoFSR = .false.
  call shower%add_child (prt2%parent%parent, 2)
end if

end subroutine shower_prepare_for_simulate_isr_ana_test

```

```

(Shower core: procedures)+≡
subroutine shower_add_children_of_emitted_timelike_parton (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), pointer :: prt

  if (prt%t > prt%mass_squared () + shower%settings%min_virtuality) then
    if (prt%is_quark ()) then
      !!! q -> qg
      call shower%add_child (prt, 1)
      prt%child1%type = prt%type
      prt%child1%momentum%p(0) = prt%z * prt%momentum%p(0)
      prt%child1%t = prt%t
      call shower%add_child (prt, 2)
      prt%child2%type = GLUON
      prt%child2%momentum%p(0) = (one - prt%z) * prt%momentum%p(0)
      prt%child2%t = prt%t
    else
      if (int (prt%x) > 0) then
        call shower%add_child (prt, 1)
        prt%child1%type = int (prt%x)
        prt%child1%momentum%p(0) = prt%z * prt%momentum%p(0)
        prt%child1%t = prt%t
        call shower%add_child (prt, 2)
        prt%child2%type = -int (prt%x)
        prt%child2%momentum%p(0) = (one - prt%z) * prt%momentum%p(0)
        prt%child2%t = prt%t
      else
        call shower%add_child (prt, 1)
        prt%child1%type = GLUON
        prt%child1%momentum%p(0) = prt%z * prt%momentum%p(0)
        prt%child1%t = prt%t
        call shower%add_child (prt, 2)
        prt%child2%type = GLUON
        prt%child2%momentum%p(0) = (one - prt%z) * prt%momentum%p(0)
        prt%child2%t = prt%t
      end if
    end if
  end if
end subroutine shower_add_children_of_emitted_timelike_parton

```

```

(Shower core: procedures)+≡
subroutine shower_simulate_children_ana (shower,prt)
  type(shower_t), intent(inout), target :: shower
  type(parton_t), intent(inout) :: prt
  real(default), dimension(1:2) :: random, integral
  integer, dimension(1:2) :: gtoqq
  integer :: daughter
  type(parton_t), pointer :: daughterprt
  integer :: n_loop

  if (signal_is_pending ()) return
  if (debug2_active (D_SHOWER)) &
    print *, "D: shower_simulate_children_ana: for parton " , prt%nr
  gtoqq = 0

```

```

if (.not. associated (prt%child1) .or. .not. associated (prt%child2)) then
  call msg_error ("Shower: error in simulate_children_ana: no children.")
  return
end if

<Set beam-remnants and internal partons as simulated>

integral = zero

!!! impose constraints by angular ordering -> cf. (26) of Gaining analytic control
!!! check if no branchings are possible
if (.not. prt%child1%simulated) then
  prt%child1%t = min (prt%child1%t, &
    0.5_default * prt%child1%momentum%p(0)**2 * (one - &
    prt%get_costheta ()))
  if (.not. associated (prt%child1%settings)) &
    prt%child1%settings => shower%settings
  if (min (prt%child1%t, prt%child1%momentum%p(0)**2) < &
    prt%child1%mass_squared () + &
    prt%child1%settings%min_virtuality) then
    prt%child1%t = prt%child1%mass_squared ()
    call prt%child1%set_simulated ()
  end if
end if
if (.not. prt%child2%simulated) then
  prt%child2%t = min (prt%child2%t, &
    0.5_default * prt%child2%momentum%p(0)**2 * (one - &
    prt%get_costheta ()))
  if (.not. associated (prt%child2%settings)) &
    prt%child2%settings => shower%settings
  if (min (prt%child2%t, prt%child2%momentum%p(0)**2) < &
    prt%child2%mass_squared () + &
    prt%child2%settings%min_virtuality) then
    prt%child2%t = prt%child2%mass_squared ()
    call prt%child2%set_simulated ()
  end if
end if

call shower%rng%generate (random)

n_loop = 0
do
  if (signal_is_pending ()) return
  n_loop = n_loop + 1
  if (n_loop > 900) then
    !!! try with massless quarks
    treat_duscb_quarks_massless = .true.
  end if
  if (n_loop > 1000) then
    call msg_message ("simulate_children_ana failed for parton ", prt%nr)
    call msg_warning ("too many loops in simulate_children_ana")
    call shower%write ()
    shower%valid = .false.
    return
  end if
end do

```

```

end if

!!! check if a branching in the range t(i) to t(i) - tstep(i) occurs
if (.not. prt%child1%simulated) then
    call parton_simulate_stept &
        (prt%child1, shower%rng, integral(1), random(1), gtoqq(1))
end if
if (.not. prt%child2%simulated) then
    call parton_simulate_stept &
        (prt%child2, shower%rng, integral(2), random(2), gtoqq(2))
end if

if (prt%child1%simulated .and. prt%child2%simulated) then
    if (sqrt (prt%t) <= sqrt (prt%child1%t) + sqrt (prt%child2%t)) then
        <Repeat the simulation for the parton with the lower virtuality>
    else
        exit
    end if
end if
end do

call parton_apply_costheta (prt, shower%rng)

<Add children>
call shower_parton_update_color_connections (shower, prt)
end subroutine shower_simulate_children_ana

<Set beam-remnants and internal partons as simulated>≡
if (HADRON_REMNANT <= abs (prt%type) .and. abs (prt%type) <= HADRON_REMNANT_OCTET) then
    !!! prt is beam-remnant
    call prt%set_simulated ()
    return
end if

!!! check if partons are "internal" -> fixed scale
if (prt%child1%type == INTERNAL) then
    call prt%child1%set_simulated ()
end if
if (prt%child2%type == INTERNAL) then
    call prt%child2%set_simulated ()
end if

<Repeat the simulation for the parton with the lower virtuality>≡
!!! virtuality : t - m**2 (assuming it's not fixed)
if (prt%child1%type == INTERNAL .and. prt%child2%type == INTERNAL) then
    call msg_fatal &
        ("Shower: both partons fixed, but momentum not conserved")
else if (prt%child1%type == INTERNAL) then
    !!! reset child2
    call prt%child2%set_simulated (.false.)
    prt%child2%t = min (prt%child1%t, (sqrt (prt%t) - &
        sqrt (prt%child1%t))**2)
    integral(2) = zero
    call shower%rng%generate (random(2))

```

```

else if (prt%child2%type == INTERNAL) then
  ! reset child1
  call prt%child1%set_simulated (.false.)
  prt%child1%t = min (prt%child2%t, (sqrt (prt%t) - &
    sqrt (prt%child2%t))**2)
  integral(1) = zero
  call shower%rng%generate (random(1))
else if (prt%child1%t - prt%child1%mass_squared () > &
  prt%child2%t - prt%child2%mass_squared ()) then
  !!! reset child2
  call prt%child2%set_simulated (.false.)
  prt%child2%t = min (prt%child1%t, (sqrt (prt%t) - &
    sqrt (prt%child1%t))**2)
  integral(2) = zero
  call shower%rng%generate (random(2))
else
  !!! reset child1 ! TODO choose child according to their t
  call prt%child1%set_simulated (.false.)
  prt%child1%t = min (prt%child2%t, (sqrt (prt%t) - &
    sqrt (prt%child2%t))**2)
  integral(1) = zero
  call shower%rng%generate (random(1))
end if

<Add children>≡
if (.not. associated (prt%child1%settings)) &
  prt%child1%settings => shower%settings
if (.not. associated (prt%child2%settings)) &
  prt%child2%settings => shower%settings
do daughter = 1, 2
  if (signal_is_pending ()) return
  if (daughter == 1) then
    daughterprt => prt%child1
  else
    daughterprt => prt%child2
  end if
  if (daughterprt%t < daughterprt%mass_squared () + &
    daughterprt%settings%min_virtuality) then
    cycle
  end if
  if (.not. (daughterprt%is_quark () .or. daughterprt%is_gluon ())) then
    cycle
  end if
  if (daughterprt%is_quark ()) then
    !!! q -> qg
    call shower%add_child (daughterprt, 1)
    daughterprt%child1%type = daughterprt%type
    daughterprt%child1%momentum%p(0) = daughterprt%z * &
      daughterprt%momentum%p(0)
    daughterprt%child1%t = daughterprt%t
    call shower%add_child (daughterprt, 2)
    daughterprt%child2%type = GLUON
    daughterprt%child2%momentum%p(0) = (one - daughterprt%z) * &
      daughterprt%momentum%p(0)
    daughterprt%child2%t = daughterprt%t
  end if
end do

```



```

else if (daughterprt%is_gluon ()) then
  if (gtoqq(daughter) > 0) then
    call shower%add_child (daughterprt, 1)
    daughterprt%child1%type = gtoqq (daughter)
    daughterprt%child1%momentum%p(0) = &
      daughterprt%z * daughterprt%momentum%p(0)
    daughterprt%child1%t = daughterprt%t
    call shower%add_child (daughterprt, 2)
    daughterprt%child2%type = - gtoqq (daughter)
    daughterprt%child2%momentum%p(0) = (one - &
      daughterprt%z) * daughterprt%momentum%p(0)
    daughterprt%child2%t = daughterprt%t
  else
    call shower%add_child (daughterprt, 1)
    daughterprt%child1%type = GLUON
    daughterprt%child1%momentum%p(0) = &
      daughterprt%z * daughterprt%momentum%p(0)
    daughterprt%child1%t = daughterprt%t
    call shower%add_child (daughterprt, 2)
    daughterprt%child2%type = GLUON
    daughterprt%child2%momentum%p(0) = (one - &
      daughterprt%z) * daughterprt%momentum%p(0)
    daughterprt%child2%t = daughterprt%t
  end if
end if
end do

```

The recoiler is `otherprt`. Instead of the random number and the exponential of the integral, we compare the logarithm of the random number and the integral.

(Shower core: procedures) +=

```

subroutine shower_isr_step_pt (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), target, intent(inout) :: prt
  type(parton_t), pointer :: otherprt

  real(default) :: scale, scalestep
  real(default), volatile :: integral
  real(default) :: random, factor
  real(default) :: temprand1, temprand2

  otherprt => shower%find_recoiler (prt)

  scale = prt%scale
  call shower%rng%generate (temprand1)
  call shower%rng%generate (temprand2)
  scalestep = max (abs (scalefactor1 * scale) * temprand1, &
    scalefactor2 * temprand2 * D_Min_scale)
  call shower%rng%generate (random)
  random = - twopi * log(random)
  integral = zero

  if (scale - 0.5_default * scalestep < D_Min_scale) then
    !!! close enough to cut-off scale -> ignore
    prt%scale = zero
  end if
end subroutine shower_isr_step_pt

```

```

    prt%t = prt%mass_squared ()
    call prt%set_simulated ()
else
    prt%scale = scale - 0.5_default * scalestep
    factor = scalestep * (D_alpha_s_isr (prt%scale, &
        shower%settings) / (prt%scale * &
        shower%get_pdf (prt%initial%type, prt%x, prt%scale, prt%type)))
    integral = integral + factor * integral_over_z_isr_pt &
        (prt, otherprt, (random - integral) / factor)
    if (integral > random) then
        !!! prt%scale set above and prt%z set in integral_over_z_isr_pt
        call prt%set_simulated ()
        prt%t = - prt%scale / (one - prt%z)
    else
        prt%scale = scale - scalestep
    end if
end if

contains

function integral_over_z_isr_pt (prt, otherprt, final) &
    result (integral)
    type(parton_t), intent(inout) :: prt, otherprt
    real(default), intent(in) :: final
    real(default), volatile :: integral
    real(default) :: mbr, r
    real(default) :: zmin, zmax, z, zstep
    integer :: n_bin
    integer, parameter :: n_total_bins = 100
    real(default) :: quarkpdfsum
    real(default) :: temprand
    integer :: quark, d_nf

    quarkpdfsum = zero
    d_nf = shower%settings%max_n_flavors
    if (debug2_active (D_SHOWER)) then
        print *, "D: integral_over_z_isr_pt: for scale = ", prt%scale
    end if

    integral = zero
    mbr = (prt%momentum + otherprt%momentum)**1
    zmin = prt%x
    zmax = min (one - (sqrt (prt%scale) / mbr) * &
        (sqrt(one + 0.25_default * prt%scale / mbr**2) - &
        0.25_default * sqrt(prt%scale) / mbr), shower%settings%isr_z_cutoff)
    zstep = (zmax - zmin) / n_total_bins

    if (debug_active (D_SHOWER)) then
        if (zmin > zmax) then
            call msg_bug(" error in integral_over_z_isr_pt: zmin > zmax ")
            integral = zero
        end if
    end if
end if

```

```

!!! divide the range [zmin:zmax] in n_total_bins
BINS: do n_bin = 1, n_total_bins
  z = zmin + zstep * (n_bin - 0.5_default)
  !!! z-value in the middle of the bin

  if (prt%is_gluon ()) then
    QUARKS: do quark = -d_nf, d_nf
      if (quark == 0) cycle quarks
      quarkpdfsum = quarkpdfsum + shower%get_pdf &
        (prt%initial%type, prt%x / z, prt%scale, quark)
    end do QUARKS
    !!! g -> gg or q -> gq
    integral = integral + (zstep / z) * ((P_ggg (z) + &
      P_ggg (one - z)) * shower%get_pdf (prt%initial%type, &
      prt%x / z, prt%scale, GLUON) + P_qqg (one - z) * quarkpdfsum)
  else if (prt%is_quark ()) then
    !!! q -> qg or g -> qq
    integral = integral + (zstep / z) * ( P_qqg (z) * &
      shower%get_pdf (prt%initial%type, prt%x / z, prt%scale, &
      prt%type) + &
      P_gqq(z) * shower%get_pdf (prt%initial%type, prt%x / z, &
      prt%scale, GLUON))
  else
    ! call msg_fatal ("Bug neither quark nor gluon in" &
    !               // " integral_over_z_isr_pt")
  end if
  if (integral > final) then
    prt%z = z
    call shower%rng%generate (temprand)
    !!! decide type of father partons
    if (prt%is_gluon ()) then
      if (temprand > (P_qqg (one - z) * quarkpdfsum) / &
        ((P_ggg (z) + P_ggg (one - z)) * shower%get_pdf &
        (prt%initial%type, prt%x / z, prt%scale, GLUON) &
        + P_qqg (one - z) * quarkpdfsum)) then
        !!! gluon => gluon + gluon
        prt%aux_pt = GLUON
      else
        !!! quark => quark + gluon
        !!! decide which quark flavor the parent is
        r = temprand * quarkpdfsum
        WHICH_QUARK: do quark = -d_nf, d_nf
          if (quark == 0) cycle WHICH_QUARK
          if (r > quarkpdfsum - shower%get_pdf (prt%initial%type, &
            prt%x / z, prt%scale, quark)) then
            prt%aux_pt = quark
            exit WHICH_QUARK
          else
            quarkpdfsum = quarkpdfsum - shower%get_pdf &
              (prt%initial%type, prt%x / z, prt%scale, quark)
          end if
        end do WHICH_QUARK
      end if
    end if
  end if
end if

```

```

else if (prt%is_quark ()) then
  if (temprand > (P_qqg (z) * shower%get_pdf (prt%initial%type, &
    prt%x / z, prt%scale, prt%type)) / &
    (P_qqg (z) * shower%get_pdf (prt%initial%type, prt%x / z, &
    prt%scale, prt%type) + &
    P_gqq (z) * shower%get_pdf (prt%initial%type, prt%x / z, &
    prt%scale, GLUON))) then
    !!! gluon => quark + antiquark
    prt%aux_pt = GLUON
  else
    !!! quark => quark + gluon
    prt%aux_pt = prt%type
  end if
end if
exit BINS
end if
end do BINS
end function integral_over_z_isr_pt
end subroutine shower_isr_step_pt

```

This function returns a pointer to the parton with the next ISR branching, while FSR branchings are ignored.

(Shower core: shower: TBP)+≡

```

procedure :: generate_next_isr_branching_veto => &
  shower_generate_next_isr_branching_veto

```

(Shower core: procedures)+≡

```

function shower_generate_next_isr_branching_veto &
  (shower) result (next_brancher)
  class(shower_t), intent(inout) :: shower
  type(parton_pointer_t) :: next_brancher
  integer :: i
  type(parton_t), pointer :: prt
  real(default) :: random
  !!! pointers to branchable partons
  type(parton_pointer_t), dimension(:), allocatable :: partons
  integer :: n_partons
  real(default) :: weight
  real(default) :: temp1, temp2, temp3, E3

  if (signal_is_pending ()) return

  if (shower%settings%isr_pt_ordered) then
    next_brancher = shower%generate_next_isr_branching ()
    return
  end if
  next_brancher%p => null()
  !!! branchable partons
  n_partons = 0
  do i = 1, size (shower%partons)
    prt => shower%partons(i)%p
    if (.not. associated (prt)) cycle
    if (prt%belongstoFSR) cycle
    if (prt%is_final ()) cycle

```

```

        if (.not. prt%belongstoFSR .and. prt%simulated) cycle
        n_partons = n_partons + 1
    end do
    if (n_partons == 0) then
        return
    end if
    allocate (partons(1:n_partons))
    n_partons = 1
    do i = 1, size (shower%partons)
        prt => shower%partons(i)%p
        if (.not. associated (prt)) cycle
        if (prt%belongstoFSR) cycle
        if (prt%is_final ()) cycle
        if (.not. prt%belongstoFSR .and. prt%simulated) cycle
        partons(n_partons)%p => shower%partons(i)%p
        n_partons = n_partons + 1
    end do
    !!! generate initial trial scales
    do i = 1, size (partons)
        if (signal_is_pending ()) return
        call generate_next_trial_scale (partons(i)%p)
    end do

    do
        !!! search for parton with the highest trial scale
        prt => partons(1)%p
        do i = 1, size (partons)
            if (prt%t >= zero) cycle
            if (abs (partons(i)%p%t) > abs (prt%t)) then
                prt => partons(i)%p
            end if
        end do

        if (prt%t >= zero) then
            next_brancher%p => null()
            exit
        end if
        !!! generate trial z and type of mother prt
        call generate_trial_z_and_typ (prt)

        !!! weight with pdf and alpha_s
        temp1 = (D_alpha_s_isr ((one - prt%z) * abs(prt%t), &
            shower%settings) / sqrt (alphaspdfmax))
        temp2 = shower%get_xpdf (prt%initial%type, prt%x, prt%t, &
            prt%type) / sqrt (alphaspdfmax)
        temp3 = shower%get_xpdf (prt%initial%type, prt%child1%x, prt%child1%t, &
            prt%child1%type) / &
            shower%get_xpdf (prt%initial%type, prt%child1%x, prt%t, &
            prt%child1%type)
        ! TODO: (bcn 2015-02-19) ???
        if (temp1 * temp2 * temp3 > one) then
            print *, "weights:", temp1, temp2, temp3
        end if
        weight = (D_alpha_s_isr ((one - prt%z) * abs(prt%t), &

```

```

        shower%settings)) * &
        shower%get_xpdf (prt%initial%type, prt%x, prt%t, prt%type) * &
        shower%get_xpdf (prt%initial%type, prt%child1%x, prt%child1%t, &
        prt%child1%type) / &
        shower%get_xpdf &
        (prt%initial%type, prt%child1%x, prt%t, prt%child1%type)
if (weight > alphasxpdfmax) then
    print *, "Setting alphasxpdfmax from ", alphasxpdfmax, " to ", weight
    alphasxpdfmax = weight
end if
weight = weight / alphasxpdfmax
call shower%rng%generate (random)
if (weight < random) then
    !!! discard branching
    call generate_next_trial_scale (prt)
    cycle
end if
!!! branching accepted so far
!!! generate emitted parton
prt%child2%t = abs(prt%t)
prt%child2%momentum%p(0) = sqrt (abs(prt%t))
if (shower%settings%isr_only_onshell_emitted_partons) then
    prt%child2%t = prt%child2%mass_squared ()
else
    call prt%child2%next_t_ana (shower%rng)
end if

if (thetabar (prt, shower%find_recoiler (prt), &
    shower%settings%isr_angular_ordered, E3)) then
    prt%momentum%p(0) = E3
    prt%child2%momentum%p(0) = E3 - prt%child1%momentum%p(0)

    !!! found branching
    call prt%generate_ps_ini (shower%rng)
    next_brancher%p => prt
    call prt%set_simulated ()
    exit
else
    call generate_next_trial_scale (prt)
    cycle
end if
end do
if (.not. associated (next_brancher%p)) then
    !!! no further branching found -> all partons emitted by hadron
    print *, "--all partons emitted by hadrons---"
    do i = 1, size(partons)
        call shower_replace_parent_by_hadron (shower, partons(i)%p%child1)
    end do
end if
!!! some bookkeeping
call shower%sort_partons ()
! call shower%boost_to_CMframe ()      ! really necessary?
! call shower%rotate_to_z ()          ! really necessary?
contains

```

```

subroutine generate_next_trial_scale (prt)
  type(parton_t), pointer, intent(inout) :: prt
  real(default) :: random, F
  real(default) :: zmax = 0.99_default !! ??
  call shower%rng%generate (random)
  F = one !!! TODO
  F = alphaspdfmax / (two * pi)
  if (prt%child1%is_quark ()) then
    F = F * (integral_over_P_gqq (prt%child1%x, zmax) + &
              integral_over_P_qqq (prt%child1%x, zmax))
  else if (prt%child1%is_gluon ()) then
    F = F * (integral_over_P_ggg (prt%child1%x, zmax) + &
              two * shower%settings%max_n_flavors * &
              integral_over_P_qqq (one - zmax, one - prt%child1%x))
  else
    call msg_bug("neither quark nor gluon in generate_next_trial_scale")
  end if
  F = F / shower%get_xpdf (prt%child1%initial%type, prt%child1%x, &
                           prt%child1%t, prt%child1%type)
  prt%t = prt%t * random**(one / F)
  if (abs (prt%t) - prt%mass_squared () < &
      prt%settings%min_virtuality) then
    prt%t = prt%mass_squared ()
  end if
end subroutine generate_next_trial_scale

subroutine generate_trial_z_and_typ (prt)
  type(parton_t), pointer, intent(inout) :: prt
  real(default) :: random
  real(default) :: z, zstep, zmin, integral
  real(default) :: zmax = 0.99_default !! ??
  if (debug_on) call msg_debug (D_SHOWER, "generate_trial_z_and_typ")
  call shower%rng%generate (random)
  integral = zero
  !!! decide which branching a->bc occurs
  if (prt%child1%is_quark ()) then
    if (random < integral_over_P_qqq (prt%child1%x, zmax) / &
        (integral_over_P_qqq (prt%child1%x, zmax) + &
         integral_over_P_gqq (prt%child1%x, zmax))) then
      prt%type = prt%child1%type
      prt%child2%type = GLUON
      integral = integral_over_P_qqq (prt%child1%x, zmax)
    else
      prt%type = GLUON
      prt%child2%type = - prt%child1%type
      integral = integral_over_P_gqq (prt%child1%x, zmax)
    end if
  else if (prt%child1%is_gluon ()) then
    if (random < integral_over_P_ggg (prt%child1%x, zmax) / &
        (integral_over_P_ggg (prt%child1%x, zmax) + two * &
         shower%settings%max_n_flavors * &
         integral_over_P_qqq (one - zmax, &
                              one - prt%child1%x))) then

```

```

    prt%type = GLUON
    prt%child2%type = GLUON
    integral = integral_over_P_ggg (prt%child1%x, zmax)
else
    call shower%rng%generate (random)
    prt%type = 1 + floor(random * shower%settings%max_n_flavors)
    call shower%rng%generate (random)
    if (random > 0.5_default) prt%type = - prt%type
    prt%child2%type = prt%type
    integral = integral_over_P_qqg (one - zmax, &
        one - prt%child1%x)
end if
else
    call msg_bug("neither quark nor gluon in generate_next_trial_scale")
end if
!!! generate the z-value
!!! z between prt%child1%x and zmax
! prt%z = one - random * (one - prt%child1%x)      ! TODO

call shower%rng%generate (random)
zmin = prt%child1%x
zstep = max(0.1_default, 0.5_default * (zmax - zmin))
z = zmin
if (zmin > zmax) then
    print *, " zmin = ", zmin, " zmax = ", zmax
    call msg_fatal ("Shower: zmin greater than zmax")
end if
!!! procedure pointers would be helpful here
if (prt%is_quark () .and. prt%child1%is_quark ()) then
    do
        zstep = min(zstep, 0.5_default * (zmax - z))
        if (abs(zstep) < 0.00001) exit
        if (integral_over_P_qqg (zmin, z) < random * integral) then
            if (integral_over_P_qqg (zmin, min(z + zstep, zmax)) &
                < random * integral) then
                z = min (z + zstep, zmax)
                cycle
            else
                zstep = zstep * 0.5_default
                cycle
            end if
        end if
    end do
else if (prt%is_quark () .and. prt%child1%is_gluon ()) then
    do
        zstep = min(zstep, 0.5_default * (zmax - z))
        if (abs(zstep) < 0.00001) exit
        if (integral_over_P_qqg (zmin, z) < random * integral) then
            if (integral_over_P_qqg (zmin, min(z + zstep, zmax)) &
                < random * integral) then
                z = min(z + zstep, zmax)
                cycle
            else
                zstep = zstep * 0.5_default

```



```

        cycle
      end if
    end if
  end do
else if (prt%is_gluon () .and. prt%child1%is_quark ()) then
  do
    zstep = min(zstep, 0.5_default * (zmax - z))
    if (abs (zstep) < 0.00001) exit
    if (integral_over_P_gqq (zmin, z) < random * integral) then
      if (integral_over_P_gqq (zmin, min(z + zstep, zmax)) &
        < random * integral) then
        z = min (z + zstep, zmax)
        cycle
      else
        zstep = zstep * 0.5_default
        cycle
      end if
    end if
  end do
else if (prt%is_gluon () .and. prt%child1%is_gluon ()) then
  do
    zstep = min(zstep, 0.5_default * (zmax - z))
    if (abs (zstep) < 0.00001) exit
    if (integral_over_P_ggg (zmin, z) < random * integral) then
      if (integral_over_P_ggg (zmin, min(z + zstep, zmax)) &
        < random * integral) then
        z = min(z + zstep, zmax)
        cycle
      else
        zstep = zstep * 0.5_default
        cycle
      end if
    end if
  end do
else
  end if
prt%z = z
prt%x = prt%child1%x / prt%z
end subroutine generate_trial_z_and_typ
end function shower_generate_next_isr_branching_veto

```

<Shower core: shower: TBP>+≡

```
procedure :: find_recoiler => shower_find_recoiler
```

<Shower core: procedures>+≡

```
function shower_find_recoiler (shower, prt) result(recoiler)
  class(shower_t), intent(inout) :: shower
  type(parton_t), intent(inout), target :: prt
  type(parton_t), pointer :: recoiler
  type(parton_t), pointer :: otherprt1, otherprt2
  integer :: n_int
  otherprt1 => null()
  otherprt2 => null()
  DO_INTERACTIONS: do n_int = 1, size(shower%interactions)

```

```

otherprt1 => shower%interactions(n_int)%i%partons(1)%p
otherprt2 => shower%interactions(n_int)%i%partons(2)%p
PARTON1: do
  if (associated (otherprt1%parent)) then
    if (.not. otherprt1%parent%is_proton () .and. &
        otherprt1%parent%simulated) then
      otherprt1 => otherprt1%parent
      if (associated (otherprt1, prt)) then
        exit PARTON1
      end if
    else
      exit PARTON1
    end if
  else
    exit PARTON1
  end if
end do PARTON1
PARTON2: do
  if (associated (otherprt2%parent)) then
    if (.not. otherprt2%parent%is_proton () .and. &
        otherprt2%parent%simulated) then
      otherprt2 => otherprt2%parent
      if (associated (otherprt2, prt)) then
        exit PARTON2
      end if
    else
      exit PARTON2
    end if
  else
    exit PARTON2
  end if
end do PARTON2

if (associated (otherprt1, prt) .or. associated (otherprt2, prt)) then
  exit DO_INTERACTIONS
end if
if (associated (otherprt1%parent, prt) .or. &
    associated (otherprt2%parent, prt)) then
  exit DO_INTERACTIONS
end if
end do DO_INTERACTIONS

recoiler => null()
if (associated (otherprt1%parent, prt)) then
  recoiler => otherprt2
else if (associated (otherprt2%parent, prt)) then
  recoiler => otherprt1
else if (associated (otherprt1, prt)) then
  recoiler => otherprt2
else if (associated (otherprt2, prt)) then
  recoiler => otherprt1
else
  call shower%write ()
  call prt%write ()

```

```

        call msg_error ("shower_find_recoiler: no otherparton found")
    end if
end function shower_find_recoiler

```

(Shower core: procedures)+≡

```

subroutine shower_isr_step (shower, prt)
    type(shower_t), intent(inout) :: shower
    type(parton_t), target, intent(inout) :: prt
    type(parton_t), pointer :: otherprt => null()
    real(default) :: t, tstep
    real(default), volatile :: integral
    real(default) :: random
    real(default) :: temprand1, temprand2
    otherprt => shower%find_recoiler (prt)
    ! if (.not. otherprt%child1%belongstointeraction) then
    !     otherprt => otherprt%child1
    ! end if

    if (signal_is_pending ()) return
    t = max(prt%t, prt%child1%t)
    call shower%rng%generate (random)
    ! compare Integral and log(random) instead of random and exp(-Integral)
    random = - twopi * log(random)
    integral = zero
    call shower%rng%generate (temprand1)
    call shower%rng%generate (temprand2)
    tstep = max (abs (0.02_default * t) * temprand1, &
        0.02_default * temprand2 * shower%settings%min_virtuality)
    if (t + 0.5_default * tstep > - shower%settings%min_virtuality) then
        prt%t = prt%mass_squared ()
        call prt%set_simulated ()
    else
        prt%t = t + 0.5_default * tstep
        integral = integral + tstep * &
            integral_over_z_isr (shower, prt, otherprt, (random - integral) / tstep)
        if (integral > random) then
            prt%t = t + 0.5_default * tstep
            prt%x = prt%child1%x / prt%z
            call prt%set_simulated ()
        else
            prt%t = t + tstep
        end if
    end if
end subroutine shower_isr_step

```

(Shower core: procedures)+≡

```

function integral_over_z_isr (shower, prt, otherprt, final) result (integral)
    type(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout) :: prt, otherprt
    real(default), intent(in) :: final
    !!! !!! !!! volatile argument: gfortran 7 aggressive optimization (#809)
    real(default), volatile :: integral
    real(default) :: minz, maxz, shat,s

```

```

integer :: quark

!!! calculate shat -> s of parton-parton system
shat = (otherprt%momentum + prt%child1%momentum)**2
!!! calculate s -> s of hadron-hadron system
s = (otherprt%initial%momentum + prt%initial%momentum)**2
integral = zero
minz = prt%child1%x
maxz = maxx (shat, s, shower%settings%isr_z_cutoff, &
             shower%settings%isr_minenergy)

!!! for gluon
if (prt%child1%is_gluon ()) then
  !!! 1: g->gg
  prt%type = GLUON
  prt%child2%type = GLUON
  prt%child2%t = abs(prt%t)
  call integral_over_z_part_isr &
    (shower, prt, otherprt, shat, minz, maxz, integral, final)
  if (integral > final) then
    return
  else
    !!! 2: q->qq
    do quark = - shower%settings%max_n_flavors, &
      shower%settings%max_n_flavors
      if (quark == 0) cycle
      prt%type = quark
      prt%child2%type = quark
      prt%child2%t = abs(prt%t)
      call integral_over_z_part_isr &
        (shower, prt, otherprt, shat, minz, maxz, integral, final)
      if (integral > final) then
        return
      end if
    end do
  end if
else if (prt%child1%is_quark ()) then
  !!! 1: q->qg
  prt%type = prt%child1%type
  prt%child2%type = GLUON
  prt%child2%t = abs(prt%t)
  call integral_over_z_part_isr &
    (shower, prt, otherprt, shat, minz, maxz, integral, final)
  if (integral > final) then
    return
  else
    !!! 2: g->qqbar
    prt%type = GLUON
    prt%child2%type = -prt%child1%type
    prt%child2%t = abs(prt%t)
    call integral_over_z_part_isr &
      (shower, prt, otherprt, shat, minz, maxz, integral, final)
  end if
end if
end if

```

```
end function integral_over_z_isr
```

(Shower core: procedures)+≡

```
subroutine integral_over_z_part_isr &
  (shower, prt, otherprt, shat ,minz, maxz, retvalue, final)
  type(shower_t), intent(inout) :: shower
  type(parton_t), intent(inout) :: prt, otherprt
  real(default), intent(in) :: shat, minz, maxz, final
  real(default), intent(inout) :: retvalue
  real(default) :: z, zstep
  real(default) :: r1,r3,s1,s3
  real(default) :: pdf_divisor
  real(default) :: temprand
  real(default), parameter :: zstepfactor = 0.1_default
  real(default), parameter :: zstepmin = 0.0001_default
  if (debug_on) call msg_debug2 (D_SHOWER, "integral_over_z_part_isr")
  if (signal_is_pending ()) return
  pdf_divisor = shower%get_pdf &
    (prt%initial%type, prt%child1%x, prt%t, prt%child1%type)
  z = minz
  s1 = shat + abs(otherprt%t) + abs(prt%child1%t)
  r1 = sqrt (s1**2 - four * abs(otherprt%t * prt%child1%t))
  ZLOOP: do
    if (signal_is_pending ()) return
    if (z >= maxz) then
      exit
    end if
    call shower%rng%generate (temprand)
    if (prt%child1%is_gluon ()) then
      if (prt%is_gluon ()) then
        !!! g-> gg -> divergencies at z->0 and z->1
        zstep = max(zstepmin, temprand * zstepfactor * z * (one - z))
      else
        !!! q-> gq -> divergencies at z->0
        zstep = max(zstepmin, temprand * zstepfactor * (one - z))
      end if
    else
      if (prt%is_gluon ()) then
        !!! g-> qqbar -> no divergencies
        zstep = max(zstepmin, temprand * zstepfactor)
      else
        !!! q-> qg -> divergencies at z->1
        zstep = max(zstepmin, temprand * zstepfactor * (one - z))
      end if
    end if
    zstep = min(zstep, maxz - z)
    prt%z = z + 0.5_default * zstep
    s3 = shat / prt%z + abs(otherprt%t) + abs(prt%t)
    r3 = sqrt (s3**2 - four * abs(otherprt%t * prt%t))
    !!! TODO: WHY is this if needed?
    if (abs(otherprt%t) > eps0) then
      prt%child2%t = min ((s1 * s3 - r1 * r3) / &
        (two * abs(otherprt%t)) - abs(prt%child1%t) - &
        abs(prt%t), abs(prt%child1%t))
    end if
  end do
  retvalue = pdf_divisor * r1 * r3
```

```

else
  prt%child2%t = abs(prt%child1%t)
end if
do
  prt%child2%momentum%p(0) = sqrt (abs(prt%child2%t))
  if (shower%settings%isr_only_onshell_emitted_partons) then
    prt%child2%t = prt%child2%mass_squared ()
  else
    call prt%child2%next_t_ana (shower%rng)
  end if
  !!! take limits by recoiler into account
  prt%momentum%p(0) = (shat / prt%z + &
    abs(otherprt%t) - abs(prt%child1%t) - &
    prt%child2%t) / (two * sqrt(shat))
  prt%child2%momentum%p(0) = &
    prt%momentum%p(0) - prt%child1%momentum%p(0)
  !!! check if E and t of prt%child2 are consistent
  if (prt%child2%momentum%p(0)**2 < prt%child2%t &
    .and. prt%child2%t > prt%child2%mass_squared ()) then
    !!! E is too small to have  $p_T^2 = E^2 - t > 0$ 
    !!!      -> cycle to find another solution
    cycle
  else
    !!! E is big enough -> exit
    exit
  end if
end do
if (thetabar (prt, otherprt, shower%settings%isr_angular_ordered) &
  .and. pdf_divisor > zero &
  .and. prt%child2%momentum%p(0) > zero) then
  retvalue = retvalue + (zstep / prt%z) * &
    (D_alpha_s_isr ((one - prt%z) * prt%t, &
      shower%settings) * &
    P_prt_to_child1 (prt) * &
    shower%get_pdf (prt%initial%type, prt%child1%x / prt%z, &
      prt%t, prt%type)) / (abs(prt%t) * pdf_divisor)
end if
if (retvalue > final) then
  exit
else
  z = z + zstep
end if
end do ZLOOP
end subroutine integral_over_z_part_isr

```

This returns a pointer to the parton with the next ISR branching, again FSR branchings are ignored.

(Shower core: shower: TBP)+≡

```

  procedure :: generate_next_isr_branching => &
    shower_generate_next_isr_branching

```

(Shower core: procedures)+≡

```

  function shower_generate_next_isr_branching &
    (shower) result (next_brancher)

```

```

class(shower_t), intent(inout) :: shower
type(parton_pointer_t) :: next_brancher
integer i, index
type(parton_t), pointer :: prt
next_brancher%p => null()
do
  if (signal_is_pending ()) return
  if (shower_isr_is_finished (shower)) exit
  !!! find mother with highest |t| or pt to be simulated
  index = 0
  call shower%sort_partons ()
  do i = 1,size (shower%partons)
    prt => shower%partons(i)%p
    if (.not. associated (prt)) cycle
    if (.not. shower%settings%isr_pt_ordered) then
      if (prt%belongstointeraction) cycle
    end if
    if (prt%belongstoFSR) cycle
    if (prt%is_final ()) cycle
    if (.not. prt%belongstoFSR .and. prt%simulated) cycle
    index = i
    exit
  end do
  if (debug_active (D_SHOWER)) then
    if (index == 0) then
      call msg_fatal(" no branchable partons found")
    end if
  end if

  prt => shower%partons(index)%p

  !!! ISR simulation
  if (shower%settings%isr_pt_ordered) then
    call shower_isr_step_pt (shower, prt)
  else
    call shower_isr_step (shower, prt)
  end if
  if (prt%simulated) then
    if (prt%t < zero) then
      next_brancher%p => prt
      if (.not. shower%settings%isr_pt_ordered) &
        call prt%generate_ps_ini (shower%rng)
      exit
    else
      if (.not. shower%settings%isr_pt_ordered) then
        call shower_replace_parent_by_hadron (shower, prt%child1)
      else
        call shower_replace_parent_by_hadron (shower, prt)
      end if
    end if
  end if
end do

!!! some bookkeeping

```

```

    call shower%sort_partons ()
    call shower%boost_to_CMframe ()      !!! really necessary?
    call shower%rotate_to_z ()          !!! really necessary?
end function shower_generate_next_isr_branching

```

This is a loop which searches for all emitted and branched partons.

```

<Shower core: shower: TBP>+≡
    procedure :: generate_fsr_for_isr_partons => &
        shower_generate_fsr_for_partons_emitted_in_ISR

<Shower core: procedures>+≡
    subroutine shower_generate_fsr_for_partons_emitted_in_ISR (shower)
        class(shower_t), intent(inout) :: shower
        integer :: n_int, i
        type(parton_t), pointer :: prt
        if (shower%settings%isr_only_onshell_emitted_partons) return
        if (debug_on) call msg_debug (D_SHOWER, "shower_generate_fsr_for_partons_emitted_in_ISR")
        INTERACTIONS_LOOP: do n_int = 1, size (shower%interactions)
            INCOMING_PARTONS_LOOP: do i = 1, 2
                if (signal_is_pending ()) return
                prt => shower%interactions(n_int)%i%partons(i)%p
                PARENT_PARTONS_LOOP: do
                    if (associated (prt%parent)) then
                        if (.not. prt%parent%is_proton ()) then
                            prt => prt%parent
                        else
                            exit
                        end if
                    else
                        exit
                    end if
                    if (associated (prt%child2)) then
                        if (prt%child2%is_branched ()) then
                            call shower_parton_generate_fsr (shower, prt%child2)
                        end if
                    else
                        ! call msg_fatal ("Shower: no child2 associated?")
                    end if
                end do PARENT_PARTONS_LOOP
            end do INCOMING_PARTONS_LOOP
        end do INTERACTIONS_LOOP
    end subroutine shower_generate_fsr_for_partons_emitted_in_ISR

```

This executes the branching generated by `shower_generate_next_isr_branching`, that means it generates the flavors, momenta, etc.

```

<Shower core: shower: TBP>+≡
    procedure :: execute_next_isr_branching => shower_execute_next_isr_branching

<Shower core: procedures>+≡
    subroutine shower_execute_next_isr_branching (shower, prtp)
        class(shower_t), intent(inout) :: shower
        type(parton_pointer_t), intent(inout) :: prtp
        type(parton_t), pointer :: prt, otherprt
        type(parton_t), pointer :: prta, prtb, prtc, prtr

```



```

real(default) :: mbr
real(default) :: phirand
if (debug_on) call msg_debug (D_SHOWER, "shower_execute_next_isr_branching")
if (.not. associated (prtp%p)) then
    call msg_fatal ("Shower: prtp not associated")
end if

prt => prtp%p

if ((.not. shower%settings%isr_pt_ordered .and. &
    prt%t > - shower%settings%min_virtuality) .or. &
    (shower%settings%isr_pt_ordered .and. prt%scale < D_Min_scale)) then
    call msg_error ("Shower: no branching to be executed.")
end if

otherprt => shower%find_recoiler (prt)
if (shower%settings%isr_pt_ordered) then
    !!! get the recoiler
    otherprt => shower%find_recoiler (prt)
    if (associated (otherprt%parent)) then
        !!! Why only for pt ordered
        if (.not. otherprt%parent%is_proton () .and. &
            shower%settings%isr_pt_ordered) otherprt => otherprt%parent
    end if
    if (.not. associated (prt%parent)) then
        call shower%add_parent (prt)
    end if
    prt%parent%belongstoFSR = .false.
    if (.not. associated (prt%parent%child2)) then
        call shower%add_child (prt%parent, 2)
    end if

    prta => prt%parent          !!! new parton a with branching a->bc
    prtb => prt                 !!! former parton
    prtc => prt%parent%child2    !!! emitted parton
    prtr => otherprt            !!! recoiler

    mbr = (prtb%momentum + prtr%momentum)**1

    !!! 1. assume you are in the restframe
    !!! 2. rotate by random phi
    call shower%rng%generate (phirand)
    phirand = twopi * phirand
    call shower_apply_lorentztrafo (shower, &
        rotation(cos(phirand), sin(phirand), vector3_canonical(3)))
    !!! 3. Put the b off-shell
    !!! and
    !!! 4. construct the massless a
    !!! and the parton (eventually emitted by a)

    !!! generate the flavor of the parent (prta)
    if (prtb%aux_pt /= 0) prta%type = prtb%aux_pt
    if (prtb%is_quark ()) then
        if (prta%type == prtb%type) then

```

```

        !!! (anti)-quark -> (anti-)quark + gluon
        prta%type = prtb%type      ! quarks have same flavor
        prtc%type = GLUON          ! emitted gluon
    else
        !!! gluon -> quark + antiquark
        prta%type = GLUON
        prtc%type = - prtb%type
    end if
else if (prtb%is_gluon ()) then
    prta%type = GLUON
    prtc%type = GLUON
else
    ! STOP "Bug in shower_execute_next_branching: neither quark nor gluon"
end if

prta%initial => prtb%initial
prta%belongstoFSR = .false.
prta%scale = prtb%scale
prta%x = prtb%x / prtb%z

prtb%momentum = vector4_moving ((mbr**2 + prtb%t) / (two * mbr), &
    vector3_canonical(3) * &
    sign ((mbr**2 - prtb%t) / (two * mbr), &
    prtb%momentum%p(3)))
prtr%momentum = vector4_moving ((mbr**2 - prtb%t) / (two * mbr), &
    vector3_canonical(3) * &
    sign( (mbr**2 - prtb%t) / (two * mbr), &
    prtr%momentum%p(3)))

prta%momentum = vector4_moving ((0.5_default / mbr) * &
    ((mbr**2 / prtb%z) + prtb%t - prtc%mass_squared ()), &
    vector3_null)
prta%momentum = vector4_moving (prta%momentum%p(0), &
    vector3_canonical(3) * &
    (0.5_default / prtb%momentum%p(3)) * &
    ((mbr**2 / prtb%z) - two &
    * prtr%momentum%p(0) * prta%momentum%p(0) ) )
if (prta%momentum%p(0)**2 - prta%momentum%p(3)**2 - &
    prtc%mass_squared () > zero) then
    !!! This SHOULD be always fulfilled???
    prta%momentum = vector4_moving (prta%momentum%p(0), &
        vector3_moving([sqrt (prta%momentum%p(0)**2 - &
        prta%momentum%p(3)**2 - &
        prtc%mass_squared ()), zero, &
        prta%momentum%p(3)]))
end if
prtc%momentum = prta%momentum - prtb%momentum

!!! 5. rotate to have a along z-axis
call shower%boost_to_CMframe ()
call shower%rotate_to_z ()
!!! 6. rotate back in phi
call shower_apply_lorentztrafo (shower, rotation &
    (cos(-phirand), sin(-phirand), vector3_canonical(3)))

```

```

else
  if (prt%child2%t > prt%child2%mass_squared ()) then
    call shower_add_children_of_emitted_timelike_parton &
      (shower, prt%child2)
    call prt%child2%set_simulated ()
  end if

  call shower%add_parent (prt)
  call shower%add_child (prt%parent, 2)

  prt%parent%momentum = prt%momentum
  prt%parent%t = prt%t
  prt%parent%x = prt%x
  prt%parent%initial => prt%initial
  prt%parent%belongstoFSR = .false.

  prta => prt
  prtb => prt%child1
  prtc => prt%child2
end if
if (signal_is_pending ()) return
if (shower%settings%isr_pt_ordered) then
  call prt%parent%generate_ps_ini (shower%rng)
else
  call prt%generate_ps_ini (shower%rng)
end if

!!! add color connections
if (prtb%is_quark ()) then

  if (prta%type == prtb%type) then
    if (prtb%type > 0) then
      !!! quark -> quark + gluon
      prtc%c2 = prtb%c1
      prtc%c1 = shower%get_next_color_nr ()
      prta%c1 = prtc%c1
    else
      !!! antiquark -> antiquark + gluon
      prtc%c1 = prtb%c2
      prtc%c2 = shower%get_next_color_nr ()
      prta%c2 = prtc%c2
    end if
  else
    !!! gluon -> quark + antiquark
    if (prtb%type > 0) then
      !!! gluon -> quark + antiquark
      prta%c1 = prtb%c1
      prtc%c1 = 0
      prtc%c2 = shower%get_next_color_nr ()
      prta%c2 = prtc%c2
    else
      !!! gluon -> antiquark + quark
      prta%c2 = prtb%c2
      prtc%c1 = shower%get_next_color_nr ()

```

```

        prtc%c2 = 0
        prta%c1 = prtc%c1
    end if
end if
else if (prtb%is_gluon ()) then
    if (prta%is_gluon ()) then
        !!! g -> gg
        prtc%c2 = prtb%c1
        prtc%c1 = shower%get_next_color_nr ()
        prta%c1 = prtc%c1
        prta%c2 = prtb%c2
    else if (prta%is_quark ()) then
        if (prta%type > 0) then
            prta%c1 = prtb%c1
            prta%c2 = 0
            prtc%c1 = prtb%c2
            prtc%c2 = 0
        else
            prta%c1 = 0
            prta%c2 = prtb%c2
            prtc%c1 = 0
            prtc%c2 = prtb%c1
        end if
    end if
end if

call shower%sort_partons ()
call shower%boost_to_CMframe ()
call shower%rotate_to_z ()

end subroutine shower_execute_next_isr_branching

```

(Shower core: procedures) +=

```

subroutine shower_remove_parents_and_stuff (shower, prt)
    type(shower_t), intent(inout) :: shower
    type(parton_t), intent(inout), target :: prt
    type(parton_t), pointer :: actprt, nextprt
    nextprt => prt%parent
    actprt => null()
    !!! remove children of emitted timelike parton
    if (associated (prt%child2)) then
        if (associated (prt%child2%child1)) then
            call shower_remove_parton_from_partons_recursive &
                (shower, prt%child2%child1)
        end if
        prt%child2%child1 => null()
        if (associated (prt%child2%child2)) then
            call shower_remove_parton_from_partons_recursive &
                (shower, prt%child2%child2)
        end if
        prt%child2%child2 => null()
    end if
end if
do
    actprt => nextprt

```

```

        if (.not. associated (actprt)) then
            exit
        else if (actprt%is_proton ()) then
            !!! remove beam-remnant
            call shower_remove_parton_from_partons (shower, actprt%child2)
            exit
        end if
        if (associated (actprt%parent)) then
            nextprt => actprt%parent
        else
            nextprt => null()
        end if
        call shower_remove_parton_from_partons_recursive &
            (shower, actprt%child2)
        call shower_remove_parton_from_partons (shower, actprt)

    end do
    prt%parent=>null()

end subroutine shower_remove_parents_and_stuff

<Shower core: shower: TBP>+=
    procedure :: get_ISR_scale => shower_get_ISR_scale

<Shower core: procedures>+=
    function shower_get_ISR_scale (shower) result (scale)
        class(shower_t), intent(in) :: shower
        real(default) :: scale
        type(parton_t), pointer :: prt1, prt2
        integer :: i
        scale = zero
        do i = 1, size (shower%interactions)
            call interaction_find_partons_nearest_to_hadron &
                (shower%interactions(i)%i, prt1, prt2, &
                 shower%settings%isr_pt_ordered)
            if (.not. prt1%simulated .and. abs(prt1%scale) > scale) &
                scale = abs(prt1%scale)
            if (.not. prt1%simulated .and. abs(prt2%scale) > scale) &
                scale = abs(prt2%scale)
        end do
    end function shower_get_ISR_scale

<Shower core: shower: TBP>+=
    procedure :: set_max_isr_scale => shower_set_max_isr_scale

<Shower core: procedures>+=
    subroutine shower_set_max_isr_scale (shower, newscale)
        class(shower_t), intent(inout) :: shower
        real(default), intent(in) :: newscale
        real(default) :: scale
        type(parton_t), pointer :: prt
        integer :: i,j
        if (debug_on) call msg_debug (D_SHOWER, "shower_set_max_isr_scale: newscale", &
            newscale)

```

```

if (shower%settings%isr_pt_ordered) then
  scale = newscale
else
  scale = - abs (newscale)
end if

INTERACTIONS: do i = 1, size (shower%interactions)
  PARTONS: do j = 1, 2
    prt => shower%interactions(i)%i%partons(j)%p
    do
      if (.not. shower%settings%isr_pt_ordered) then
        if (prt%belongstointeraction) prt => prt%parent
      end if
      if (prt%t < scale) then
        if (associated (prt%parent)) then
          prt => prt%parent
        else
          exit   !!! unresolved prt found
        end if
      else
        exit   !!! prt with scale above newscale found
      end if
    end do
    if (.not. shower%settings%isr_pt_ordered) then
      if (prt%child1%belongstointeraction .or. &
        prt%is_proton ()) then
        !!! don't reset scales of "first" spacelike partons
        !!!   in virtuality ordered shower or hadrons
        cycle
      end if
    else
      if (prt%is_proton ()) then
        !!! don't reset scales of hadrons
        cycle
      end if
    end if
    if (shower%settings%isr_pt_ordered) then
      prt%scale = scale
    else
      prt%t = scale
    end if
    call prt%set_simulated (.false.)
    call shower_remove_parents_and_stuff (shower, prt)
  end do PARTONS
end do INTERACTIONS
end subroutine shower_set_max_isr_scale

```

<Shower core: shower: TBP>+≡

```

  procedure :: interaction_generate_fsr_2ton => &
    shower_interaction_generate_fsr_2ton

```

<Shower core: procedures>+≡

```

  subroutine shower_interaction_generate_fsr_2ton (shower, interaction)
    class(shower_t), intent(inout) :: shower

```

```

type(shower_interaction_t), intent(inout) :: interaction
type(parton_t), pointer :: prt
prt => interaction%partons(3)%p
do
  if (.not. associated (prt%parent)) exit
  prt => prt%parent
end do
call shower_parton_generate_fsr (shower, prt)
call shower_parton_update_color_connections (shower, prt)
end subroutine shower_interaction_generate_fsr_2ton

```

Perform the FSR for one parton, it is assumed, that the parton already branched. Hence, its children are to be simulated. This procedure is intended for branched FSR-partons emitted in the ISR.

(Shower core: procedures)+≡

```

subroutine shower_parton_generate_fsr (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), intent(inout), target :: prt
  type(parton_pointer_t), dimension(:), allocatable :: partons
  logical :: single_emission = .false.
  if (debug_on) call msg_debug (D_SHOWER, "shower_parton_generate_fsr")
  if (signal_is_pending ()) return
  if (debug_active (D_SHOWER)) then
    if (.not. prt%is_branched ()) then
      call msg_error ("shower_parton_generate_fsr: parton not branched")
      return
    end if
    if (prt%child1%simulated .or. &
      prt%child2%simulated) then
      print *, "children already simulated for parton ", prt%nr
      return
    end if
  end if
  allocate (partons(1))
  partons(1)%p => prt
  if (single_emission) then
    call shower%parton_pointer_array_generate_fsr (partons, partons)
  else
    call shower%parton_pointer_array_generate_fsr_recursive (partons)
  end if
end subroutine shower_parton_generate_fsr

```

(Shower core: shower: TBP)+≡

```

procedure :: parton_pointer_array_generate_fsr_recursive => &
  shower_parton_pointer_array_generate_fsr_recursive

```

(Shower core: procedures)+≡

```

recursive subroutine shower_parton_pointer_array_generate_fsr_recursive &
  (shower, partons)
  class(shower_t), intent(inout) :: shower
  type(parton_pointer_t), dimension(:), allocatable, intent(inout) :: &
    partons
  type(parton_pointer_t), dimension(:), allocatable :: partons_new

```

```

        if (debug_on) call msg_debug (D_SHOWER, "shower_parton_pointer_array_generate_fsr_recursive"
        if (signal_is_pending ()) return
        if (size (partons) == 0) return
        call shower%parton_pointer_array_generate_fsr (partons, partons_new)
        call shower%parton_pointer_array_generate_fsr_recursive (partons_new)
    end subroutine shower_parton_pointer_array_generate_fsr_recursive

    <Shower core: shower: TBP>+≡
    procedure :: parton_pointer_array_generate_fsr => &
        shower_parton_pointer_array_generate_fsr

    <Shower core: procedures>+≡
    subroutine shower_parton_pointer_array_generate_fsr &
        (shower, partons, partons_new)
    class(shower_t), intent(inout) :: shower
    type(parton_pointer_t), dimension(:), allocatable, intent(inout) :: &
        partons
    type(parton_pointer_t), dimension(:), allocatable, intent(out) :: &
        partons_new
    integer :: i, size_partons, size_partons_new
    if (debug_on) call msg_debug (D_SHOWER, "shower_parton_pointer_array_generate_fsr")
    !!! Simulate highest/first parton
    call shower_simulate_children_ana (shower, partons(1)%p)
    !!! check for new daughters to be included in new_partons
    size_partons = size (partons)
    size_partons_new = size_partons - 1    !!! partons(1) not needed anymore
    if (partons(1)%p%child1%is_branched ()) &
        size_partons_new = size_partons_new + 1
    if (partons(1)%p%child2%is_branched ()) &
        size_partons_new = size_partons_new + 1

    allocate (partons_new (1:size_partons_new))

    if (size_partons > 1) then
        do i = 2, size_partons
            partons_new (i - 1)%p => partons(i)%p
        end do
    end if
    if (partons(1)%p%child1%is_branched ()) &
        partons_new (size_partons)%p => partons(1)%p%child1
    if (partons(1)%p%child2%is_branched ()) then
        !!! check if child1 is already included
        if (size_partons_new == size_partons) then
            partons_new (size_partons)%p => partons(1)%p%child2
        else if (size_partons_new == size_partons + 1) then
            partons_new (size_partons + 1)%p => partons(1)%p%child2
        else
            call msg_fatal ("Shower: wrong sizes in" &
                // "shower_parton_pointer_array_generate_fsr")
        end if
    end if
    deallocate (partons)

end subroutine shower_parton_pointer_array_generate_fsr

```



```

(Shower core: procedures)+≡
recursive subroutine shower_parton_update_color_connections &
  (shower, prt)
  type(shower_t), intent(inout) :: shower
  type(parton_t), intent(inout) :: prt
  real(default) :: temprand
  if (.not. associated (prt%child1) .or. &
      .not. associated (prt%child2)) return

  if (signal_is_pending ()) return
  if (prt%is_gluon ()) then
    if (prt%child1%is_quark ()) then
      !!! give the quark the colorpartner and the antiquark
      !!! the anticolorpartner
      if (prt%child1%type > 0) then
        !!! child1 is quark, child2 is antiquark
        prt%child1%c1 = prt%c1
        prt%child2%c2 = prt%c2
      else
        !!! child1 is antiquark, child2 is quark
        prt%child1%c2 = prt%c2
        prt%child2%c1 = prt%c1
      end if
    else
      !!! g -> gg splitting -> random choosing of partners
      call shower%rng%generate (temprand)
      if (temprand > 0.5_default) then
        prt%child1%c1 = prt%c1
        prt%child1%c2 = shower%get_next_color_nr ()
        prt%child2%c1 = prt%child1%c2
        prt%child2%c2 = prt%c2
      else
        prt%child1%c2 = prt%c2
        prt%child2%c1 = prt%c1
        prt%child2%c2 = shower%get_next_color_nr ()
        prt%child1%c1 = prt%child2%c2
      end if
    end if
  else if (prt%is_quark ()) then
    if (prt%child1%is_quark ()) then
      if (prt%child1%type > 0) then
        !!! q -> q + g
        prt%child2%c1 = prt%c1
        prt%child2%c2 = shower%get_next_color_nr ()
        prt%child1%c1 = prt%child2%c2
      else
        !!! qbar -> qbar + g
        prt%child2%c2 = prt%c2
        prt%child2%c1 = shower%get_next_color_nr ()
        prt%child1%c2 = prt%child2%c1
      end if
    else
      if (prt%child2%type > 0) then
        !!! q -> g + q

```

```

        prt%child1%c1 = prt%c1
        prt%child1%c2 = shower%get_next_color_nr ()
        prt%child2%c1 = prt%child1%c2
    else
        !!! qbar -> g + qbar
        prt%child1%c2 = prt%c2
        prt%child1%c1 = shower%get_next_color_nr ()
        prt%child2%c2 = prt%child1%c1
    end if
end if
end if

call shower_parton_update_color_connections (shower, prt%child1)
call shower_parton_update_color_connections (shower, prt%child2)
end subroutine shower_parton_update_color_connections

```

The next two routines are for PDFs. Wrapper function to return parton densities.

```

<Shower core: shower: TBP>+≡
    procedure :: get_pdf => shower_get_pdf

<Shower core: procedures>+≡
    function shower_get_pdf (shower, mother, x, Q2, daughter) result (pdf)
        <get pdf>
        if (x > eps0) then
            pdf = pdf / x
        end if
    end function shower_get_pdf

<Shower core: shower: TBP>+≡
    procedure :: get_xpdf => shower_get_xpdf

<Shower core: procedures>+≡
    function shower_get_xpdf (shower, mother, x, Q2, daughter) result (pdf)
        <get pdf>
    end function shower_get_xpdf

<get pdf>≡
    class(shower_t), intent(inout), target :: shower
    integer, intent(in) :: mother, daughter
    real(default), intent(in) :: x, Q2
    real(default) :: pdf
    real(double), save :: f(-6:6) = 0._double
    real(double), save :: lastx, lastQ2 = 0._double
    pdf = zero
    if (debug_active (D_SHOWER)) then
        if (abs (mother) /= PROTON) then
            if (debug_on) call msg_debug (D_SHOWER, "mother", mother)
            call msg_fatal ("Shower: pdf only implemented for (anti-)proton")
        end if
        if (.not. (abs (daughter) >= 1 .and. abs (daughter) <= 6 .or. &
            daughter == GLUON)) then
            if (debug_on) call msg_debug (D_SHOWER, "daughter", daughter)
            call msg_fatal ("Shower: error in pdf, unknown daughter")
        end if
    end if

```

```

        end if
    end if
    if (x > zero .and. x < one) then
        if ((dble(Q2) - lastQ2) > eps0 .or. (dble(x) - lastx) > eps0) then
            call shower%pdf_data%evolve &
                (dble(x), sqrt (abs (dble(Q2))), f)
        end if
        if (abs (daughter) >= 1 .and. abs (daughter) <= 6) then
            pdf = max (f(daughter * sign (1,mother)), tiny_10)
        else
            pdf = max (f(0), tiny_10)
        end if
    end if
    lastQ2 = dble(Q2)
    lastx = dble(x)

```

Convert Whizard shower to Pythia6. Currently only works for one interaction.

```

<Shower core: shower: TBP>+≡
    procedure :: converttopythia => shower_converttopythia

<Shower core: procedures>+≡
    subroutine shower_converttopythia (shower)
        class(shower_t), intent(in) :: shower
        <PYJETS COMMON BLOCK>
        type(parton_t), pointer :: pp, ppparent
        integer :: i
        K = 0
        do i = 1, 2
            !!! get history of the event
            pp => shower%interactions(1)%i%partons(i)%p
            !!! add these partons to the event record
            if (associated (pp%initial)) then
                !!! add hadrons
                K(i,1) = 21
                K(i,2) = pp%initial%type
                K(i,3) = 0
                P(i,1:5) = pp%initial%momentum_to_pythia6 ()
                !!! add partons emitted by the hadron
                ppparent => pp
                do while (associated (ppparent%parent))
                    if (ppparent%parent%is_proton ()) then
                        exit
                    else
                        ppparent => ppparent%parent
                    end if
                end do
                K(i+2,1) = 21
                K(i+2,2) = ppparent%type
                K(i+2,3) = i
                P(i+2,1:5) = ppparent%momentum_to_pythia6 ()
                !!! add partons in the initial state of the ME
                K(i+4,1) = 21
                K(i+4,2) = pp%type
                K(i+4,3) = i
                P(i+4,1:5) = pp%momentum_to_pythia6 ()
            end if
        end do
    end subroutine

```

```

else
  !!! for e+e- without ISR all entries are the same
  K(i,1) = 21
  K(i,2) = pp%type
  K(i,3) = 0
  P(i,1:5) = pp%momentum_to_pythia6 ()
  P(i+2,:) = P(1,:)
  K(i+2,:) = K(1,:)
  K(i+2,3) = i
  P(i+4,:) = P(1,:)
  K(i+4,:) = K(1,:)
  K(i+4,3) = i
  P(i+4,5) = 0.
end if
end do
N = 6
!!! create intermediate (fake) Z-Boson
!K(7,1) = 21
!K(7,2) = 23
!K(7,3) = 0
!P(7,1:4) = P(5,1:4) + P(6,1:4)
!P(7,5) = P(7,4)**2 - P(7,3)**2 - P(7,2)**2 - P(7,1)**2
!N = 7
!!! include partons in the final state of the hard matrix element
do i = 1, size (shower%interactions(1)%i%partons) - 2
  !!! get partons that are in the final state of the hard matrix element
  pp => shower%interactions(1)%i%partons(2+i)%p
  !!! add these partons to the event record
  K(7+I,1) = 21
  K(7+I,2) = pp%type
  K(7+I,3) = 7
  P(7+I,1:5) = pp%momentum_to_pythia6 ()
  !N = 7 + I
  N = 6 + I
end do
!!! include "Z" (again)
!N = N + 1
!K(N,1) = 11
!K(N,2) = 23
!K(N,3) = 7
!P(N,1:5) = P(7,1:5)
!nz = N
!!! include partons from the final state of the parton shower
call shower_transfer_final_partons_to_pythia (shower, 8)
!!! set "children" of "Z"
!K(nz,4) = 11
!K(nz,5) = N

!!! be sure to remove the next partons (=first obsolete partons)
!!! otherwise they might be interpreted as thrust information
K(N+1:N+3,1:3) = 0
end subroutine shower_converttopythia

```

(Shower core: procedures) +=

```

subroutine shower_transfer_final_partons_to_pythia (shower, first)
<PYJETS COMMON BLOCK>
  type(shower_t), intent(in) :: shower
  integer, intent(in) :: first
  type(parton_t), pointer :: prt
  integer :: i, j, n_finals
  type(parton_t), dimension(:), allocatable :: final_partons
  type(parton_t) :: temp_parton
  integer :: minindex, maxindex

  prt => null()

  !!! get total number of final partons
  n_finals = 0
  do i = 1, size (shower%partons)
    if (.not. associated (shower%partons(i)%p)) cycle
    prt => shower%partons(i)%p
    if (.not. prt%belongstoFSR) cycle
    if (associated (prt%child1)) cycle
    n_finals = n_finals + 1
  end do

  allocate (final_partons(1:n_finals))
  j = 1
  do i = 1, size (shower%partons)
    if (.not. associated (shower%partons(i)%p)) cycle
    prt => shower%partons(i)%p
    if (.not. prt%belongstoFSR) cycle
    if (associated (prt%child1)) cycle
    final_partons(j) = shower%partons(i)%p
    j = j + 1
  end do

  !!! move quark to front as beginning of color string
  minindex = 1
  maxindex = size (final_partons)
  FIND_Q: do i = minindex, maxindex
    if (final_partons(i)%type >= 1 .and. final_partons(i)%type <= 6) then
      temp_parton = final_partons(minindex)
      final_partons(minindex) = final_partons(i)
      final_partons(i) = temp_parton
      exit FIND_Q
    end if
  end do FIND_Q

  !!! sort so that connected partons are next to each other, don't care about zeros
  do i = 1, size (final_partons)
    !!! ensure that final_partons begins with a color (not an anticolor)
    if (final_partons(i)%c1 > 0 .and. final_partons(i)%c2 == 0) then
      if (i == 1) then
        exit
      else
        temp_parton = final_partons(1)
        final_partons(1) = final_partons(i)

```

```

        final_partons(i) = temp_parton
        exit
    end if
end if
end do

do i = 1, size (final_partons) - 1
    !!! search for color partner and move it to i + 1
    PARTNERS: do j = i + 1, size (final_partons)
        if (final_partons(j)%c2 == final_partons(i)%c1) exit PARTNERS
    end do PARTNERS
    if (j > size (final_partons)) then
        print *, "no color connected parton found" !WRONG???
        print *, "particle: ", final_partons(i)%nr, " index: ", &
            final_partons(i)%c1
        exit
    end if
    temp_parton = final_partons(i + 1)
    final_partons(i + 1) = final_partons(j)
    final_partons(j) = temp_parton
end do

!!! transferring partons
do i = 1, size (final_partons)
    prt = final_partons(i)
    N = N + 1
    K(N,1) = 2
    if (prt%c1 == 0) K(N,1) = 1          !!! end of color string
    K(N,2) = prt%type
    !K(N,3) = first
    K(N,3) = 0
    K(N,4) = 0
    K(N,5) = 0
    P(N,1:5) = prt%momentum_to_pythia6()
end do
deallocate (final_partons)
end subroutine shower_transfer_final_partons_to_pythia

```

22.4 Interface to PYTHIA 6

*<shower_pythia6.f90>≡
<File header>*

module shower_pythia6

<Use kinds with double>

<Use strings>

<Use debug>

use constants

use numeric_utils, only: vanishes

use io_units

use physics_defs

```

    use diagnostics
    use os_interface
    use lorentz
    use subevents
    use shower_base
    use particles
    use model_data
    use hep_common
    use pdf
    use helicities
    use tauola_interface

    <Standard module head>

    <Shower pythia6: public>
    <Shower pythia6: variables>
    <Shower pythia6: types>

    contains

    <Shower pythia6: procedures>

    end module shower_pythia6

    <PYJETS COMMON BLOCK>≡
    integer :: N, NPAD, K
    real(double) :: P, V
    COMMON/PYJETS/N,NPAD,K(4000,5),P(4000,5),V(4000,5)
    SAVE /PYJETS/

    <Shower pythia6: variables>≡
    integer :: N_old

```

The PYTHIA6 shower type.

```

    <Shower pythia6: public>≡
    public :: shower_pythia6_t

    <Shower pythia6: types>≡
    type, extends (shower_base_t) :: shower_pythia6_t
    integer :: initialized_for_NPRUP = 0
    logical :: warning_given = .false.
    contains
    <Shower pythia6: shower pythia6: TBP>
    end type shower_pythia6_t

```

Initialize the PYTHIA6 shower.

```

    <Shower pythia6: shower pythia6: TBP>≡
    procedure :: init => shower_pythia6_init

    <Shower pythia6: procedures>≡
    subroutine shower_pythia6_init (shower, settings, taudec_settings, pdf_data, os_data)
    class(shower_pythia6_t), intent(out) :: shower
    type(shower_settings_t), intent(in) :: settings
    type(taudec_settings_t), intent(in) :: taudec_settings

```

```

type(pdf_data_t), intent(in) :: pdf_data
type(os_data_t), intent(in) :: os_data
if (debug_on) call msg_debug (D_SHOWER, "shower_pythia6_init")
shower%settings = settings
shower%taudec_settings = taudec_settings
shower%os_data = os_data
call pythia6_set_verbose (settings%verbose)
call shower%pdf_data%init (pdf_data)
shower%name = "PYTHIA6"
call shower%write_msg ()
end subroutine shower_pythia6_init

```

<Shower pythia6: shower pythia6: TBP>+≡

```

procedure :: import_particle_set => shower_pythia6_import_particle_set

```

<Shower pythia6: procedures>+≡

```

subroutine shower_pythia6_import_particle_set &
  (shower, particle_set)
class(shower_pythia6_t), target, intent(inout) :: shower
type(particle_set_t), intent(in) :: particle_set
type(particle_set_t) :: pset_reduced
if (debug_on) call msg_debug (D_SHOWER, "shower_pythia6_import_particle_set")
if (debug_active (D_SHOWER)) then
  print *, 'IDBMUP(1:2) = ', IDBMUP(1:2)
  print *, 'EBMUP, PDFGUP = ', EBMUP, PDFGUP
  print *, 'PDFSUP, IDWTUP = ', PDFSUP, IDWTUP
  print *, "NPRUP = ", NPRUP
  call particle_set%write (summary=.true., compressed=.true.)
end if
call particle_set%reduce (pset_reduced)
if (debug2_active (D_SHOWER)) then
  print *, 'After particle_set%reduce: pset_reduced'
  call pset_reduced%write (summary=.true., compressed=.true.)
end if
call hepeup_from_particle_set (pset_reduced, tauola_convention=.true.)
call hepeup_set_event_parameters (proc_id = 1)
call hepeup_set_event_parameters (scale = shower%fac_scale)
end subroutine shower_pythia6_import_particle_set

```

<Shower pythia6: shower pythia6: TBP>+≡

```

procedure :: generate_emissions => shower_pythia6_generate_emissions

```

<Shower pythia6: procedures>+≡

```

subroutine shower_pythia6_generate_emissions &
  (shower, valid, number_of_emissions)
IMPLICIT DOUBLE PRECISION(A-H, O-Z)
IMPLICIT INTEGER(I-N)
COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
SAVE/PYDAT1/
class(shower_pythia6_t), intent(inout), target :: shower
logical, intent(out) :: valid
integer, optional, intent(in) :: number_of_emissions
integer :: N, NPAD, K
real(double) :: P, V

```



```

common /PYJETS/ N, NPAD, K(4000,5), P(4000,5), V(4000,5)
COMMON/PYDAT2/KCHG(500,4),PMAS(500,4),PARF(2000),VCKM(4,4)
COMMON/PYINT4/MWID(500),WIDS(500,5)
save /PYJETS/,/PYDAT2/,/PYINT4/
integer :: u_W2P
integer :: i
real(double) :: beta_z, pz_in, E_in
integer, parameter :: lower = 5
real(double), parameter :: beta_x = 0.0_double
real(double), parameter :: beta_y = 0.0_double
real(double), parameter :: theta = 0.0_double
real(double), parameter :: phi = 0.0_double
if (signal_is_pending ()) return
call pythia6_setup_lhe_io_units (u_W2P)
call w2p_write_lhef_event (u_W2P)
rewind (u_W2P)
call pythia6_set_last_treated_line(6)
call shower%transfer_settings ()
if (debug_active (D_SHOWER)) then
  print *, ' Before pyevnt, before boosting :'
  call pylist(2)
end if
if (debug_on) call msg_debug (D_SHOWER, "calling pyevnt")
! TODO: (bcn 2015-04-24) doesnt change anything I think
! P(1,1:5) = pset_reduced%prt(1)%momentum_to_pythia6 ()
! P(2,1:5) = pset_reduced%prt(2)%momentum_to_pythia6 ()
call pyevnt ()
call pyedit(12)
do i = 1, n
  if (K(i,1) == 14 .and. abs(K(i,2)) >= 11 .and. abs(K(i,2)) <= 16) then
    if (K(i,4) > 0 .and. K(i,5) > 0 .and. K(i,4) < N .and. K(i,5) < N) then
      K(i,1) = 11
      K(i,4) = K(K(i,4),3)
      K(i,5) = K(K(i,5),3)
    end if
  end if
end do
if (.not. shower%settings%hadron_collision) then
  pz_in = pup(3,1) + pup(3,2)
  E_in = pup(4,1) + pup(4,2)
  beta_z = pz_in / E_in
  call pyrobo (lower, N, theta, phi, beta_x, beta_y, beta_z)
end if
if (debug_active (D_SHOWER)) then
  print *, ' After pyevnt, after boosting :'
  call pylist(2)
  if (debug2_active (D_SHOWER)) then
    call pystat (5)
    do i = 1, 200
      print *, 'MSTJ (', i, ') = ', MSTJ(i)
      print *, 'MSTU (', i, ') = ', MSTU(i)
      print *, 'PMAS (', i, ') = ', PMAS(i,1), PMAS(i,2)
      print *, 'MWID (', i, ') = ', MWID(i)
      print *, 'PARJ (', i, ') = ', PARJ(i)
    end do
  end if
end if

```

```

        end do
      end if
    end if
    close (u_W2P)
    valid = pythia6_handle_errors ()
  end subroutine shower_pythia6_generate_emissions

```

```

<Shower pythia6: shower pythia6: TBP>+≡
  procedure :: make_particle_set => shower_pythia6_make_particle_set

```

```

<Shower pythia6: procedures>+≡
  subroutine shower_pythia6_make_particle_set &
    (shower, particle_set, model, model_hadrons)
    class(shower_pythia6_t), intent(in) :: shower
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    class(model_data_t), intent(in), target :: model_hadrons
    call shower%combine_with_particle_set (particle_set, model, model_hadrons)
  end subroutine shower_pythia6_make_particle_set

```

```

<Shower pythia6: shower pythia6: TBP>+≡
  procedure :: transfer_settings => shower_pythia6_transfer_settings

```

```

<Shower pythia6: procedures>+≡
  subroutine shower_pythia6_transfer_settings (shower)
    class(shower_pythia6_t), intent(inout) :: shower
    character(len=10) :: buffer
    real(default) :: rand
    logical, save :: tauola_initialized = .false.
    if (debug_on) call msg_debug (D_SHOWER, "shower_pythia6_transfer_settings")
    !!! We repeat these as they are overwritten by the hadronization
    call pygive ("MSTP(111)=1")      !!! Allow hadronization and decays
    call pygive ("MSTJ(1)=0")       !!! No jet fragmentation
    call pygive ("MSTJ(21)=1")      !!! Allow decays but no jet fragmentation

    if (shower%initialized_for_NPRUP >= NPRUP) then
      if (debug_on) call msg_debug (D_SHOWER, "calling upinit")
      call upinit ()
    else
      if (shower%settings%isr_active) then
        call pygive ("MSTP(61)=1")
      else
        call pygive ("MSTP(61)=0") !!! switch off ISR
      end if
      if (shower%settings%fsr_active) then
        call pygive ("MSTP(71)=1")
      else
        call pygive ("MSTP(71)=0") !!! switch off FSR
      end if
      call pygive ("MSTP(11)=0")     !!! Disable Pythias QED-ISR per default
      call pygive ("MSTP(171)=1")    !!! Allow variable energies

      write (buffer, "(F10.5)") sqrt (abs (shower%settings%min_virtuality))
      call pygive ("PARJ(82)=" // buffer)
    end if
  end subroutine shower_pythia6_transfer_settings

```

```

write (buffer, "(F10.5)") shower%settings%isr_tscalefactor
call pygive ("PARP(71)=" // buffer)
write (buffer, "(F10.5)") shower%settings%fsr_lambda
call pygive ("PARP(72)=" // buffer)
write(buffer, "(F10.5)") shower%settings%isr_lambda
call pygive ("PARP(61)=" // buffer)
write (buffer, "(I10)") shower%settings%max_n_flavors
call pygive ("MSTJ(45)=" // buffer)
if (shower%settings%isr_alphas_running) then
  call pygive ("MSTP(64)=2")
else
  call pygive ("MSTP(64)=0")
end if
if (shower%settings%fsr_alphas_running) then
  call pygive ("MSTJ(44)=2")
else
  call pygive ("MSTJ(44)=0")
end if
write (buffer, "(F10.5)") shower%settings%fixed_alpha_s
call pygive ("PARU(111)=" // buffer)
write (buffer, "(F10.5)") shower%settings%isr_primordial_kt_width
call pygive ("PARP(91)=" // buffer)
write (buffer, "(F10.5)") shower%settings%isr_primordial_kt_cutoff
call pygive ("PARP(93)=" // buffer)
write (buffer, "(F10.5)") 1._double - shower%settings%isr_z_cutoff
call pygive ("PARP(66)=" // buffer)
write (buffer, "(F10.5)") shower%settings%isr_minenergy
call pygive ("PARP(65)=" // buffer)
if (shower%settings%isr_only_onshell_emitted_partons) then
  call pygive ("MSTP(63)=0")
else
  call pygive ("MSTP(63)=2")
end if
if (shower%settings%mlm_matching) then
  call pygive ("MSTP(62)=2")
  call pygive ("MSTP(67)=0")
end if
call pythia6_set_config (shower%settings%pythia6_pygive)
if (debug_on) call msg_debug (D_SHOWER, "calling pyinit")
call PYINIT ("USER", "", "", ODO)
call shower%rng%generate (rand)
write (buffer, "(I10)") floor (rand*900000000)
call pygive ("MRPY(1)=" // buffer)
call pygive ("MRPY(2)=0")
call pythia6_set_config (shower%settings%pythia6_pygive)
shower%initialized_for_NPRUP = NPRUP
end if
if (shower%settings%tau_dec) then
  call pygive ("MSTJ(28)=2")
end if
if (pythia6_tauola_active() .and. .not. tauola_initialized) then
  call wo_tauola_init_call (shower%tauddec_settings)
  tauola_initialized = .true.
end if

```

```
end subroutine shower_pythia6_transfer_settings
```

<Shower pythia6: shower pythia6: TBP>+≡

```
procedure :: combine_with_particle_set => &
    shower_pythia6_combine_with_particle_set
```

<Shower pythia6: procedures>+≡

```
subroutine shower_pythia6_combine_with_particle_set &
    (shower, particle_set, model_in, model_hadrons)
class(shower_pythia6_t), intent(in) :: shower
type(particle_set_t), intent(inout) :: particle_set
class(model_data_t), intent(in), target :: model_in
class(model_data_t), intent(in), target :: model_hadrons
call pythia6_combine_with_particle_set &
    (particle_set, model_in, model_hadrons, shower%settings)
end subroutine shower_pythia6_combine_with_particle_set
```

K(I,1) pythia status code

1 = undecayed particle or unfragmented parton
 (single or last of parton system)
 2 = unfragmented parton
 (followed by more partons in the same color singlet)
 3 = unfragmented parton (color info in K(I,4), K(I,5))
 11 = decayed particle or fragmented parton
 12 = fragmented parton
 13 = fragmented parton that has been removed
 14 = branched parton with color info like 3
 21 = documentation lines

The first two

K(I,2) PDG code

K(I,3) Parent where known else 0. Unphysical to assign
 particles partons as parents

K(I,4) Normally first daughter

K(I,5) Normally last daughter

particles are always the beams, in Pythia and Whizard. We remove all beam remnants (including the ISR photons) since those are added back in by Pythia.

<Shower pythia6: public>+≡

```
public :: pythia6_combine_with_particle_set
```

<Shower pythia6: procedures>+≡

```
subroutine pythia6_combine_with_particle_set (particle_set, model_in, &
    model_hadrons, settings)
type(particle_set_t), intent(inout) :: particle_set
class(model_data_t), intent(in), target :: model_in
class(model_data_t), intent(in), target :: model_hadrons
type(shower_settings_t), intent(in) :: settings
class(model_data_t), pointer :: model
type(vector4_t) :: momentum
type(particle_t), dimension(:), allocatable :: particles, beams
integer :: dangling_col, dangling_anti_col, color, anti_color
integer :: i, j, py_entries, next_color, n_tot_old, parent, real_parent
integer :: pdg, status, child, hadro_start, i_py, i_whz
integer, allocatable, dimension(:) :: py_index, whz_index
logical, allocatable, dimension(:) :: valid
```

```

real(default), parameter :: py_tiny = 1E-10_default
integer :: N, NPAD, K
real(double) :: P, V
common /PYJETS/ N, NPAD, K(4000,5), P(4000,5), V(4000,5)
save /PYJETS/
integer, parameter :: KSUSY1 = 1000000, KSUSY2 = 2000000

if (signal_is_pending ()) return
if (debug_active (D_SHOWER)) then
  call msg_debug (D_SHOWER, 'Combine PYTHIA6 with particle set')
  call msg_debug (D_SHOWER, 'Particle set before replacing')
  call particle_set%write (summary=.true., compressed=.true.)
  call pylist (3)
  call msg_debug (D_SHOWER, string = "settings%hadron_collision", &
    value = settings%hadron_collision)
end if
if (settings%method == PS_PYTHIA6 .and. settings%hadron_collision) then
  call pythia6_set_last_treated_line(2)
  allocate (beams(2))
  beams = particle_set%prt(1:2)
  call particle_set%replace (beams)
  if (debug_active (D_SHOWER)) then
    call msg_debug (D_SHOWER, 'Resetting particle set to')
    call particle_set%write (summary=.true., compressed=.true.)
  end if
end if
call fill_hepevt_block_from_pythia ()
call count_valid_entries_in_pythia_record ()
call particle_set%without_hadronic_remnants &
  (particles, n_tot_old, py_entries)
if (debug_active (D_SHOWER)) then
  print *, 'n_tot_old = ', n_tot_old
  print *, 'py_entries = ', py_entries
end if
call add_particles_of_pythia ()
call particle_set%replace (particles)
if (settings%hadron_collision) then
  call set_parent_child_relations_from_K ()
  call set_parent_child_relations_of_color_strings_to_hadrons ()
  !!! call particle_set%remove_duplicates (py_tiny * 100.0_default)
else
  call set_parent_child_relations_from_hepevt ()
end if
!call fix_nonemitting_outgoings ()
if (settings%method == PS_WHIZARD) then
  call fudge_whizard_partons_in_hadro ()
end if
where ((particle_set%prt%status == PRT_OUTGOING .or. &
  particle_set%prt%status == PRT_VIRTUAL .or. &
  particle_set%prt%status == PRT_BEAM_REMNANT) .and. &
  particle_set%prt%has_children ()) &
  particle_set%prt%status = PRT_RESONANT
if (debug_active (D_SHOWER)) then
  print *, 'Particle set after replacing'

```

```

        call particle_set%write (summary=.true., compressed=.true.)
        print *, ' pythia6_set_last_treated_line will set to: ', N
    end if
    call pythia6_set_last_treated_line(N)

```

contains

<Shower pythia6: combine with particle set: procedures>

end subroutine pythia6_combine_with_particle_set

<Shower pythia6: combine with particle set: procedures>≡

```

subroutine count_valid_entries_in_pythia_record ()
<HEPEVT BLOCK>
    integer :: pset_idx
    logical :: comes_from_cmshower, emitted_zero_momentum_photon, &
        direct_decendent
    integer, parameter :: cmshower = 94
    hadro_start = 0
    allocate (valid(N))
    valid = .false.
    FIND: do i_py = 5, N
        !if (K(i_py,2) >= 91 .and. K(i_py,2) <= 94) then
        if (K(i_py,2) >= 91 .and. K(i_py,2) <= 93) then
            hadro_start = i_py
            exit FIND
        end if
    end do FIND
    do i_py = N, N_old+1, -1
        status = K(i_py,1)
        if (any (P(i_py,1:4) > 1E-8_default * P(1,4)) .and. &
            (status >= 1 .and. status <= 21)) then
            pset_idx = find_pythia_particle (i_py, more_fuzzy=.false.)
            direct_decendent = IDHEP(JMOHEP(1,i_py)) == cmshower .and. &
                JMOHEP(2,i_py) == 0
            emitted_zero_momentum_photon = find_pythia_particle &
                (JMOHEP(1,i_py), more_fuzzy=.false.) == pset_idx
            comes_from_cmshower = status == 1 .and. &
                (direct_decendent .or. emitted_zero_momentum_photon)
            valid(i_py) = pset_idx == 0 .or. comes_from_cmshower
        end if
    end do
    py_entries = count (valid)
    allocate (py_index (py_entries))
    allocate (whz_index (N))
    whz_index = 0
end subroutine count_valid_entries_in_pythia_record

```

<Shower pythia6: combine with particle set: procedures>+≡

```

subroutine add_particles_of_pythia ()
    integer :: whizard_status
    integer :: pset_idx, start_in_py
    integer :: ihelicity

```

```

type(helicity_t) :: hel
real(default) :: lifetime
type(vector4_t) :: vertex
dangling_col = 0
dangling_anti_col = 0
next_color = 500
i_whz = 1
if (settings%method == PS_PYTHIA6 .and. settings%hadron_collision) then
    start_in_py = 3
else
    start_in_py = 7
end if
do i_py = start_in_py, N
    status = K(i_py,1)
    if (valid(i_py)) then
        call assign_colors (color, anti_color)
        momentum = real ([P(i_py,4), P(i_py,1:3)], kind=default)
        pdg = K(i_py,2)
        parent = K(i_py,3)
        call find_model (model, pdg, model_in, model_hadrons)
        if (i_py <= 4) then
            whizard_status = PRT_INCOMING
        else
            if (status <= 10) then
                whizard_status = PRT_OUTGOING
            else
                whizard_status = PRT_VIRTUAL
            end if
        end if
        call particles(n_tot_old+i_whz)%init &
            (whizard_status, pdg, model, color, anti_color, momentum)
        lifetime = V(i_py,5)
        vertex = [real (V(i_py,4), kind=default), &
            real (V(i_py,1), kind=default), &
            real (V(i_py,2), kind=default), &
            real (V(i_py,3), kind=default)]
        if (.not. vanishes(lifetime)) &
            call particles(n_tot_old+i_whz)%set_lifetime (lifetime)
        if (any (.not. vanishes(real(V(i_py,1:4), kind = default)))) &
            call particles(n_tot_old+i_whz)%set_vertex (vertex)
        !!! Set tau helicity set by TAUOLA
        if (abs (pdg) == 15) then
            call wo_tauola_get_helicity (i_py, ihelicity)
            call hel%init (ihelicity)
            call particles(n_tot_old+i_whz)%set_helicity(hel)
            call particles(n_tot_old+i_whz)%set_polarization(PRT_DEFINITE_HELICITY)
        end if
        py_index(i_whz) = i_py
        whz_index(i_py) = n_tot_old + i_whz
        i_whz = i_whz + 1
    else
        pset_idx = find_pythia_particle (i_py, more_fuzzy=.true.)
        whz_index(i_py) = pset_idx
    end if
end if

```

```

end do
end subroutine add_particles_of_pythia

```

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine assign_colors (color, anti_color)
integer, intent(out) :: color, anti_color
if ((K(i_py,2) == 21) .or. (abs (K(i_py,2)) <= 8) .or. &
    (abs (K(i_py,2)) >= KSUSY1+1 .and. abs (K(i_py,2)) <= KSUSY1+8) .or. &
    (abs (K(i_py,2)) >= KSUSY2+1 .and. abs (K(i_py,2)) <= KSUSY2+8) .or. &
    (abs (K(i_py,2)) >= 1000 .and. abs (K(i_py,2)) <= 9999) .and. &
    hadro_start == 0) then
if (dangling_col == 0 .and. dangling_anti_col == 0) then
! new color string
! Gluon and gluino only color octets implemented so far
if (K(i_py,2) == 21 .or. K(i_py,2) == 1000021) then
color = next_color
dangling_col = color
next_color = next_color + 1
anti_color = next_color
dangling_anti_col = anti_color
next_color = next_color + 1
else if (K(i_py,2) > 0) then ! particles have color
color = next_color
dangling_col = color
anti_color = 0
next_color = next_color + 1
else if (K(i_py,2) < 0) then ! antiparticles have anticolor
anti_color = next_color
dangling_anti_col = anti_color
color = 0
next_color = next_color + 1
end if
else if(status == 1) then
! end of string
color = dangling_anti_col
anti_color = dangling_col
dangling_col = 0
dangling_anti_col = 0
else
! inside the string
if(dangling_col /= 0) then
anti_color = dangling_col
color = next_color
dangling_col = next_color
next_color = next_color +1
else if(dangling_anti_col /= 0) then
color = dangling_anti_col
anti_color = next_color
dangling_anti_col = next_color
next_color = next_color +1
else
call msg_bug ("Couldn't assign colors")
end if
end if
end if

```



```

else
  color = 0
  anti_color = 0
end if
end subroutine assign_colors

```

```

<Shower pythia6: combine with particle set: procedures>+≡
subroutine fill_hepevt_block_from_pythia ()
  integer :: first_daughter, second_mother_of_first_daughter, i_hep
  logical :: inconsistent_mother, more_than_one_points_to_first_daughter
  <HEPEVT BLOCK>
  call pyhepc(1)
  do i_hep = 1, NHEP
    first_daughter = JDAHEP(1,i_hep)
    if (first_daughter > 0) then
      more_than_one_points_to_first_daughter = &
        count (JDAHEP(1,i_hep:NHEP) == first_daughter) > 1
      if (more_than_one_points_to_first_daughter) then
        second_mother_of_first_daughter = JMOHEP(2,first_daughter)
        ! Only entries with codes 91-94 should have a second mother
        if (second_mother_of_first_daughter == 0) then
          inconsistent_mother = JMOHEP(1,first_daughter) /= i_hep
          if (inconsistent_mother) then
            JMOHEP(1,first_daughter) = i_hep
            do j = i_hep + 1, NHEP
              if (JDAHEP(1,j) == first_daughter) then
                JMOHEP(2,first_daughter) = j
              end if
            end do
          end if
        end if
      end if
    end if
  end do
end subroutine fill_hepevt_block_from_pythia

```

```

<HEPEVT BLOCK>≡
integer, parameter :: NMXHEP = 4000
integer :: NEVHEP
integer :: NHEP
integer, dimension(NMXHEP) :: ISTHEP
integer, dimension(NMXHEP) :: IDHEP
integer, dimension(2, NMXHEP) :: JMOHEP
integer, dimension(2, NMXHEP) :: JDAHEP
double precision, dimension(5, NMXHEP) :: PHEP
double precision, dimension(4, NMXHEP) :: VHEP
common /HEPEVT/ &
  NEVHEP, NHEP, ISTHEP, IDHEP, &
  JMOHEP, JDAHEP, PHEP, VHEP
save /HEPEVT/

```

Use HEPEVT for parent-child informations

```

<Shower pythia6: combine with particle set: procedures>+≡

```

```

subroutine set_parent_child_relations_from_hepevt ()
  integer, allocatable, dimension(:) :: parents
  <HEPEVT BLOCK>
  integer :: parent2, parent1, npar
  integer :: jsearch
  if (debug_on) call msg_debug (D_SHOWER, &
    "set_parent_child_relations_from_hepevt")
  if (debug_active (D_SHOWER)) then
    print *, 'NHEP, n, py_entries:', NHEP, n, py_entries
    call pylist(5)
  end if
  do i_whz = 1, py_entries
    parent1 = JMOHEP(1,py_index(i_whz))

    if (IDHEP(py_index(i_whz)) == 94) then
      firstmother: do jsearch = parent1-1, 1, -1
        if (JDAHEP(1,jsearch) /= py_index(i_whz)) then
          exit firstmother
        end if
        parent1 = jsearch
      end do firstmother
    end if

    parent2 = parent1
    if (JMOHEP(2,py_index(i_whz)) > 0) then
      parent2 = JMOHEP(2,py_index(i_whz))
    end if
    if (IDHEP(py_index(i_whz)) == 94) then
      lastmother: do jsearch = parent1+1, py_index(i_whz)
        if (JDAHEP(1,jsearch) /= py_index(i_whz)) then
          exit lastmother
        end if
        parent2 = jsearch
      end do lastmother
    end if

    allocate (parents(parent2-parent1+1))
    parents = 0
    child = n_tot_old + i_whz
    npar = 0
    do parent = parent1, parent2
      if (parent > 0) then
        if (parent <= 2) then
          call particle_set%parent_add_child (parent, child)
        else
          if (whz_index(parent) > 0) then
            npar = npar + 1
            parents(npar) = whz_index(parent)
            call particle_set%prt(whz_index(parent))%add_child (child)
          end if
        end if
      end if
    end do
    parents = pack (parents, parents > 0)
  end do
end subroutine

```

```

        if (npar > 0) call particle_set%prt(child)%set_parents (parents)
        if (allocated (parents)) deallocate (parents)
    end do
    NHEP = 0
end subroutine set_parent_child_relations_from_hepevt

```

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine fix_nonemitting_outgoings ()
    integer, dimension(1) :: child
    integer, parameter :: cmshower = 94
    do i = 1, size (particle_set%prt)
        associate (p => particle_set%prt(i))
            if (p%get_n_children () == 1) then
                child = p%get_children ()
                if (particle_set%prt(child(1))%get_pdg () == cmshower) then
                    j = particle_set%reverse_find_particle (p%get_pdg (), p%p)
                    if (j == i) then
                        deallocate (p%child)
                        p%status = PRT_OUTGOING
                    end if
                end if
            end if
        end associate
    end do
end subroutine fix_nonemitting_outgoings

```

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine set_parent_child_relations_from_K ()
    do j = 1, py_entries
        parent = K(py_index(j),3)
        child = n_tot_old + j
        if (parent > 0) then
            if (parent >= 1 .and. parent <= 2) then
                call particle_set%parent_add_child (parent, child)
            else
                real_parent = whz_index (parent)
                if (real_parent > 0 .and. real_parent /= child) then
                    call particle_set%parent_add_child (real_parent, child)
                end if
            end if
        end if
    end do
end subroutine set_parent_child_relations_from_K

```

(Shower pythia6: combine with particle set: procedures)+≡

```

subroutine set_parent_child_relations_of_color_strings_to_hadrons ()
    integer :: begin_string, end_string, old_start, next_start, real_child
    integer, allocatable, dimension(:) :: parents
    if (debug_on) call msg_debug (D_SHOWER, "set_parent_child_relations_of_color_strings_to_hadron
    if (debug_on) call msg_debug (D_SHOWER, "hadro_start", hadro_start)
    if (hadro_start > 0) then
        old_start = hadro_start
    do

```

```

next_start = 0
FIND: do i = old_start + 1, N
  if (K(i,2) >= 91 .and. K(i,2) <= 94) then
    next_start = i
    exit FIND
  end if
end do FIND
begin_string = K(old_start,3)
end_string = N
do i = begin_string, N
  if (K(i,1) == 11) then
    end_string = i
    exit
  end if
end do
allocate (parents (end_string - begin_string + 1))
parents = 0
real_child = whz_index (old_start)
do i = begin_string, end_string
  real_parent = whz_index (i)
  if (real_parent > 0) then
    call particle_set%prt(real_parent)%add_child (real_child)
    parents (i - begin_string + 1) = real_parent
  end if
end do
call particle_set%prt(real_child)%set_parents (parents)
deallocate (parents)
if (next_start == 0) exit
old_start = next_start
end do
end if
end subroutine set_parent_child_relations_of_color_strings_to_hadrons

```

We allow to be more_fuzzy when finding particles for parent child relations than when deciding whether we add particles or not.

(Shower pythia6: combine with particle set: procedures)+≡

```

function find_pythia_particle (i_py, more_fuzzy) result (j)
  integer :: j
  integer, intent(in) :: i_py
  logical, intent(in) :: more_fuzzy
  real(default) :: rel_small
  pdg = K(i_py,2)
  momentum = real([P(i_py,4), P(i_py,1:3)], kind=default)
  if (more_fuzzy) then
    rel_small = 1E-6_default
  else
    rel_small = 1E-10_default
  end if
  j = particle_set%reverse_find_particle (pdg, momentum, &
    abs_smallness = py_tiny, &
    rel_smallness = rel_small)
end function find_pythia_particle

```

Outgoing partons after hadronization shouldn't happen and is a dirty fix to missing mother daughter relation. I suspect that it has to do with the ordering of the color string but am not sure.

<Shower pythia6: combine with particle set: procedures>+≡

```
subroutine fudge_whizard_partons_in_hadro ()
  do i = 1, size (particle_set%prt)
    if (particle_set%prt(i)%status == PRT_OUTGOING .and. &
        (particle_set%prt(i)%flv%get_pdg () == GLUON .or. &
         particle_set%prt(i)%flv%get_pdg_abs () < 6) .or. &
         particle_set%prt(i)%status == PRT_BEAM_REMNANT) then
      particle_set%prt(i)%status = PRT_VIRTUAL
    end if
  end do
end subroutine fudge_whizard_partons_in_hadro
```

<Shower pythia6: shower pythia6: TBP>+≡

```
procedure :: get_final_colored_ME_momenta => shower_pythia6_get_final_colored_ME_momenta
```

<Shower pythia6: procedures>+≡

```
subroutine shower_pythia6_get_final_colored_ME_momenta &
  (shower, momenta)
  class(shower_pythia6_t), intent(in) :: shower
  type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
  <PYJETS COMMON BLOCK>
  integer :: i, j, n_jets
  if (signal_is_pending ()) return

  i = 7 !!! final ME partons start in 7th row of event record
  n_jets = 0
  do
    if (K(I,1) /= 21) exit
    if ((K(I,2) == 21) .or. (abs(K(I,2)) <= 6)) then
      n_jets = n_jets + 1
    end if
    i = i + 1
  end do
  if (n_jets == 0) return
  allocate (momenta(1:n_jets))
  i = 7
  j = 1
  do
    if (K(I,1) /= 21) exit
    if ((K(I,2) == 21) .or. (abs(K(I,2)) <= 6)) then
      momenta(j) = real ([P(i,4), P(i,1:3)], kind=default)
      j = j + 1
    end if
    i = i + 1
  end do
end subroutine shower_pythia6_get_final_colored_ME_momenta
```

<Shower pythia6: public>+≡

```
public :: pythia6_setup_lhe_io_units
```

```

<Shower pythia6: procedures>+≡
subroutine pythia6_setup_lhe_io_units (u_W2P, u_P2W)
  integer, intent(out) :: u_W2P
  integer, intent(out), optional :: u_P2W
  character(len=10) :: buffer
  u_W2P = free_unit ()
  if (debug_active (D_SHOWER)) then
    open (unit=u_W2P, status="replace", file="whizardout.lhe", &
      action="readwrite")
  else
    open (unit=u_W2P, status="scratch", action="readwrite")
  end if
  write (buffer, "(I10)") u_W2P
  call pygive ("MSTP(161)=" // buffer) !!! Unit for PYUPIN (LHA)
  call pygive ("MSTP(162)=" // buffer) !!! Unit for PYUPEV (LHA)
  if (present (u_P2W)) then
    u_P2W = free_unit ()
    write (buffer, "(I10)") u_P2W
    call pygive ("MSTP(163)=" // buffer)
    if (debug_active (D_SHOWER)) then
      open (unit=u_P2W, file="pythiaout2.lhe", status="replace", &
        action="readwrite")
    else
      open (unit=u_P2W, status="scratch", action="readwrite")
    end if
  end if
end subroutine pythia6_setup_lhe_io_units

<Shower pythia6: public>+≡
public :: pythia6_set_config

<Shower pythia6: procedures>+≡
subroutine pythia6_set_config (pygive_all)
  type(string_t), intent(in) :: pygive_all
  type(string_t) :: pygive_remaining, pygive_partial
  if (len (pygive_all) > 0) then
    pygive_remaining = pygive_all
    do while (len (pygive_remaining) > 0)
      call split (pygive_remaining, pygive_partial, ";")
      call pygive (char (pygive_partial))
    end do
    if (pythia6_get_error() /= 0) then
      call msg_fatal &
        (" PYTHIA6 did not recognize ps_PYTHIA_PYGIVE setting.")
    end if
  end if
end subroutine pythia6_set_config

```

Exchanging error messages with PYTHIA6.

```

<Shower pythia6: public>+≡
public :: pythia6_set_error

<Shower pythia6: procedures>+≡
subroutine pythia6_set_error (mstu23)

```

```

    IMPLICIT DOUBLE PRECISION(A-H, 0-Z)
    IMPLICIT INTEGER(I-N)
    COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
    SAVE/PYDAT1/
    integer, intent(in) :: mstu23
    MSTU(23) = mstu23
end subroutine pythia6_set_error

```

```

<Shower pythia6: public>+≡
    public :: pythia6_get_error

```

```

<Shower pythia6: procedures>+≡
    function pythia6_get_error () result (mstu23)
        IMPLICIT DOUBLE PRECISION(A-H, 0-Z)
        IMPLICIT INTEGER(I-N)
        COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
        SAVE/PYDAT1/
        integer :: mstu23
        mstu23 = MSTU(23)
    end function pythia6_get_error

```

```

<Shower pythia6: public>+≡
    public :: pythia6_tauola_active

```

```

<Shower pythia6: procedures>+≡
    function pythia6_tauola_active () result (active)
        IMPLICIT DOUBLE PRECISION(A-H, 0-Z)
        IMPLICIT INTEGER(I-N)
        COMMON/PYDAT1/MSTU(200),PARU(200),MSTJ(200),PARJ(200)
        SAVE/PYDAT1/
        logical :: active
        active = MSTJ(28) == 2
    end function pythia6_tauola_active

```

```

<Shower pythia6: public>+≡
    public :: pythia6_handle_errors

```

```

<Shower pythia6: procedures>+≡
    function pythia6_handle_errors () result (valid)
        logical :: valid
        valid = pythia6_get_error () == 0
        if (.not. valid) then
            call pythia6_set_error (0)
        end if
    end function pythia6_handle_errors

```

```

<Shower pythia6: public>+≡
    public :: pythia6_set_verbose

```

```

<Shower pythia6: procedures>+≡
    subroutine pythia6_set_verbose (verbose)
        logical, intent(in) :: verbose
        if (verbose) then
            call pygive ('MSTU(13)=1')
        end if
    end subroutine pythia6_set_verbose

```

```

        else
            call pygive ('MSTU(12)=12345') !!! No title page is written
            call pygive ('MSTU(13)=0')      !!! No information is written
        end if
    end subroutine pythia6_set_verbose

<Shower pythia6: public>+≡
    public :: pythia6_set_last_treated_line

<Shower pythia6: procedures>+≡
    subroutine pythia6_set_last_treated_line (last_line)
        integer,intent(in) :: last_line
        N_old = last_line
    end subroutine pythia6_set_last_treated_line

<pythia6_up.f>≡
    C...UPINIT
    C...Is supposed to fill the HEPRUP commonblock with info
    C...on incoming beams and allowed processes.

        SUBROUTINE UPINIT

    C...Double precision and integer declarations.
        IMPLICIT DOUBLE PRECISION(A-H, O-Z)
        IMPLICIT INTEGER(I-N)

    C...PYTHIA commonblock: only used to provide read unit MSTP(161).
        COMMON/PYPARS/MSTP(200),PARP(200),MSTI(200),PARI(200)
        SAVE /PYPARS/

    C...User process initialization commonblock.
        INTEGER MAXPUP
        PARAMETER (MAXPUP=100)
        INTEGER IDBMUP,PDFGUP,PDFSUP,IDWTUP,NPRUP,LPRUP
        DOUBLE PRECISION EBMUP,XSECUP,XERRUP,XMAXUP
        COMMON/HEPRUP/IDBMUP(2),EBMUP(2),PDFGUP(2),PDFSUP(2),
        &IDWTUP,NPRUP,XSECUP(MAXPUP),XERRUP(MAXPUP),XMAXUP(MAXPUP),
        &LPRUP(MAXPUP)
        SAVE /HEPRUP/

    C...Lines to read in assumed never longer than 200 characters.
        PARAMETER (MAXLEN=200)
        CHARACTER*(MAXLEN) STRING

    C...Format for reading lines.
        CHARACTER(len=6) STRFMT
        STRFMT='(A000)'
        WRITE(STRFMT(3:5),'(I3)') MAXLEN

    C...Loop until finds line beginning with "<init>" or "<init ".
    100 READ(MSTP(161),STRFMT,END=130,ERR=130) STRING
        IBEG=0
    110 IBEG=IBEG+1

```



```

C...Allow indentation.
      IF (STRING (IBEG:IBEG).EQ.' '.AND.IBEG.LT.MAXLEN-5) GOTO 110
      IF (STRING (IBEG:IBEG+5).NE.'<init>'.AND.
&STRING (IBEG:IBEG+5).NE.'<init '>) GOTO 100

C...Read first line of initialization info.
      READ (MSTP (161),*,END=130,ERR=130) IDBMUP (1),IDBMUP (2),EBMUP (1),
&EBMUP (2),PDFGUP (1),PDFGUP (2),PDFSUP (1),PDFSUP (2),IDWTUP,NPRUP

C...Read NPRUP subsequent lines with information on each process.
      DO 120 IPR=1,NPRUP
        READ (MSTP (161),*,END=130,ERR=130) XSECUP (IPR),XERRUP (IPR),
& XMAXUP (IPR),LPRUP (IPR)
120 CONTINUE
      RETURN

C...Error exit: give up if initialization does not work.
130 WRITE (*,*) ' Failed to read LHEF initialization information.'
      WRITE (*,*) ' Event generation will be stopped.'
      CALL PYSTOP (12)

      RETURN
      END

(pythia6.up.f)+≡
C...UPEVNT
C...Dummy routine, to be replaced by a user implementing external
C...processes. Depending on cross section model chosen, it either has
C...to generate a process of the type IDPRUP requested, or pick a type
C...itself and generate this event. The event is to be stored in the
C...HEPEUP commonblock, including (often) an event weight.

C...New example: handles a standard Les Houches Events File.

      SUBROUTINE UPEVNT

C...Double precision and integer declarations.
      IMPLICIT DOUBLE PRECISION (A-H, O-Z)
      IMPLICIT INTEGER (I-N)

C...PYTHIA commonblock: only used to provide read unit MSTP (162).
      COMMON /PYPARS /MSTP (200),PARP (200),MSTI (200),PARI (200)
      SAVE /PYPARS /

C...Added by WHIZARD
      COMMON /PYDAT1 /MSTU (200),PARU (200),MSTJ (200),PARJ (200)
      SAVE /PYDAT1 /

C...User process event common block.
      INTEGER MAXNUP
      PARAMETER (MAXNUP=500)
      INTEGER NUP,IDPRUP,IDUP,ISTUP,MOTHUP,ICOLUP
      DOUBLE PRECISION XWGTUP,SCALUP,AQEDUP,AQCDUP,PUP,VTIMUP,SPINUP
      COMMON /HEPEUP /NUP,IDPRUP,XWGTUP,SCALUP,AQEDUP,AQCDUP,IDUP (MAXNUP),

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```

        &ISTUP(MAXNUP),MOTHUP(2,MAXNUP),ICOLUP(2,MAXNUP),PUP(5,MAXNUP),
        &VTIMUP(MAXNUP),SPINUP(MAXNUP)
        SAVE /HEPEUP/

C...Lines to read in assumed never longer than 200 characters.
        PARAMETER (MAXLEN=200)
        CHARACTER*(MAXLEN) STRING

C...Format for reading lines.
        CHARACTER(len=6) STRFMT
        STRFMT='(A000)'
        WRITE(STRFMT(3:5),'(I3)') MAXLEN

C...Loop until finds line beginning with "<event>" or "<event ".
        100 READ(MSTP(162),STRFMT,END=130,ERR=130) STRING
            IBEG=0
        110 IBEG=IBEG+1
C...Allow indentation.
            IF(STRING(IBEG:IBEG).EQ.' '.AND.IBEG.LT.MAXLEN-6) GOTO 110
            IF(STRING(IBEG:IBEG+6).NE.'<event>'.AND.
            &STRING(IBEG:IBEG+6).NE.'<event ') GOTO 100

C...Read first line of event info.
            READ(MSTP(162),*,END=130,ERR=130) NUP,IDPRUP,XWGTUP,SCALUP,
            &AQEDUP,AQCDUP

C...Read NUP subsequent lines with information on each particle.
            DO 120 I=1,NUP
                READ(MSTP(162),*,END=130,ERR=130) IDUP(I),ISTUP(I),
                & MOTHUP(1,I),MOTHUP(2,I),ICOLUP(1,I),ICOLUP(2,I),
                & (PUP(J,I),J=1,5),VTIMUP(I),SPINUP(I)
            120 CONTINUE
            RETURN

C...Error exit, typically when no more events.
        130 CONTINUE
C        WRITE(*,*) ' Failed to read LHEF event information.'
C        WRITE(*,*) ' Will assume end of file has been reached.'
        NUP=0
        MSTI(51)=1
C...Added by WHIZARD, mark these failed events
        MSTU(23)=1

        RETURN
        END

(pythia6_up.f)+≡
C...UPVETO
C...Dummy routine, to be replaced by user, to veto event generation
C...on the parton level, after parton showers but before multiple
C...interactions, beam remnants and hadronization is added.
C...If resonances like W, Z, top, Higgs and SUSY particles are handed
C...undecayed from UPEVNT, or are generated by PYTHIA, they will also
C...be undecayed at this stage; if decayed their decay products will

```

C...have been allowed to shower.

C...All partons at the end of the shower phase are stored in the
C...HEPEVT commonblock. The interesting information is
C...NHEP = the number of such partons, in entries $1 \leq i \leq NHEP$,
C...IDHEP(I) = the particle ID code according to PDG conventions,
C...PHEP(J,I) = the (p_x, p_y, p_z, E, m) of the particle.
C...All ISTHEP entries are 1, while the rest is zeroed.

C...The user decision is to be conveyed by the IVETO value.
C...IVETO = 0 : retain current event and generate in full;
C... = 1 : abort generation of current event and move to next.

SUBROUTINE UPVETO(IVETO)

C...HEPEVT commonblock.
PARAMETER (NMXHEP=4000)
COMMON/HEPEVT/NEVHEP,NHEP,ISTHEP(NMXHEP),IDHEP(NMXHEP),
&JMOHEP(2,NMXHEP),JDAHEP(2,NMXHEP),PHEP(5,NMXHEP),VHEP(4,NMXHEP)
DOUBLE PRECISION PHEP,VHEP
SAVE /HEPEVT/

C...Next few lines allow you to see what info PYVETO extracted from
C...the full event record for the first two events.

C...Delete if you don't want it.
DATA NLIST/0/
SAVE NLIST
IF(NLIST.LE.2) THEN
WRITE(*,*) ' Full event record at time of UPVETO call:'
CALL PYLIST(1)
WRITE(*,*) ' Part of event record made available to UPVETO:'
CALL PYLIST(5)
NLIST=NLIST+1
ENDIF

C...Make decision here.
IVETO = 0

RETURN
END

(ktclus.f90)≡
(File header)

module ktclus

(Use kinds)

(KTCLUS: public)

contains

(KTCLUS: procedures)

```

end module ktclus
<KTCLUS: procedures>=
!C-----
!C-----
!C-----
!C      KTCLUS: written by Mike Seymour, July 1992.
!C      Last modified November 2000.
!C      Please send comments or suggestions to Mike.Seymour@rl.ac.uk
!C
!C      This is a general-purpose kt clustering package.
!C      It can handle ee, ep and pp collisions.
!C      It is loosely based on the program of Siggi Bethke.
!C
!C      The time taken (on a 10MIP machine) is (0.2microsec)*N**3
!C      where N is the number of particles.
!C      Over 90 percent of this time is used in subroutine KTPMIN, which
!C      simply finds the minimum member of a one-dimensional array.
!C      It is well worth thinking about optimization: on the SPARCstation
!C      a factor of two increase was obtained simply by increasing the
!C      optimization level from its default value.
!C
!C      The approach is to separate the different stages of analysis.
!C      KTCLUS does all the clustering and records a merging history.
!C      It returns a simple list of the y values at which each merging
!C      occurred. Then the following routines can be called to give extra
!C      information on the most recently analysed event.
!C      KTCLUR is identical but includes an R parameter, see below.
!C      KTYCUT gives the number of jets at each given YCUT value.
!C      KTYSUB gives the number of sub-jets at each given YCUT value.
!C      KTBEAM gives same info as KTCLUS but only for merges with the beam
!C      KTJOIN gives same info as KTCLUS but for merges of sub-jets.
!C      KTRECO reconstructs the jet momenta at a given value of YCUT.
!C      It also gives information on which jets at scale YCUT belong to
!C      which macro-jets at scale YMAC, for studying sub-jet properties.
!C      KTINCL reconstructs the jet momenta according to the inclusive jet
!C      definition of Ellis and Soper.
!C      KTISUB, KTIJOI and KTIREC are like KTYSUB, KTJOIN and KTRECO,
!C      except that they only apply to one inclusive jet at a time,
!C      with the pt of that jet automatically used for ECUT.
!C      KTWICH gives a list of which particles ended up in which jets.
!C      KTWCHS gives the same thing, but only for subjets.
!C      Note that the numbering of jets used by these two routines is
!C      guaranteed to be the same as that used by KTRECO.
!C
!C      The collision type and analysis type are indicated by the first
!C      argument of KTCLUS. IMODE=<TYPE><ANGLE><MONO><RECOM> where
!C      TYPE:  1=>ee, 2=>ep with p in -z direction, 3=>pe, 4=>pp
!C      ANGLE: 1=>angular kt def., 2=>DeltaR, 3=>f(DeltaEta,DeltaPhi)
!C              where f()=2(cosh(eta)-cos(phi)) is the QCD emission metric
!C      MONO:  1=>derive relative pseudoparticle angles from jets
!C              2=>monotonic definitions of relative angles
!C      RECOM: 1=>E recombination scheme, 2=>pt scheme, 3=>pt**2 scheme
!C
!C      There are also abbreviated forms for the most common combinations:

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!C      IMODE=1 => E scheme in e+e-                      (=1111)
!C      2 => E scheme in ep                             (=2111)
!C      3 => E scheme in pe                             (=3111)
!C      4 => E scheme in pp                             (=4111)
!C      5 => covariant E scheme in pp                   (=4211)
!C      6 => covariant pt-scheme in pp                  (=4212)
!C      7 => covariant monotonic pt**2-scheme in pp     (=4223)
!C
!C      KTRECO no longer needs to reconstruct the momenta according to the
!C      same recombination scheme in which they were clustered. Its first
!C      argument gives the scheme, taking the same values as RECOM above.
!C
!C      Note that unlike previous versions, all variables which hold y
!C      values have been named in a consistent way:
!C      Y() is the output scale at which jets were merged,
!C      YCUT is the input scale at which jets should be counted, and
!C      jet-momenta reconstructed etc,
!C      YMAC is the input macro-jet scale, used in determining whether
!C      or not each jet is a sub-jet.
!C      The original scheme defined in our papers is equivalent to always
!C      setting YMAC=1.
!C      Whenever a YCUT or YMAC variable is used, it is rounded down
!C      infinitesimally, so that for example, setting YCUT=Y(2) refers
!C      to the scale where the event is 2-jet, even if rounding errors
!C      have shifted its value slightly.
!C
!C      An R parameter can be used in hadron-hadron collisions by
!C      calling KTCLUR instead of KTCLUS. This is as suggested by
!C      Ellis and Soper, but implemented slightly differently,
!C      as in M.H. Seymour, LU TP 94/2 (submitted to Nucl. Phys. B.).
!C      R**2 multiplies the single Kt everywhere it is used.
!C      Calling KTCLUR with R=1 is identical to calling KTCLUS.
!C      R plays a similar role to the jet radius in a cone-type algorithm,
!C      but is scaled up by about 40% (ie R=0.7 in a cone algorithm is
!C      similar to this algorithm with R=1).
!C      Note that R.EQ.1 must be used for the e+e- and ep versions,
!C      and is strongly recommended for the hadron-hadron version.
!C      However, R values smaller than 1 have been found to be useful for
!C      certain applications, particularly the mass reconstruction of
!C      highly-boosted colour-singlets such as high-pt hadronic Ws,
!C      as in M.H. Seymour, LU TP 93/8 (to appear in Z. Phys. C.).
!C      Situations in which R<1 is useful are likely to also be those in
!C      which the inclusive reconstruction method is more useful.
!C
!C      Also included is a set of routines for doing Lorentz boosts:
!C      KTLBST finds the boost matrix to/from the cm frame of a 4-vector
!C      KTRROT finds the rotation matrix from one vector to another
!C      KTMMUL multiplies together two matrices
!C      KTMVUL multiplies a vector by a matrix
!C      KTINVT inverts a transformation matrix (nb NOT a general 4 by 4)
!C      KTFRAM boosts a list of vectors between two arbitrary frames
!C      KTBREI boosts a list of vectors between the lab and Breit frames
!C      KTHADR boosts a list of vectors between the lab and hadronic cmf
!C      The last two need the momenta in the +z direction of the lepton

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!C      and hadron beams, and the 4-momentum of the outgoing lepton.
!C
!C      The main reference is:
!C      S. Catani, Yu.L. Dokshitzer, M.H. Seymour and B.R. Webber,
!C      Nucl.Phys.B406(1993)187.
!C      The ep version was proposed in:
!C      S. Catani, Yu.L. Dokshitzer and B.R. Webber,
!C      Phys.Lett.285B(1992)291.
!C      The inclusive reconstruction method was proposed in:
!C      S.D. Ellis and D.E. Soper,
!C      Phys.Rev.D48(1993)3160.
!C
!C-----
!C-----
!C-----

<KTCLUS: public>≡
      public :: ktclur

<KTCLUS: procedures>+≡
      SUBROUTINE KTCLUR(IMODE,PP,NN,R,ECUT,Y,*)
      use io_units
      IMPLICIT NONE
!C---DO CLUSTER ANALYSIS OF PARTICLES IN PP
!C
!C   IMODE   = INPUT   : DESCRIBED ABOVE
!C   PP(I,J) = INPUT   : 4-MOMENTUM OF Jth PARTICLE: I=1,4 => PX,PY,PZ,E
!C   NN      = INPUT   : NUMBER OF PARTICLES
!C   R        = INPUT   : ELLIS AND SOPER'S R PARAMETER, SEE ABOVE.
!C   ECUT     = INPUT   : DENOMINATOR OF KT MEASURE. IF ZERO, ETOT IS USED
!C   Y(J)     = OUTPUT  : VALUE OF Y FOR WHICH EVENT CHANGES FROM BEING
!C                       J JET TO J-1 JET
!C   LAST ARGUMENT IS LABEL TO JUMP TO IF FOR ANY REASON THE EVENT
!C   COULD NOT BE PROCESSED (MOST LIKELY DUE TO TOO MANY PARTICLES)
!C
!C   NOTE THAT THE MOMENTA ARE DECLARED DOUBLE PRECISION,
!C   AND ALL OTHER FLOATING POINT VARIABLES ARE DECLARED DOUBLE PRECISION
!C
      INTEGER NMAX,IM,IMODE,TYPE,ANGL,MONO,RECO,N,I,J,NN, &
      IMIN,JMIN,KMIN,NUM,HIST,INJET,IABBR,NABBR
      PARAMETER (NMAX=512,NABBR=7)
      DOUBLE PRECISION PP(4,*)
      integer :: u
!CHANGE      DOUBLE PRECISION R,ECUT,Y(*),P,KT,ETOT,RSQ,KTP,KTS,KTPAIR,KTSING, &
      DOUBLE PRECISION R,ECUT,Y(*),P,KT,ETOT,RSQ,KTP,KTS, &
      KTMIN,ETSQ,KTLAST,KTMAX,KTTMP
      LOGICAL FIRST
      CHARACTER TITLE(4,4)*10
!C---KT RECORDS THE KT**2 OF EACH MERGING.
!C---KTLAST RECORDS FOR EACH MERGING, THE HIGHEST ECUT**2 FOR WHICH THE
!C   RESULT IS NOT MERGED WITH THE BEAM (COULD BE LARGER THAN THE
!C   KT**2 AT WHICH IT WAS MERGED IF THE KT VALUES ARE NOT MONOTONIC).
!C   THIS MAY SOUND POINTLESS, BUT ITS USEFUL FOR DETERMINING WHETHER
!C   SUB-JETS SURVIVED TO SCALE Y=YMAC OR NOT.
!C---HIST RECORDS MERGING HISTORY:

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!C  N=>DELETED TRACK N, M*NMAX+N=>MERGED TRACKS M AND N (M<N).
COMMON /KTCOMM/ETOT,RSQ,P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX), &
      KT(NMAX),KTLAST(NMAX),HIST(NMAX),NUM
DIMENSION INJET(NMAX),IABBR(NABBR)
DATA FIRST,TITLE,IABBR/.TRUE., &
      'e+e-      ', 'ep      ', 'pe      ', 'pp      ', &
      'angle      ', 'DeltaR    ', 'f(DeltaR) ', '*****', &
      'no          ', 'yes          ', '*****', '*****', &
      'E           ', 'Pt           ', 'Pt**2     ', '*****', &
      1111,2111,3111,4111,4211,4212,4223/
!C---CHECK INPUT
IM=IMODE
IF (IM.GE.1.AND.IM.LE.NABBR) IM=IABBR(IM)
TYPE=MOD(IM/1000,10)
ANGL=MOD(IM/100 ,10)
MONO=MOD(IM/10 ,10)
RECO=MOD(IM ,10)
IF (NN.GT.NMAX) CALL KTWARN('KT-MAX',100,*999)
IF (NN.LT.1) CALL KTWARN('KT-LT1',100,*999)
IF (NN.LT.2.AND.TYPE.EQ.1) CALL KTWARN('KT-LT2',100,*999)
IF (TYPE.LT.1.OR.TYPE.GT.4.OR.ANGL.LT.1.OR.ANGL.GT.4.OR. &
      MONO.LT.1.OR.MONO.GT.2.OR.RECO.LT.1.OR.RECO.GT.3) CALL KTWARN('KTCLUS',101,*999)
u = given_output_unit ()
IF (FIRST) THEN
  WRITE (u,'(/,1X,54(''*'')/A)') &
    ' KTCLUS: written by Mike Seymour, July 1992.'
  WRITE (u,'(A)') &
    ' Last modified November 2000.'
  WRITE (u,'(A)') &
    ' Please send comments or suggestions to Mike.Seymour@rl.ac.uk'
  WRITE (u,'(/A,I2,2A)') &
    ' Collision type =',TYPE,' = ',TITLE(TYPE,1)
  WRITE (u,'(A,I2,2A)') &
    ' Angular variable =',ANGL,' = ',TITLE(ANGL,2)
  WRITE (u,'(A,I2,2A)') &
    ' Monotonic definition =',MONO,' = ',TITLE(MONO,3)
  WRITE (u,'(A,I2,2A)') &
    ' Recombination scheme =',RECO,' = ',TITLE(RECO,4)
  IF (R.NE.1) THEN
    WRITE (u,'(A,F5.2)') &
      ' Radius parameter =',R
    IF (TYPE.NE.4) WRITE (u,'(A)') &
      ' R.NE.1 is strongly discouraged for this collision type!'
  ENDIF
  WRITE (u,'(1X,54(''*'')/)')
  FIRST=.FALSE.
ENDIF
!C---COPY PP TO P
N=NN
NUM=NN
CALL KTCOPY(PP,N,P,(RECO.NE.1))
ETOT=0
DO I=1,N
  ETOT=ETOT+P(4,I)

```

```

      END DO
      IF (ETOT.EQ.0) CALL KTWARN('KTCLUS',102,*999)
      IF (ECUT.EQ.0) THEN
        ETSQ=1/ETOT**2
      ELSE
        ETSQ=1/ECUT**2
      ENDIF
      RSQ=R**2
!C---CALCULATE ALL PAIR KT's
      DO I=1,N-1
        DO J=I+1,N
          KTP(J,I)=-1
          KTP(I,J)=KTPAIR(ANGL,P(1,I),P(1,J),KTP(J,I))
        END DO
      END DO
!C---CALCULATE ALL SINGLE KT's
      DO I=1,N
        KTS(I)=KTSING(ANGL,TYPE,P(1,I))
      END DO
      KTMAX=0
!C---MAIN LOOP
300 CONTINUE
!C---FIND MINIMUM MEMBER OF KTP
      CALL KTPMIN(KTP,NMAX,N,IMIN,JMIN)
!C---FIND MINIMUM MEMBER OF KTS
      CALL KTSMIN(KTS,NMAX,N,KMIN)
!C---STORE Y VALUE OF TRANSITION FROM N TO N-1 JETS
      KTMIN=KTP(IMIN,JMIN)
      KTTMP=RSQ*KTS(KMIN)
      IF ((TYPE.GE.2.AND.TYPE.LE.4).AND. &
        (KTTMP.LE.KTMIN.OR.N.EQ.1)) &
        KTMIN=KTTMP
      KT(N)=KTMIN
      Y(N)=KT(N)*ETSQ
!C---IF MONO.GT.1, SEQUENCE IS SUPPOSED TO BE MONOTONIC, IF NOT, WARN
      IF (KTMIN.LT.KTMAX.AND.MONO.GT.1) CALL KTWARN('KTCLUS',1,*999)
      IF (KTMIN.GE.KTMAX) KTMAX=KTMIN
!C---IF LOWEST KT IS TO A BEAM, THROW IT AWAY AND MOVE LAST ENTRY UP
      IF (KTMIN.EQ.KTTMP) THEN
        CALL KTMOVE(P,KTP,KTS,NMAX,N,KMIN,1)
!C---UPDATE HISTORY AND CROSS-REFERENCES
        HIST(N)=KMIN
        INJET(N)=KMIN
        DO I=N,NN
          IF (INJET(I).EQ.KMIN) THEN
            KTLAST(I)=KTMAX
            INJET(I)=0
          ELSEIF (INJET(I).EQ.N) THEN
            INJET(I)=KMIN
          ENDIF
        END DO
!C---OTHERWISE MERGE JETS IMIN AND JMIN AND MOVE LAST ENTRY UP
      ELSE
        CALL KTMERG(P,KTP,KTS,NMAX,IMIN,JMIN,N,TYPE,ANGL,MONO,RECO)
      END IF

```



```

      CALL KTMOVE(P,KTP,KTS,NMAX,N,JMIN,1)
!C---UPDATE HISTORY AND CROSS-REFERENCES
      HIST(N)=IMIN*NMAX+JMIN
      INJET(N)=IMIN
      DO I=N,NN
        IF (INJET(I).EQ.JMIN) THEN
          INJET(I)=IMIN
        ELSEIF (INJET(I).EQ.N) THEN
          INJET(I)=JMIN
        ENDIF
      END DO
    ENDIF
  !C---THATS ALL THERE IS TO IT
  N=N-1
  IF (N.GT.1 .OR. N.GT.0.AND.(TYPE.GE.2.AND.TYPE.LE.4)) GOTO 300
  IF (N.EQ.1) THEN
    KT(N)=1D20
    Y(N)=KT(N)*ETSQ
  ENDIF
  RETURN
999 RETURN 1
END SUBROUTINE KTCLUR
!C-----

<KTCLUS: public>+≡
  public :: ktreco

<KTCLUS: procedures>+≡
!C-----
      SUBROUTINE KTRECO(RECO,PP,NN,ECUT,YCUT,YMAC,PJET,JET,NJET,NSUB,*)
      IMPLICIT NONE
!C---RECONSTRUCT KINEMATICS OF JET SYSTEM, WHICH HAS ALREADY BEEN
!C ANALYSED BY KTCLUS. NOTE THAT NO CONSISTENCY CHECK IS MADE: USER
!C IS TRUSTED TO USE THE SAME PP VALUES AS FOR KTCLUS
!C
!C RECO      = INPUT : RECOMBINATION SCHEME (NEED NOT BE SAME AS KTCLUS)
!C PP(I,J)   = INPUT : 4-MOMENTUM OF Jth PARTICLE: I=1,4 => PX,PY,PZ,E
!C NN        = INPUT : NUMBER OF PARTICLES
!C ECUT      = INPUT : DENOMINATOR OF KT MEASURE. IF ZERO, ETOT IS USED
!C YCUT      = INPUT : Y VALUE AT WHICH TO RECONSTRUCT JET MOMENTA
!C YMAC      = INPUT : Y VALUE USED TO DEFINE MACRO-JETS, TO DETERMINE
!C              WHICH JETS ARE SUB-JETS
!C PJET(I,J)=OUTPUT : 4-MOMENTUM OF Jth JET AT SCALE YCUT
!C JET(J)    =OUTPUT : THE MACRO-JET WHICH CONTAINS THE Jth JET,
!C              SET TO ZERO IF JET IS NOT A SUB-JET
!C NJET      =OUTPUT : THE NUMBER OF JETS
!C NSUB      =OUTPUT : THE NUMBER OF SUB-JETS (EQUAL TO THE NUMBER OF
!C              NON-ZERO ENTRIES IN JET())
!C LAST ARGUMENT IS LABEL TO JUMP TO IF FOR ANY REASON THE EVENT
!C COULD NOT BE PROCESSED
!C
!C NOTE THAT THE MOMENTA ARE DECLARED DOUBLE PRECISION,
!C AND ALL OTHER FLOATING POINT VARIABLES ARE DECLARED DOUBLE PRECISION
!C
      INTEGER NMAX,RECO,NUM,N,NN,NJET,NSUB,JET(*),HIST,IMIN,JMIN,I,J

```

```

PARAMETER (NMAX=512)
DOUBLE PRECISION PP(4,*),PJET(4,*)
DOUBLE PRECISION ECUT,P,KT,KTP,KTS,ETOT,RSQ,ETSQ,YCUT,YMAC,KTLAST, &
    ROUND
PARAMETER (ROUND=0.99999D0)
COMMON /KTCOMM/ETOT,RSQ,P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX), &
    KT(NMAX),KTLAST(NMAX),HIST(NMAX),NUM
!C---CHECK INPUT
    IF (RECO.LT.1.OR.RECO.GT.3) THEN
        PRINT *, 'RECO=',RECO
        CALL KTWARN('KTRECO',100,*999)
    ENDIF
!C---COPY PP TO P
    N=NN
    IF (NUM.NE.NN) CALL KTWARN('KTRECO',101,*999)
    CALL KTCOPY(PP,N,P,(RECO.NE.1))
    IF (ECUT.EQ.0) THEN
        ETSQ=1/ETOT**2
    ELSE
        ETSQ=1/ECUT**2
    ENDIF
!C---KEEP MERGING UNTIL YCUT
100  IF (ETSQ*KT(N).LT.ROUND*YCUT) THEN
        IF (HIST(N).LE.NMAX) THEN
            CALL KTMOVE(P,KTP,KTS,NMAX,N,HIST(N),0)
        ELSE
            IMIN=HIST(N)/NMAX
            JMIN=HIST(N)-IMIN*NMAX
            CALL KTMERG(P,KTP,KTS,NMAX,IMIN,JMIN,N,0,0,0,RECO)
            CALL KTMOVE(P,KTP,KTS,NMAX,N,JMIN,0)
        ENDIF
        N=N-1
        IF (N.GT.0) GOTO 100
    ENDIF
!C---IF YCUT IS TOO LARGE THERE ARE NO JETS
    NJET=N
    NSUB=N
    IF (N.EQ.0) RETURN
!C---SET UP OUTPUT MOMENTA
    DO I=1,NJET
        IF (RECO.EQ.1) THEN
            DO J=1,4
                PJET(J,I)=P(J,I)
            END DO
        ELSE
            PJET(1,I)=P(6,I)*COS(P(8,I))
            PJET(2,I)=P(6,I)*SIN(P(8,I))
            PJET(3,I)=P(6,I)*SINH(P(7,I))
            PJET(4,I)=P(6,I)*COSH(P(7,I))
        ENDIF
        JET(I)=I
    END DO
!C---KEEP MERGING UNTIL YMAC TO FIND THE FATE OF EACH JET
300  IF (ETSQ*KT(N).LT.ROUND*YMAC) THEN

```

```

      IF (HIST(N).LE.NMAX) THEN
        IMIN=0
        JMIN=HIST(N)
        NSUB=NSUB-1
      ELSE
        IMIN=HIST(N)/NMAX
        JMIN=HIST(N)-IMIN*NMAX
        IF (ETSQ*KTLAST(N).LT.ROUND*YMAC) NSUB=NSUB-1
      ENDIF
      DO I=1,NJET
        IF (JET(I).EQ.JMIN) JET(I)=IMIN
        IF (JET(I).EQ.N) JET(I)=JMIN
      END DO
      N=N-1
      IF (N.GT.0) GOTO 300
    ENDIF
    RETURN
999  RETURN 1
    END SUBROUTINE KTRECO
!C-----
<KTCLUS: procedures>+≡
!C-----
      FUNCTION KTPAIR(ANGL,P,Q,ANGLE)
        IMPLICIT NONE
!C---CALCULATE LOCAL KT OF PAIR, USING ANGULAR SCHEME:
!C  1=>ANGULAR, 2=>DeltaR, 3=>f(DeltaEta,DeltaPhi)
!C  WHERE f(eta,phi)=2(COSH(eta)-COS(phi)) IS THE QCD EMISSION METRIC
!C---IF ANGLE<0, IT IS SET TO THE ANGULAR PART OF THE LOCAL KT ON RETURN
!C  IF ANGLE>0, IT IS USED INSTEAD OF THE ANGULAR PART OF THE LOCAL KT
      INTEGER ANGL
!  CHANGE      DOUBLE PRECISION P(9),Q(9),KTPAIR,R,KTMDPI,ANGLE,ETA,PHI,ESQ
      DOUBLE PRECISION P(9),Q(9),KTPAIR,R,ANGLE,ETA,PHI,ESQ
!C---COMPONENTS OF MOMENTA ARE PX,PY,PZ,E,1/P,PT,ETA,PHI,PT**2
      R=ANGLE
      IF (ANGL.EQ.1) THEN
        IF (R.LE.0) R=2*(1-(P(1)*Q(1)+P(2)*Q(2)+P(3)*Q(3))*(P(5)*Q(5)))
        ESQ=MIN(P(4),Q(4))**2
      ELSEIF (ANGL.EQ.2.OR.ANGL.EQ.3) THEN
        IF (R.LE.0) THEN
          ETA=P(7)-Q(7)
          PHI=KTMDPI(P(8)-Q(8))
          IF (ANGL.EQ.2) THEN
            R=ETA**2+PHI**2
          ELSE
            R=2*(COSH(ETA)-COS(PHI))
          ENDIF
        ENDIF
        ESQ=MIN(P(9),Q(9))
      ELSEIF (ANGL.EQ.4) THEN
        ESQ=(1d0/(P(5)*Q(5))-P(1)*Q(1)-P(2)*Q(2)- &
          P(3)*Q(3))*2D0/(P(5)*Q(5))/(0.0001D0+1d0/P(5)+1d0/Q(5))**2
        R=1d0
      ELSE
        CALL KTWARN('KTPAIR',200,*999)

```

```

        STOP
      ENDIF
      KTPAIR=ESQ*R
      IF (ANGLE.LT.0) ANGLE=R
999 END FUNCTION KTPAIR
!C-----
      FUNCTION KTSING(ANGL,TYPE,P)
        IMPLICIT NONE
!C---CALCULATE KT OF PARTICLE, USING ANGULAR SCHEME:
!C  1=>ANGULAR, 2=>DeltaR, 3=>f(DeltaEta,DeltaPhi)
!C---TYPE=1 FOR E+E-, 2 FOR EP, 3 FOR PE, 4 FOR PP
!C  FOR EP, PROTON DIRECTION IS DEFINED AS -Z
!C  FOR PE, PROTON DIRECTION IS DEFINED AS +Z
        INTEGER ANGL,TYPE
        DOUBLE PRECISION P(9),KTSING,COSTH,R,SMALL
        DATA SMALL/1D-4/
        IF (ANGL.EQ.1.OR.ANGL.EQ.4) THEN
          COSTH=P(3)*P(5)
          IF (TYPE.EQ.2) THEN
            COSTH=-COSTH
          ELSEIF (TYPE.EQ.4) THEN
            COSTH=ABS(COSTH)
          ELSEIF (TYPE.NE.1.AND.TYPE.NE.3) THEN
            CALL KTWARN('KTSING',200,*999)
            STOP
          ENDIF
          R=2*(1-COSTH)
!C---IF CLOSE TO BEAM, USE APPROX  $2*(1-\cos(\theta))=\sin^2(\theta)$ 
          IF (R.LT.SMALL) R=(P(1)**2+P(2)**2)*P(5)**2
          KTSING=P(4)**2*R
        ELSEIF (ANGL.EQ.2.OR.ANGL.EQ.3) THEN
          KTSING=P(9)
        ELSE
          CALL KTWARN('KTSING',201,*999)
          STOP
        ENDIF
999 END FUNCTION KTSING
!C-----
      SUBROUTINE KTPMIN(A,NMAX,N,IMIN,JMIN)
        IMPLICIT NONE
!C---FIND THE MINIMUM MEMBER OF A(NMAX,NMAX) WITH IMIN < JMIN <= N
        INTEGER NMAX,N,IMIN,JMIN,KMIN,I,J,K
!C---REMEMBER THAT  $A(X+(Y-1)*NMAX)=A(X,Y)$ 
!C  THESE LOOPING VARIABLES ARE J=Y-2, I=X+(Y-1)*NMAX
        DOUBLE PRECISION A(*),AMIN
        K=1+NMAX
        KMIN=K
        AMIN=A(KMIN)
        DO J=0,N-2
          DO I=K,K+J
            IF (A(I).LT.AMIN) THEN
              KMIN=I
              AMIN=A(KMIN)
            ENDIF
          ENDIF
        ENDIF

```

```

        END DO
        K=K+NMAX
    END DO
    JMIN=KMIN/NMAX+1
    IMIN=KMIN-(JMIN-1)*NMAX
END SUBROUTINE KTPMIN
!C-----
SUBROUTINE KTSMIN(A,NMAX,N,IMIN)
    IMPLICIT NONE
!C---FIND THE MINIMUM MEMBER OF A
    INTEGER N,NMAX,IMIN,I
    DOUBLE PRECISION A(NMAX)
    IMIN=1
    DO I=1,N
        IF (A(I).LT.A(IMIN)) IMIN=I
    END DO
END SUBROUTINE KTSMIN
!C-----
SUBROUTINE KTCOPY(A,N,B,ONSHLL)
    IMPLICIT NONE
!C---COPY FROM A TO B. 5TH=1/(3-MTM), 6TH=PT, 7TH=ETA, 8TH=PHI, 9TH=PT**2
!C IF ONSHLL IS .TRUE. PARTICLE ENTRIES ARE PUT ON-SHELL BY SETTING E=P
    INTEGER I,N
    DOUBLE PRECISION A(4,N)
    LOGICAL ONSHLL
    DOUBLE PRECISION B(9,N),ETAMAX,SINMIN,EPS
    DATA ETAMAX,SINMIN,EPS/10,0,1D-6/
!C---SINMIN GETS CALCULATED ON FIRST CALL
    IF (SINMIN.EQ.0) SINMIN=1/COSH(ETAMAX)
    DO I=1,N
        B(1,I)=A(1,I)
        B(2,I)=A(2,I)
        B(3,I)=A(3,I)
        B(4,I)=A(4,I)
        B(5,I)=SQRT(A(1,I)**2+A(2,I)**2+A(3,I)**2)
        IF (ONSHLL) B(4,I)=B(5,I)
        IF (B(5,I).EQ.0) B(5,I)=1D-10
        B(5,I)=1/B(5,I)
        B(9,I)=A(1,I)**2+A(2,I)**2
        B(6,I)=SQRT(B(9,I))
        B(7,I)=B(6,I)*B(5,I)
        IF (B(7,I).GT.SINMIN) THEN
            B(7,I)=A(4,I)**2-A(3,I)**2
            IF (B(7,I).LE.EPS*B(4,I)**2.OR.ONSHELL) B(7,I)=B(9,I)
            B(7,I)=LOG((B(4,I)+ABS(B(3,I)))**2/B(7,I))/2
        ELSE
            B(7,I)=ETAMAX+2
        ENDIF
        B(7,I)=SIGN(B(7,I),B(3,I))
        IF (A(1,I).EQ.0 .AND. A(2,I).EQ.0) THEN
            B(8,I)=0
        ELSE
            B(8,I)=ATAN2(A(2,I),A(1,I))
        ENDIF
    END DO

```

```

      END DO
      END SUBROUTINE KTCOPY
!C-----
      SUBROUTINE KTMERG(P,KTP,KTS,NMAX,I,J,N,TYPE,ANGL,MONO,RECO)
      IMPLICIT NONE
!C---MERGE THE Jth PARTICLE IN P INTO THE Ith PARTICLE
!C   J IS ASSUMED GREATER THAN I. P CONTAINS N PARTICLES BEFORE MERGING.
!C---ALSO RECALCULATING THE CORRESPONDING KTP AND KTS VALUES IF MONO.GT.0
!C   FROM THE RECOMBINED ANGULAR MEASURES IF MONO.GT.1
!C---NOTE THAT IF MONO.LE.0, TYPE AND ANGL ARE NOT USED
      INTEGER ANGL,RECO,TYPE,I,J,K,N,NMAX,MONO
      DOUBLE PRECISION P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX),PT,PTT, &
! CHANGE      KTMDPI,KTUP,PI,PJ,ANG,KTPAIR,KTSING,ETAMAX,EPS
      KTUP,PI,PJ,ANG,ETAMAX,EPS
      KTUP(I,J)=KTP(MAX(I,J),MIN(I,J))
      DATA ETAMAX,EPS/10,1D-6/
      IF (J.LE.I) CALL KTWARN('KTMERG',200,*999)
!C---COMBINE ANGULAR MEASURES IF NECESSARY
      IF (MONO.GT.1) THEN
        DO K=1,N
          IF (K.NE.I.AND.K.NE.J) THEN
            IF (RECO.EQ.1) THEN
              PI=P(4,I)
              PJ=P(4,J)
            ELSEIF (RECO.EQ.2) THEN
              PI=P(6,I)
              PJ=P(6,J)
            ELSEIF (RECO.EQ.3) THEN
              PI=P(9,I)
              PJ=P(9,J)
            ELSE
              CALL KTWARN('KTMERG',201,*999)
              STOP
            ENDIF
            IF (PI.EQ.0.AND.PJ.EQ.0) THEN
              PI=1
              PJ=1
            ENDIF
            KTP(MAX(I,K),MIN(I,K))= &
              (PI*KTUP(I,K)+PJ*KTUP(J,K))/(PI+PJ)
          ENDIF
        END DO
      ENDIF
      IF (RECO.EQ.1) THEN
!C---VECTOR ADDITION
        P(1,I)=P(1,I)+P(1,J)
        P(2,I)=P(2,I)+P(2,J)
        P(3,I)=P(3,I)+P(3,J)
!c      P(4,I)=P(4,I)+P(4,J) ! JA
        P(5,I)=SQRT(P(1,I)**2+P(2,I)**2+P(3,I)**2)
        P(4,I)=P(5,I) ! JA (Massless scheme)
        IF (P(5,I).EQ.0) THEN
          P(5,I)=1
        ELSE

```

```

        P(5,I)=1/P(5,I)
    ENDIF
    ELSEIF (RECO.EQ.2) THEN
!C---PT WEIGHTED ETA-PHI ADDITION
        PT=P(6,I)+P(6,J)
        IF (PT.EQ.0) THEN
            PTT=1
        ELSE
            PTT=1/PT
        ENDIF
        P(7,I)=(P(6,I)*P(7,I)+P(6,J)*P(7,J))*PTT
        P(8,I)=KTMDPI(P(8,I)+P(6,J)*PTT*KTMDPI(P(8,J)-P(8,I)))
        P(6,I)=PT
        P(9,I)=PT**2
    ELSEIF (RECO.EQ.3) THEN
!C---PT**2 WEIGHTED ETA-PHI ADDITION
        PT=P(9,I)+P(9,J)
        IF (PT.EQ.0) THEN
            PTT=1
        ELSE
            PTT=1/PT
        ENDIF
        P(7,I)=(P(9,I)*P(7,I)+P(9,J)*P(7,J))*PTT
        P(8,I)=KTMDPI(P(8,I)+P(9,J)*PTT*KTMDPI(P(8,J)-P(8,I)))
        P(6,I)=P(6,I)+P(6,J)
        P(9,I)=P(6,I)**2
    ELSE
        CALL KTWARN('KTMERG',202,*999)
        STOP
    ENDIF
!C---IF MONO.GT.0 CALCULATE NEW KT MEASURES. IF MONO.GT.1 USE ANGULAR ONES.
    IF (MONO.LE.0) RETURN
!C---CONVERTING BETWEEN 4-MTM AND PT,ETA,PHI IF NECESSARY
    IF (ANGL.NE.1.AND.RECO.EQ.1) THEN
        P(9,I)=P(1,I)**2+P(2,I)**2
        P(7,I)=P(4,I)**2-P(3,I)**2
        IF (P(7,I).LE.EPS*P(4,I)**2) P(7,I)=P(9,I)
        IF (P(7,I).GT.0) THEN
            P(7,I)=LOG((P(4,I)+ABS(P(3,I)))*2/P(7,I))/2
            IF (P(7,I).GT.ETAMAX) P(7,I)=ETAMAX+2
        ELSE
            P(7,I)=ETAMAX+2
        ENDIF
        P(7,I)=SIGN(P(7,I),P(3,I))
        IF (P(1,I).NE.0.AND.P(2,I).NE.0) THEN
            P(8,I)=ATAN2(P(2,I),P(1,I))
        ELSE
            P(8,I)=0
        ENDIF
    ELSEIF (ANGL.EQ.1.AND.RECO.NE.1) THEN
        P(1,I)=P(6,I)*COS(P(8,I))
        P(2,I)=P(6,I)*SIN(P(8,I))
        P(3,I)=P(6,I)*SINH(P(7,I))
        P(4,I)=P(6,I)*COSH(P(7,I))

```

```

        IF (P(4,I).NE.0) THEN
            P(5,I)=1/P(4,I)
        ELSE
            P(5,I)=1
        ENDIF
    ENDIF
    ANG=0
    DO K=1,N
        IF (K.NE.I.AND.K.NE.J) THEN
            IF (MONO.GT.1) ANG=KTUP(I,K)
            KTP(MIN(I,K),MAX(I,K))= &
                KTPAIR(ANGL,P(1,I),P(1,K),ANG)
        ENDIF
    END DO
    KTS(I)=KTSING(ANGL,TYPE,P(1,I))
999 END SUBROUTINE KTMERG
!C-----
    SUBROUTINE KTMOVE(P,KTP,KTS,NMAX,N,J,IOPT)
        IMPLICIT NONE
!C---MOVE THE Nth PARTICLE IN P TO THE Jth POSITION
!C---ALSO MOVING KTP AND KTS IF IOPT.GT.0
        INTEGER I,J,N,NMAX,IOPT
        DOUBLE PRECISION P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX)
        DO I=1,9
            P(I,J)=P(I,N)
        END DO
        IF (IOPT.LE.0) RETURN
        DO I=1,J-1
            KTP(I,J)=KTP(I,N)
            KTP(J,I)=KTP(N,I)
        END DO
        DO I=J+1,N-1
            KTP(J,I)=KTP(I,N)
            KTP(I,J)=KTP(N,I)
        END DO
        KTS(J)=KTS(N)
    END SUBROUTINE KTMOVE
!C-----
<KTCLUS: procedures>+=
    FUNCTION KTMDPI(PHI)
        IMPLICIT NONE
!C---RETURNS PHI, MOVED ONTO THE RANGE [-PI,PI)
        DOUBLE PRECISION KTMDPI,PHI,PI,TWOPI,THRPI,EPS
        PARAMETER (PI=3.14159265358979324D0,TWOPI=6.28318530717958648D0, &
            THRPI=9.42477796076937972D0)
        PARAMETER (EPS=1D-15)
        KTMDPI=PHI
        IF (KTMDPI.LE.PI) THEN
            IF (KTMDPI.GT.-PI) THEN
                GOTO 100
            ELSEIF (KTMDPI.GT.-THRPI) THEN
                KTMDPI=KTMDPI+TWOPI
            ELSE
                KTMDPI=-MOD(PI-KTMDPI,TWOPI)+PI
            ENDIF
        ENDIF
    END FUNCTION

```



```

        ENDIF
        ELSEIF (KTMDPI.LE.THRPI) THEN
            KTMDPI=KTMDPI-TWOPI
        ELSE
            KTMDPI=MOD(PI+KTMDPI,TWOPI)-PI
        ENDIF
100 IF (ABS(KTMDPI).LT.EPS) KTMDPI=0
    END FUNCTION KTMDPI
!C-----
    SUBROUTINE KTWARN(SUBRTN,ICODE,*)
!C    DEALS WITH ERRORS DURING EXECUTION
!C    SUBRTN = NAME OF CALLING SUBROUTINE
!C    ICODE = ERROR CODE:      - 99 PRINT WARNING & CONTINUE
!C                                100-199 PRINT WARNING & JUMP
!C                                200-    PRINT WARNING & STOP DEAD
!C-----
    INTEGER ICODE
    CHARACTER(len=6) SUBRTN
    WRITE (6,10) SUBRTN,ICODE
10  FORMAT(/' KTWARN CALLED FROM SUBPROGRAM ',A6,' : CODE =',I4/)
    IF (ICODE.LT.100) RETURN
    IF (ICODE.LT.200) RETURN 1
    STOP
    END SUBROUTINE KTWARN
!C-----
!C-----
!C-----

```

22.5 Interface to PYTHIA 8

`<shower_pythia8.f90>≡`

`<File header>`

`module shower_pythia8`

`<Use kinds with double>`

`<Use strings>`

`<Use debug>`

`use constants`

`use numeric_utils, only: vanishes`

`use io_units`

`use physics_defs`

`use diagnostics`

`use os_interface`

`use lorentz`

`use subevents`

`use shower_base`

`use particles`

`use model_data`

`use pdf`

`use helicities`

`use whizard_lha`

```

use pythia8
use tauola_interface, only: taudec_settings_t

<Standard module head>

<Shower pythia8: public>
<Shower pythia8: variables>
<Shower pythia8: types>

contains

<Shower pythia8: procedures>

end module shower_pythia8

<Shower pythia8: public>≡
    public :: shower_pythia8_t
<Shower pythia8: types>≡
    type, extends(shower_base_t) :: shower_pythia8_t
        private
        type(pythia8_t) :: pythia
        type(whizard_lha_t) :: lhaup
        logical :: user_process_set = .false.
        logical :: pythia_initialized = .false., &
            lhaup_initialized = .false.
        contains
        <Shower pythia8: shower pythia8: TBP>
    end type shower_pythia8_t

<Shower pythia8: shower pythia8: TBP>≡
    procedure :: init => shower_pythia8_init
<Shower pythia8: procedures>≡
    subroutine shower_pythia8_init (shower, settings, taudec_settings, pdf_data, os_data)
        class(shower_pythia8_t), intent(out) :: shower
        type(shower_settings_t), intent(in) :: settings
        type(taudec_settings_t), intent(in) :: taudec_settings
        type(pdf_data_t), intent(in) :: pdf_data
        type(os_data_t), intent(in) :: os_data
        if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_init")
        shower%settings = settings
        shower%taudec_settings = taudec_settings
        shower%os_data = os_data
        call shower%pdf_data%init (pdf_data)
        shower%name = "PYTHIA8"
        call shower%write_msg ()
        call shower%pythia%init (verbose = settings%verbose)
        call shower%lhaup%init ()
    end subroutine shower_pythia8_init

```

Setup the user process for the LHA interface.

We fill the user process with the correct information on the beams, and set the strategy of the user process to weighted events. `process_id` and `n_processes`

are not used by LHA user process for weighted (or unweighted) events, but required by the LHA user process interface. Therefore, we choose arbitrary defaults.

```

(Shower pythia8: shower pythia8: TBP)+≡
  procedure, private :: set_user_process => shower_pythia8_set_user_process

(Shower pythia8: procedures)+≡
  subroutine shower_pythia8_set_user_process (shower, pset)
    class(shower_pythia8_t), intent(inout) :: shower
    type(particle_set_t), intent(in) :: pset
    integer, dimension(2) :: beam_pdg
    real(default), dimension(2) :: beam_energy
    integer, parameter :: process_id = 1, n_processes = 1
    if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_set_user_process")
    ! TODO sbrass find correct beam entries, fallback would be first two entries
    beam_pdg = [pset%prt(1)%get_pdg (), pset%prt(2)%get_pdg ()]
    beam_energy = [energy(pset%prt(1)%p), energy(pset%prt(2)%p)]
    call shower%lhaup%set_init (beam_pdg, beam_energy, &
      n_processes, unweighted = .false., negative_weights = .false.)
    call shower%lhaup%set_process_parameters (process_id = process_id, &
      cross_section = one, error = one)
  end subroutine shower_pythia8_set_user_process

```

Import a particle set and make it accessible for PYTHIA8 as an user process. We check whether the LHA object needs to be initialized and do the appropriate steps.

```

(Shower pythia8: shower pythia8: TBP)+≡
  procedure :: import_particle_set => shower_pythia8_import_particle_set

(Shower pythia8: procedures)+≡
  subroutine shower_pythia8_import_particle_set &
    (shower, particle_set)
    class(shower_pythia8_t), target, intent(inout) :: shower
    type(particle_set_t), intent(in) :: particle_set
    type(particle_set_t) :: pset_reduced
    integer, parameter :: PROCESS_ID = 1
    logical :: keep_beams
    if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_import_particle_set")
    if (.not. shower%user_process_set) then
      call shower%set_user_process (particle_set)
      shower%user_process_set = .true.
    end if
    if (debug_active (D_SHOWER)) then
      call particle_set%write (summary=.true., compressed=.true.)
    end if
    call shower%lhaup%set_event_process (process_id = PROCESS_ID, scale = shower%fac_scale, &
      alpha_qcd = shower%alpha_s, alpha_qed = -one, weight = -one)
    call shower%lhaup%set_event (process_id = PROCESS_ID, particle_set = particle_set, &
      keep_beams = .false., keep_remnants = .true., polarization = .true.)
    if (debug_active (D_SHOWER)) then
      call shower%lhaup%list_init ()
      call shower%lhaup%list_event ()
    end if
  end subroutine shower_pythia8_import_particle_set

```

```

<Shower pythia8: shower pythia8: TBP>+≡
  procedure :: generate_emissions => shower_pythia8_generate_emissions

<Shower pythia8: procedures>+≡
  subroutine shower_pythia8_generate_emissions &
    (shower, valid, number_of_emissions)
    class(shower_pythia8_t), intent(inout), target :: shower
    logical, intent(out) :: valid
    integer, optional, intent(in) :: number_of_emissions
    if (signal_is_pending ()) return
    call shower%transfer_settings ()
    call shower%pythia%next (valid)
  end subroutine shower_pythia8_generate_emissions

<Shower pythia8: shower pythia8: TBP>+≡
  procedure :: make_particle_set => shower_pythia8_make_particle_set

<Shower pythia8: procedures>+≡
  subroutine shower_pythia8_make_particle_set &
    (shower, particle_set, model, model_hadrons)
    class(shower_pythia8_t), intent(in) :: shower
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    class(model_data_t), intent(in), target :: model_hadrons
    type(particle_t), dimension(:), allocatable :: beam
    integer :: n_whizard, n_tot_pythia
    if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_make_particle_set")
    if (signal_is_pending ()) return
    associate (settings => shower%settings)
      if (debug_active (D_SHOWER)) then
        call msg_debug (D_SHOWER, 'Combine PYTHIA8 with particle set')
        call msg_debug (D_SHOWER, 'Particle set before replacing')
        call particle_set%write (summary=.true., compressed=.true.)
        call shower%pythia%list_event ()
        call msg_debug (D_SHOWER, string = "settings%hadron_collision", &
          value = settings%hadron_collision)
      end if
    end associate
    call shower%pythia%get_shower_particles (&
      model, model_hadrons, particle_set, &
      helicity = PRT_DEFINITE_HELICITY, &
      recover_beams = shower%settings%hadron_collision)
    if (debug_active (D_SHOWER)) then
      print *, 'Particle set after replacing'
      call particle_set%write (summary=.true., compressed=.true.)
    end if
  end subroutine shower_pythia8_make_particle_set

```

Transfer WHIZARD shower settings to Pythia8. Import a pointer to shower%rng and initialize Pythia itself, at once.

```

<Shower pythia8: shower pythia8: TBP>+≡
  procedure, private :: transfer_settings => shower_pythia8_transfer_settings

```

<Shower pythia8: procedures>+≡

```

subroutine shower_pythia8_transfer_settings (shower)
  class(shower_pythia8_t), intent(inout), target :: shower
  if (debug_on) call msg_debug (D_SHOWER, "shower_pythia8_transfer_settings")
  if (debug_on) call msg_debug2 (D_SHOWER, "pythia_initialized", shower%pythia_initialized)
  if (shower%pythia_initialized) return
  associate (pythia => shower%pythia)
    call pythia%set_lhaup_ptr (shower%lhaup)
    call pythia%import_rng (shower%rng)
    call shower%pythia%parse_and_set_config (shower%settings%pythia8_config)
    if (len (shower%settings%pythia8_config_file) > 0) &
      call pythia%read_file (shower%settings%pythia8_config_file)
    call pythia%read_string (var_str ("Beams:frameType = 5"))
    ! call pythia%read_string (var_str ("ParticleDecays:allowPhotonRadiation = off"))
    call pythia%read_string (var_str ("HadronLevel:all = off"))
    if (.not. shower%settings%verbose) then
      call pythia%read_string (var_str ("Print:quiet = on"))
    end if
    if (.not. shower%settings%isr_active) then
      call pythia%read_string (var_str ("PartonLevel:ISR = off"))
    else
      call pythia%read_string (var_str ("PartonLevel:ISR = on"))
    end if
    if (.not. shower%settings%fsr_active) then
      call pythia%read_string (var_str ("PartonLevel:FSR = off"))
    else
      call pythia%read_string (var_str ("PartonLevel:FSR = on"))
    end if
    call pythia%init_pythia ()
  end associate
  shower%pythia_initialized = .true.
end subroutine shower_pythia8_transfer_settings

```

<Shower pythia8: shower pythia8: TBP>+≡

```

procedure :: get_final_colored_ME_momenta => shower_pythia8_get_final_colored_ME_momenta

```

<Shower pythia8: procedures>+≡

```

subroutine shower_pythia8_get_final_colored_ME_momenta &
  (shower, momenta)
  class(shower_pythia8_t), intent(in) :: shower
  type(vector4_t), dimension(:), allocatable, intent(out) :: momenta
  if (debug_on) call msg_debug (D_MATCHING, "shower_pythia8_get_final_colored_ME_momenta")
  call shower%pythia%get_final_colored_ME_momenta (momenta)
end subroutine shower_pythia8_get_final_colored_ME_momenta

```

Chapter 23

Multiple Interactions (MPI) Code

23.1 The Multiple Interactions main module

This file contains the module `muli` which is the multiple parton interactions interface module to `WHIZARD`. `muli` is supposed to run together with initial state radiation. Both share a momentum evolution variable and compete for beam momentum, so the generation of this scale variable must be fully transparent to `WHIZARD`. This here is a stub as long as there is no working `WHIZARD` implementation for multiple interactions. It gives an interface for the necessary routines.

```
<muli.f90>≡  
  <File header>  
  
  module muli  
    use, intrinsic :: iso_fortran_env  
    <Use kinds>  
  
    <Standard module head>  
  
    <Muli: variables>  
  
    <Muli: public>  
  
    <Muli: types>  
  
    contains  
  
    <Muli: procedures>  
  
  end module muli
```

23.1.1 The main Multiple Interactions type

```
<Muli: public>≡
```

No internal dependencies

Figure 23.1: Module dependencies in `src/muli`.

```
public :: muli_t
<Muli: types>≡
  type :: muli_t
    real(default) :: GeV2_scale_cutoff
    logical :: initialized = .false.
    integer, dimension(4) :: flow
    contains
    <Muli: muli: TBP>
  end type muli_t

<Muli: muli: TBP>≡
  generic :: initialize => muli_initialize
  procedure :: muli_initialize

<Muli: procedures>≡
  subroutine muli_initialize (this, GeV2_scale_cutoff, gev2_s, &
    muli_dir, random_seed)
    class(muli_t), intent(out) :: this
    real(kind=default), intent(in) :: gev2_s, GeV2_scale_cutoff
    character(*), intent(in) :: muli_dir
    integer, intent(in), optional :: random_seed
    this%initialized = .true.
  end subroutine muli_initialize

<Muli: muli: TBP>+≡
  procedure :: apply_initial_interaction => muli_apply_initial_interaction

<Muli: procedures>+≡
  subroutine muli_apply_initial_interaction (this, GeV2_s, &
    x1, x2, pdg_f1, pdg_f2, n1, n2)
    class(muli_t), intent(inout) :: this
    real(default), intent(in) :: GeV2_s, x1, x2
    integer, intent(in):: pdg_f1, pdg_f2, n1, n2
  end subroutine muli_apply_initial_interaction
```

```

<Muli: muli: TBP>+≡
  procedure :: restart => muli_restart

<Muli: procedures>+≡
  subroutine muli_restart (this)
    class(muli_t), intent(inout) :: this
  end subroutine muli_restart

<Muli: muli: TBP>+≡
  procedure :: is_initialized => muli_is_initialized

<Muli: procedures>+≡
  elemental function muli_is_initialized (this) result (res)
    logical :: res
    class(muli_t), intent(in) :: this
    res = this%initialized
  end function muli_is_initialized

<Muli: muli: TBP>+≡
  procedure :: generate_gev2_pt2 => muli_generate_gev2_pt2

<Muli: procedures>+≡
  subroutine muli_generate_gev2_pt2 (this, gev2_start_scale, gev2_new_scale)
    class(muli_t), intent(inout) :: this
    real(kind=default), intent(in) :: gev2_start_scale
    real(kind=default), intent(out) :: gev2_new_scale
    call this%generate_next_scale ()
    gev2_new_scale = 1
  end subroutine muli_generate_gev2_pt2

<Muli: muli: TBP>+≡
  procedure :: generate_partons => muli_generate_partons

<Muli: procedures>+≡
  subroutine muli_generate_partons (this, n1, n2, x_proton_1, x_proton_2, &
    pdg_f1, pdg_f2, pdg_f3, pdg_f4)
    class(muli_t), intent(inout) :: this
    integer, intent(in) :: n1, n2
    real(kind=default), intent(out) :: x_proton_1, x_proton_2
    integer, intent(out) :: pdg_f1, pdg_f2, pdg_f3, pdg_f4
    integer, dimension(4) :: pdg_f
    call this%generate_color_flows ()
    pdg_f = 0
    pdg_f1 = 0
    pdg_f2 = 0
    pdg_f3 = 0
    pdg_f4 = 0
  end subroutine muli_generate_partons

<Muli: muli: TBP>+≡
  procedure :: generate_color_flows => muli_generate_color_flows

```



```

<Muli: procedures>+≡
  subroutine multi_generate_color_flows (this)
    class(muli_t), intent(inout) :: this
    integer, dimension(4) :: flow
  end subroutine multi_generate_color_flows

<Muli: muli: TBP>+≡
  procedure :: get_color_flow => multi_get_color_flow

<Muli: procedures>+≡
  pure function multi_get_color_flow (this) result (flow)
    class(muli_t), intent(in) :: this
    integer, dimension(4) :: flow
    flow = this%flow
  end function multi_get_color_flow

<Muli: muli: TBP>+≡
  procedure :: get_color_correlations => multi_get_color_correlations

<Muli: procedures>+≡
  subroutine multi_get_color_correlations &
    (this, start_index, final_index, flow)
    class(muli_t), intent(in) :: this
    integer, intent(in) :: start_index
    integer, intent(out) :: final_index
    integer, dimension(2,4), intent(out) :: flow
    integer :: pos, f_end, f_beginning
    final_index = start_index
    flow = reshape([0,0,0,0,0,0,0,0],[2,4])
  end subroutine multi_get_color_correlations

<Muli: muli: TBP>+≡
  procedure :: replace_parton => multi_replace_parton

<Muli: procedures>+≡
  subroutine multi_replace_parton &
    (this, proton_id, old_id, new_id, pdg_f, x_proton, gev_scale)
    class(muli_t), intent(inout) :: this
    integer, intent(in) :: proton_id, old_id, new_id, pdg_f
    real(kind=default), intent(in) :: x_proton, gev_scale
  end subroutine multi_replace_parton

<Muli: muli: TBP>+≡
  procedure :: generate_next_scale => multi_generate_next_scale

<Muli: procedures>+≡
  subroutine multi_generate_next_scale (this, integrand_kind)
    class(muli_t), intent(inout) :: this
    integer, intent(in), optional :: integrand_kind
  end subroutine multi_generate_next_scale

```

Chapter 24

BLHA Interface

The code in this chapter implements support for the BLHA record that communicates data for NLO processes.

These are the modules:

blha_config

blha_interface

blha_driver

24.1 Module definition

These modules implement the communication with one loop matrix element providers according to the Binoth LesHouches Accord Interface. The actual matrix element(s) are loaded as a dynamic library.

This module defines the common OLP-interfaces defined through the Binoth Les-Houches accord.

```
<blha_olp_interfaces.f90>≡  
  <File header>  
  
  module blha_olp_interfaces  
  
    use, intrinsic :: iso_c_binding !NODEP!  
    use, intrinsic :: iso_fortran_env  
  
    use kinds  
    <Use strings>  
    <Use debug>  
    use constants  
    use numeric_utils, only: vanishes  
    use numeric_utils, only: extend_integer_array, crop_integer_array  
    use io_units  
    use string_utils  
    use physics_defs  
    use diagnostics  
    use os_interface
```

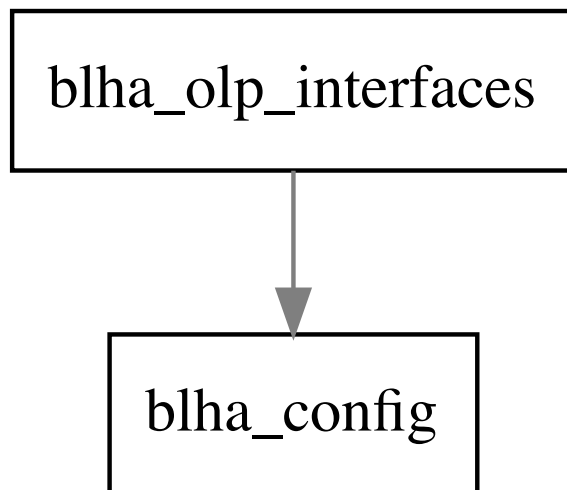


Figure 24.1: Module dependencies in `src/blha`.

```

use lorentz
use sm_qcd
use interactions
use flavors
use model_data
use pdg_arrays, only: is_gluon, is_quark, qcd_ew_interferences

use prclib_interfaces
use process_libraries
use prc_core_def
use prc_core

use prc_external

use blha_config

<Standard module head>

<BLHA OLP interfaces: public>

<BLHA OLP interfaces: public parameters>

<BLHA OLP interfaces: parameters>

<BLHA OLP interfaces: types>

<BLHA OLP interfaces: interfaces>

contains

<BLHA OLP interfaces: procedures>

end module blha_olp_interfaces

<BLHA OLP interfaces: public>≡
  public :: blha_template_t

<BLHA OLP interfaces: types>≡
  type :: blha_template_t
    integer :: I_BORN = 0
    integer :: I_REAL = 1
    integer :: I_LOOP = 2
    integer :: I_SUB = 3
    integer :: I_DGLAP = 4
    logical, dimension(0:4) :: compute_component
    logical :: include_polarizations = .false.
    logical :: switch_off_muon_yukawas = .false.
    logical :: use_internal_color_correlations = .true.
    real(default) :: external_top_yukawa = -1._default
    integer :: ew_scheme
    integer :: loop_method = BLHA_MODE_GENERIC
contains
  <BLHA OLP interfaces: blha template: TBP>
end type blha_template_t

```

```

<BLHA OLP interfaces: blha template: TBP>≡
  procedure :: write => blha_template_write

<BLHA OLP interfaces: procedures>≡
  subroutine blha_template_write (blha_template, unit)
    class(blha_template_t), intent(in) :: blha_template
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u,"(A,4(L1))") "Compute components: ", &
      blha_template%compute_component
    write (u,"(A,L1)") "Include polarizations: ", &
      blha_template%include_polarizations
    write (u,"(A,L1)") "Switch off muon yukawas: ", &
      blha_template%switch_off_muon_yukawas
    write (u,"(A,L1)") "Use internal color correlations: ", &
      blha_template%use_internal_color_correlations
  end subroutine blha_template_write

```

Compute the total number of used helicity states for the given particle PDG codes, given a model. Applies only if polarization is supported. This yields the `n_hel` value as required below.

```

<BLHA OLP interfaces: blha template: TBP>+≡
  procedure :: get_n_hel => blha_template_get_n_hel

<BLHA OLP interfaces: procedures>+≡
  function blha_template_get_n_hel (blha_template, pdg, model) result (n_hel)
    class(blha_template_t), intent(in) :: blha_template
    integer, dimension(:), intent(in) :: pdg
    class(model_data_t), intent(in), target :: model
    integer :: n_hel
    type(flavor_t) :: flv
    integer :: f
    n_hel = 1
    if (blha_template%include_polarizations) then
      do f = 1, size (pdg)
        call flv%init (pdg(f), model)
        n_hel = n_hel * flv%get_multiplicity ()
      end do
    end if
  end function blha_template_get_n_hel

```

```

<BLHA OLP interfaces: parameters>≡
  integer, parameter :: I_ALPHA_0 = 1
  integer, parameter :: I_GF = 2
  integer, parameter :: I_ALPHA_MZ = 3
  integer, parameter :: I_ALPHA_INTERNAL = 4
  integer, parameter :: I_SW2 = 5

```

```

<BLHA OLP interfaces: public>+≡
  public :: prc_blha_t

```

```

<BLHA OLP interfaces: types>+≡
type, abstract, extends (prc_external_t) :: prc_blha_t
  integer :: n_particles
  integer :: n_hel
  integer :: n_proc
  integer, dimension(:, :), allocatable :: i_tree, i_spin_c, i_color_c
  integer, dimension(:, :), allocatable :: i_virt
  integer, dimension(:, :), allocatable :: i_hel
  logical, dimension(5) :: ew_parameter_mask
  integer :: sqme_tree_pos
contains
<BLHA OLP interfaces: prc blha: TBP>
end type prc_blha_t

```

Obviously, this process-core type uses the BLHA interface.

```

<BLHA OLP interfaces: prc blha: TBP>≡
  procedure, nopass :: uses_blha => prc_blha_uses_blha

<BLHA OLP interfaces: procedures>+≡
  function prc_blha_uses_blha () result (flag)
    logical :: flag
    flag = .true.
  end function prc_blha_uses_blha

```

```

<BLHA OLP interfaces: public>+≡
  public :: blha_driver_t

<BLHA OLP interfaces: types>+≡
type, abstract, extends (prc_external_driver_t) :: blha_driver_t
  type(string_t) :: contract_file
  type(string_t) :: nlo_suffix
  logical :: include_polarizations = .false.
  logical :: switch_off_muon_yukawas = .false.
  real(default) :: external_top_yukawa = -1.0
  procedure(olp_start), nopass, pointer :: &
    blha_olp_start => null ()
  procedure(olp_eval), nopass, pointer :: &
    blha_olp_eval => null()
  procedure(olp_info), nopass, pointer :: &
    blha_olp_info => null ()
  procedure(olp_set_parameter), nopass, pointer :: &
    blha_olp_set_parameter => null ()
  procedure(olp_eval2), nopass, pointer :: &
    blha_olp_eval2 => null ()
  procedure(olp_option), nopass, pointer :: &
    blha_olp_option => null ()
  procedure(olp_polvec), nopass, pointer :: &
    blha_olp_polvec => null ()
  procedure(olp_finalize), nopass, pointer :: &
    blha_olp_finalize => null ()
  procedure(olp_print_parameter), nopass, pointer :: &
    blha_olp_print_parameter => null ()
contains
<BLHA OLP interfaces: blha driver: TBP>

```

```

end type blha_driver_t

<BLHA OLP interfaces: public>+≡
  public :: prc_blha_writer_t

<BLHA OLP interfaces: types>+≡
  type, abstract, extends (prc_external_writer_t) :: prc_blha_writer_t
  type(blha_configuration_t) :: blha_cfg
  contains
  <BLHA OLP interfaces: blha writer: TBP>
  end type prc_blha_writer_t

<BLHA OLP interfaces: public>+≡
  public :: blha_def_t

<BLHA OLP interfaces: types>+≡
  type, abstract, extends (prc_external_def_t) :: blha_def_t
  type(string_t) :: suffix
  contains
  <BLHA OLP interfaces: blha def: TBP>
  end type blha_def_t

<BLHA OLP interfaces: public>+≡
  public :: blha_state_t

<BLHA OLP interfaces: types>+≡
  type, abstract, extends (prc_external_state_t) :: blha_state_t
  contains
  <BLHA OLP interfaces: blha state: TBP>
  end type blha_state_t

<BLHA OLP interfaces: blha state: TBP>≡
  procedure :: reset_new_kinematics => blha_state_reset_new_kinematics

<BLHA OLP interfaces: procedures>+≡
  subroutine blha_state_reset_new_kinematics (object)
    class(blha_state_t), intent(inout) :: object
    object%new_kinematics = .true.
  end subroutine blha_state_reset_new_kinematics

<BLHA OLP interfaces: public parameters>≡
  integer, parameter, public :: OLP_PARAMETER_LIMIT = 10
  integer, parameter, public :: OLP_MOMENTUM_LIMIT = 50
  integer, parameter, public :: OLP_RESULTS_LIMIT = 60

<BLHA OLP interfaces: public>+≡
  public :: olp_start

```

```

<BLHA OLP interfaces: interfaces>≡
interface
  subroutine olp_start (contract_file_name, ierr) bind (C,name = "OLP_Start")
    import
    character(kind = c_char, len = 1), intent(in) :: contract_file_name
    integer(kind = c_int), intent(out) :: ierr
  end subroutine olp_start
end interface

```

```

<BLHA OLP interfaces: public>+=
public :: olp_eval

```

```

<BLHA OLP interfaces: interfaces>+=
interface
  subroutine olp_eval (label, momenta, mu, parameters, res) &
    bind (C, name = "OLP_EvalSubProcess")
    import
    integer(kind = c_int), value, intent(in) :: label
    real(kind = c_double), value, intent(in) :: mu
    real(kind = c_double), dimension(OLP_MOMENTUM_LIMIT), intent(in) :: &
      momenta
    real(kind = c_double), dimension(OLP_PARAMETER_LIMIT), intent(in) :: &
      parameters
    real(kind = c_double), dimension(OLP_RESULTS_LIMIT), intent(out) :: res
  end subroutine olp_eval
end interface

```

```

<BLHA OLP interfaces: public>+=
public :: olp_info

```

```

<BLHA OLP interfaces: interfaces>+=
interface
  subroutine olp_info (olp_file, olp_version, message) bind(C)
    import
    character(kind = c_char), intent(inout), dimension(15) :: olp_file
    character(kind = c_char), intent(inout), dimension(15) :: olp_version
    character(kind = c_char), intent(inout), dimension(255) :: message
  end subroutine olp_info
end interface

```

```

<BLHA OLP interfaces: public>+=
public :: olp_set_parameter

```

```

<BLHA OLP interfaces: interfaces>+=
interface
  subroutine olp_set_parameter &
    (variable_name, real_part, complex_part, success) bind(C)
    import
    character(kind = c_char,len = 1), intent(in) :: variable_name
    real(kind = c_double), intent(in) :: real_part, complex_part
    integer(kind = c_int), intent(out) :: success
  end subroutine olp_set_parameter
end interface

```



```

<BLHA OLP interfaces: public>+≡
    public :: olp_eval2

<BLHA OLP interfaces: interfaces>+≡
    interface
        subroutine olp_eval2 (label, momenta, mu, res, acc) bind(C)
            import
            integer(kind = c_int), intent(in) :: label
            real(kind = c_double), intent(in) :: mu
            real(kind = c_double), dimension(OLP_MOMENTUM_LIMIT), intent(in) :: momenta
            real(kind = c_double), dimension(OLP_RESULTS_LIMIT), intent(out) :: res
            real(kind = c_double), intent(out) :: acc
        end subroutine olp_eval2
    end interface

<BLHA OLP interfaces: public>+≡
    public :: olp_option

<BLHA OLP interfaces: interfaces>+≡
    interface
        subroutine olp_option (line, stat) bind(C)
            import
            character(kind = c_char, len=1), intent(in) :: line
            integer(kind = c_int), intent(out) :: stat
        end subroutine
    end interface

<BLHA OLP interfaces: public>+≡
    public :: olp_polvec

<BLHA OLP interfaces: interfaces>+≡
    interface
        subroutine olp_polvec (p, q, eps) bind(C)
            import
            real(kind = c_double), dimension(0:3), intent(in) :: p, q
            real(kind = c_double), dimension(0:7), intent(out) :: eps
        end subroutine
    end interface

<BLHA OLP interfaces: public>+≡
    public :: olp_finalize

<BLHA OLP interfaces: interfaces>+≡
    interface
        subroutine olp_finalize () bind(C)
            import
        end subroutine olp_finalize
    end interface

<BLHA OLP interfaces: public>+≡
    public :: olp_print_parameter

```

```

<BLHA OLP interfaces: interfaces>+≡
interface
  subroutine olp_print_parameter (filename) bind(C)
    import
    character(kind = c_char, len = 1), intent(in) :: filename
  end subroutine olp_print_parameter
end interface

<BLHA OLP interfaces: public>+≡
public :: blha_result_array_size

<BLHA OLP interfaces: procedures>+≡
pure function blha_result_array_size (n_part, amp_type) result (rsize)
  integer, intent(in) :: n_part, amp_type
  integer :: rsize
  select case (amp_type)
    case (BLHA_AMP_TREE)
      rsize = 1
    case (BLHA_AMP_LOOP)
      rsize = 4
    case (BLHA_AMP_COLOR_C)
      rsize = n_part * (n_part - 1) / 2
    case (BLHA_AMP_SPIN_C)
      rsize = 2 * n_part**2
    case default
      rsize = 0
  end select
end function blha_result_array_size

<BLHA OLP interfaces: prc blha: TBP>+≡
procedure :: create_momentum_array => prc_blha_create_momentum_array

<BLHA OLP interfaces: procedures>+≡
function prc_blha_create_momentum_array (object, p) result (mom)
  class(prc_blha_t), intent(in) :: object
  type(vector4_t), intent(in), dimension(:) :: p
  real(double), dimension(5*object%n_particles) :: mom
  integer :: n, i, k

  n = size (p)
  if (n > 10) call msg_fatal ("Number of external particles exceeds" &
    // "size of BLHA-internal momentum array")

  mom = zero
  k = 1
  do i = 1, n
    mom(k : k + 3) = vector4_get_components (p(i))
    mom(k + 4) = invariant_mass (p(i))
    k = k + 5
  end do
end function prc_blha_create_momentum_array

<BLHA OLP interfaces: blha template: TBP>+≡
procedure :: init => blha_template_init

```

```

<BLHA OLP interfaces: procedures>+≡
  subroutine blha_template_init (template, requires_polarizations, &
    switch_off_muon_yukawas, external_top_yukawa, ew_scheme)
    class(blha_template_t), intent(inout) :: template
    logical, intent(in) :: requires_polarizations, switch_off_muon_yukawas
    real(default), intent(in) :: external_top_yukawa
    type(string_t), intent(in) :: ew_scheme
    template%compute_component = .false.
    template%include_polarizations = requires_polarizations
    template%switch_off_muon_yukawas = switch_off_muon_yukawas
    template%external_top_yukawa = external_top_yukawa
    template%ew_scheme = ew_scheme_string_to_int (ew_scheme)
  end subroutine blha_template_init

```

```

<BLHA OLP interfaces: blha template: TBP>+≡
  procedure :: set_born => blha_template_set_born
  procedure :: set_real_trees => blha_template_set_real_trees
  procedure :: set_loop => blha_template_set_loop
  procedure :: set_subtraction => blha_template_set_subtraction
  procedure :: set_dglap => blha_template_set_dglap

```

```

<BLHA OLP interfaces: procedures>+≡
  subroutine blha_template_set_born (template)
    class(blha_template_t), intent(inout) :: template
    template%compute_component (template%I_BORN) = .true.
  end subroutine blha_template_set_born

  subroutine blha_template_set_real_trees (template)
    class(blha_template_t), intent(inout) :: template
    template%compute_component (template%I_REAL) = .true.
  end subroutine blha_template_set_real_trees

  subroutine blha_template_set_loop (template)
    class(blha_template_t), intent(inout) :: template
    template%compute_component(template%I_LOOP) = .true.
  end subroutine blha_template_set_loop

  subroutine blha_template_set_subtraction (template)
    class(blha_template_t), intent(inout) :: template
    template%compute_component (template%I_SUB) = .true.
  end subroutine blha_template_set_subtraction

  subroutine blha_template_set_dglap (template)
    class(blha_template_t), intent(inout) :: template
    template%compute_component (template%I_DGLAP) = .true.
  end subroutine blha_template_set_dglap

```

```

<BLHA OLP interfaces: blha template: TBP>+≡
  procedure :: set_internal_color_correlations &
    => blha_template_set_internal_color_correlations

```

```

<BLHA OLP interfaces: procedures>+≡
  subroutine blha_template_set_internal_color_correlations (template)
    class(blha_template_t), intent(inout) :: template

```

```

        template%use_internal_color_correlations = .true.
    end subroutine blha_template_set_internal_color_correlations

<BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: get_internal_color_correlations &
        => blha_template_get_internal_color_correlations

<BLHA OLP interfaces: procedures>+≡
    pure function blha_template_get_internal_color_correlations (template) &
        result (val)
        logical :: val
        class(blha_template_t), intent(in) :: template
        val = template%use_internal_color_correlations
    end function blha_template_get_internal_color_correlations

<BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: compute_born => blha_template_compute_born
    procedure :: compute_real_trees => blha_template_compute_real_trees
    procedure :: compute_loop => blha_template_compute_loop
    procedure :: compute_subtraction => blha_template_compute_subtraction
    procedure :: compute_dglap => blha_template_compute_dglap

<BLHA OLP interfaces: procedures>+≡
    pure function blha_template_compute_born (template) result (val)
        class(blha_template_t), intent(in) :: template
        logical :: val
        val = template%compute_component (template%I_BORN)
    end function blha_template_compute_born

    pure function blha_template_compute_real_trees (template) result (val)
        class(blha_template_t), intent(in) :: template
        logical :: val
        val = template%compute_component (template%I_REAL)
    end function blha_template_compute_real_trees

    pure function blha_template_compute_loop (template) result (val)
        class(blha_template_t), intent(in) :: template
        logical :: val
        val = template%compute_component (template%I_LOOP)
    end function blha_template_compute_loop

    pure function blha_template_compute_subtraction (template) result (val)
        class(blha_template_t), intent(in) :: template
        logical :: val
        val = template%compute_component (template%I_SUB)
    end function blha_template_compute_subtraction

    pure function blha_template_compute_dglap (template) result (val)
        class(blha_template_t), intent(in) :: template
        logical :: val
        val = template%compute_component (template%I_DGLAP)
    end function blha_template_compute_dglap

```

```

<BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: set_loop_method => blha_template_set_loop_method

<BLHA OLP interfaces: procedures>+≡
    subroutine blha_template_set_loop_method (template, master)
        class(blha_template_t), intent(inout) :: template
        class(blha_master_t), intent(in) :: master
        template%loop_method = master%blha_mode(1)
    end subroutine blha_template_set_loop_method

<BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: check => blha_template_check

<BLHA OLP interfaces: procedures>+≡
    function blha_template_check (template) result (val)
        class(blha_template_t), intent(in) :: template
        logical :: val
        val = count (template%compute_component) == 1
    end function blha_template_check

<BLHA OLP interfaces: blha template: TBP>+≡
    procedure :: reset => blha_template_reset

<BLHA OLP interfaces: procedures>+≡
    subroutine blha_template_reset (template)
        class(blha_template_t), intent(inout) :: template
        template%compute_component = .false.
    end subroutine blha_template_reset

<BLHA OLP interfaces: blha writer: TBP>≡
    procedure :: write => prc_blha_writer_write

<BLHA OLP interfaces: procedures>+≡
    subroutine prc_blha_writer_write (writer, unit)
        class(prc_blha_writer_t), intent(in) :: writer
        integer, intent(in) :: unit
        write (unit, "(1x,A)") char (writer%get_process_string ())
    end subroutine prc_blha_writer_write

<BLHA OLP interfaces: blha writer: TBP>+≡
    procedure :: get_process_string => prc_blha_writer_get_process_string

<BLHA OLP interfaces: procedures>+≡
    function prc_blha_writer_get_process_string (writer) result (s_proc)
        class(prc_blha_writer_t), intent(in) :: writer
        type(string_t) :: s_proc
        s_proc = var_str ("")
    end function prc_blha_writer_get_process_string

<BLHA OLP interfaces: blha writer: TBP>+≡
    procedure :: get_n_proc => prc_blha_writer_get_n_proc

```

```

<BLHA OLP interfaces: procedures>+≡
function prc_blha_writer_get_n_proc (writer) result (n_proc)
  class(prc_blha_writer_t), intent(in) :: writer
  integer :: n_proc
  n_proc = blha_configuration_get_n_proc (writer%blha_cfg)
end function prc_blha_writer_get_n_proc

<BLHA OLP interfaces: blha driver: TBP>≡
procedure(blha_driver_set_GF), deferred :: &
  set_GF

<BLHA OLP interfaces: interfaces>+≡
abstract interface
  subroutine blha_driver_set_GF (driver, GF)
    import
    class(blha_driver_t), intent(inout) :: driver
    real(default), intent(in) :: GF
  end subroutine blha_driver_set_GF
end interface

<BLHA OLP interfaces: blha driver: TBP>+≡
procedure(blha_driver_set_alpha_s), deferred :: &
  set_alpha_s

<BLHA OLP interfaces: interfaces>+≡
abstract interface
  subroutine blha_driver_set_alpha_s (driver, alpha_s)
    import
    class(blha_driver_t), intent(in) :: driver
    real(default), intent(in) :: alpha_s
  end subroutine blha_driver_set_alpha_s
end interface

<BLHA OLP interfaces: blha driver: TBP>+≡
procedure(blha_driver_set_weinberg_angle), deferred :: &
  set_weinberg_angle

<BLHA OLP interfaces: interfaces>+≡
abstract interface
  subroutine blha_driver_set_weinberg_angle (driver, sw2)
    import
    class(blha_driver_t), intent(inout) :: driver
    real(default), intent(in) :: sw2
  end subroutine blha_driver_set_weinberg_angle
end interface

<BLHA OLP interfaces: blha driver: TBP>+≡
procedure(blha_driver_set_alpha_qed), deferred :: set_alpha_qed

<BLHA OLP interfaces: interfaces>+≡
abstract interface
  subroutine blha_driver_set_alpha_qed (driver, alpha)
    import
    class(blha_driver_t), intent(inout) :: driver

```

```

        real(default), intent(in) :: alpha
    end subroutine blha_driver_set_alpha_qed
end interface

<BLHA OLP interfaces: blha_driver: TBP>+≡
    procedure(blha_driver_print_alpha_s), deferred :: &
        print_alpha_s

<BLHA OLP interfaces: interfaces>+≡
    abstract interface
        subroutine blha_driver_print_alpha_s (object)
            import
            class(blha_driver_t), intent(in) :: object
        end subroutine blha_driver_print_alpha_s
    end interface

<BLHA OLP interfaces: public>+≡
    public :: parameter_error_message

<BLHA OLP interfaces: procedures>+≡
    subroutine parameter_error_message (par, subr)
        type(string_t), intent(in) :: par, subr
        type(string_t) :: message
        message = "Setting of parameter " // par &
            // "failed in " // subr // "!"
        call msg_fatal (char (message))
    end subroutine parameter_error_message

<BLHA OLP interfaces: public>+≡
    public :: ew_parameter_error_message

<BLHA OLP interfaces: procedures>+≡
    subroutine ew_parameter_error_message (par)
        type(string_t), intent(in) :: par
        type(string_t) :: message
        message = "Setting of parameter " // par &
            // "failed. This happens because the chosen " &
            // "EWScheme in the BLHA file does not fit " &
            // "your parameter choice"
        call msg_fatal (char (message))
    end subroutine ew_parameter_error_message

<BLHA OLP interfaces: blha_driver: TBP>+≡
    procedure :: set_mass_and_width => blha_driver_set_mass_and_width

<BLHA OLP interfaces: procedures>+≡
    subroutine blha_driver_set_mass_and_width &
        (driver, i_pdg, mass, width)
        class(blha_driver_t), intent(inout) :: driver
        integer, intent(in) :: i_pdg
        real(default), intent(in), optional :: mass
        real(default), intent(in), optional :: width
        type(string_t) :: buf
        character(kind=c_char,len=20) :: c_string

```

```

integer :: ierr
if (present (mass)) then
  buf = 'mass(' // str (abs(i_pdg)) // ')'
  c_string = char(buf) // c_null_char
  call driver%blha_olp_set_parameter &
    (c_string, dble(mass), 0._double, ierr)
  if (ierr == 0) then
    buf = "BLHA driver: Attempt to set mass of particle " // &
      str (abs(i_pdg)) // "failed"
    call msg_fatal (char(buf))
  end if
end if
if (present (width)) then
  buf = 'width(' // str (abs(i_pdg)) // ')'
  c_string = char(buf)//c_null_char
  call driver%blha_olp_set_parameter &
    (c_string, dble(width), 0._double, ierr)
  if (ierr == 0) then
    buf = "BLHA driver: Attempt to set width of particle " // &
      str (abs(i_pdg)) // "failed"
    call msg_fatal (char(buf))
  end if
end if
end subroutine blha_driver_set_mass_and_width

```

<BLHA OLP interfaces: blha driver: TBP>+≡
 procedure(blha_driver_init_dlaccess_to_library), deferred :: &
 init_dlaccess_to_library

<BLHA OLP interfaces: interfaces>+≡
 abstract interface
 subroutine blha_driver_init_dlaccess_to_library &
 (object, os_data, dlaccess, success)
 import
 class(blha_driver_t), intent(in) :: object
 type(os_data_t), intent(in) :: os_data
 type(dlaccess_t), intent(out) :: dlaccess
 logical, intent(out) :: success
 end subroutine blha_driver_init_dlaccess_to_library
end interface

<BLHA OLP interfaces: blha driver: TBP>+≡
 procedure :: load => blha_driver_load

<BLHA OLP interfaces: procedures>+≡
 subroutine blha_driver_load (object, os_data, success)
 class(blha_driver_t), intent(inout) :: object
 type(os_data_t), intent(in) :: os_data
 logical, intent(out) :: success
 type(dlaccess_t) :: dlaccess
 type(c_funptr) :: c_funptr
 logical :: init_success

 call object%init_dlaccess_to_library (os_data, dlaccess, init_success)


```

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Start"))
call c_f_procpointer (c_fptr, object%blha_olp_start)
call check_for_error (var_str ("OLP_Start"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_EvalSubProcess"))
call c_f_procpointer (c_fptr, object%blha_olp_eval)
call check_for_error (var_str ("OLP_EvalSubProcess"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Info"))
call c_f_procpointer (c_fptr, object%blha_olp_info)
call check_for_error (var_str ("OLP_Info"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_SetParameter"))
call c_f_procpointer (c_fptr, object%blha_olp_set_parameter)
call check_for_error (var_str ("OLP_SetParameter"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_EvalSubProcess2"))
call c_f_procpointer (c_fptr, object%blha_olp_eval2)
call check_for_error (var_str ("OLP_EvalSubProcess2"))

!!! The following three functions are not implemented in OpenLoops.
!!! In another BLHA provider, they need to be implemented separately.

!!! c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Option"))
!!! call c_f_procpointer (c_fptr, object%blha_olp_option)
!!! call check_for_error (var_str ("OLP_Option"))

!!! c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Polvec"))
!!! call c_f_procpointer (c_fptr, object%blha_olp_polvec)
!!! call check_for_error (var_str ("OLP_Polvec"))

!!! c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_Finalize"))
!!! call c_f_procpointer (c_fptr, object%blha_olp_finalize)
!!! call check_for_error (var_str ("OLP_Finalize"))

c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("OLP_PrintParameter"))
call c_f_procpointer (c_fptr, object%blha_olp_print_parameter)
call check_for_error (var_str ("OLP_PrintParameter"))

success = .true.
contains
  subroutine check_for_error (function_name)
    type(string_t), intent(in) :: function_name
    if (dlaccess_has_error (dlaccess)) &
      call msg_fatal (char ("Loading of " // function_name // " failed!"))
  end subroutine check_for_error
end subroutine blha_driver_load

```

```

<BLHA OLP interfaces: parameters>+≡
  integer, parameter :: LEN_MAX_FLAVOR_STRING = 100
  integer, parameter :: N_MAX_FLAVORS = 100
<BLHA OLP interfaces: blha driver: TBP>+≡

```

```

procedure :: read_contract_file => blha_driver_read_contract_file
<BLHA OLP interfaces: procedures>+=
subroutine blha_driver_read_contract_file (driver, flavors, &
    amp_type, flv_index, hel_index, label, helicities)
class(blha_driver_t), intent(inout) :: driver
integer, intent(in), dimension(:, :) :: flavors
integer, intent(out), dimension(:), allocatable :: amp_type, &
    flv_index, hel_index, label
integer, intent(out), dimension(:, :) :: helicities
integer :: unit, filestat
character(len=LEN_MAX_FLAVOR_STRING) :: rd_line
logical :: read_flavor, give_warning
integer :: label_count, i_flv, i
integer :: i_hel, n_in
integer :: i_next, n_entries
integer, dimension(size(flavors, 1) + 2) :: i_array
integer, dimension(size(flavors, 1) + 2) :: hel_array
integer, dimension(size(flavors, 1)) :: flv_array
integer, parameter :: NO_NUMBER = -1000
integer, parameter :: PROC_NOT_FOUND = -1001
integer, parameter :: list_incr = 50
integer :: n_found
allocate (amp_type (N_MAX_FLAVORS), flv_index (N_MAX_FLAVORS), &
    hel_index (N_MAX_FLAVORS), label (N_MAX_FLAVORS))
amp_type = -1; flv_index = -1; hel_index = -1; label = -1
helicities = 0
n_in = size (helicities, dim = 2)
n_entries = size (flavors, 1) + 2
unit = free_unit ()
open (unit, file = char (driver%contract_file), status="old")
read_flavor = .false.
label_count = 1
i_hel = 1
n_found = 0
give_warning = .false.
do
    read (unit, "(A)", iostat = filestat) rd_line
    if (filestat == iostat_end) then
        exit
    else
        if (rd_line(1:13) == 'AmplitudeType') then
            if (i_hel > 2 * n_in) i_hel = 1
            i_next = find_next_word_index (rd_line, 13)
            if (label_count > size (amp_type)) &
                call extend_integer_array (amp_type, list_incr)
            if (rd_line(i_next : i_next + 4) == 'Loop') then
                amp_type(label_count) = BLHA_AMP_LOOP
            else if (rd_line(i_next : i_next + 4) == 'Tree') then
                amp_type(label_count) = BLHA_AMP_TREE
            else if (rd_line(i_next : i_next + 6) == 'ccTree') then
                amp_type(label_count) = BLHA_AMP_COLOR_C
            else if (rd_line(i_next : i_next + 6) == 'scTree' .or. &
                rd_line(i_next : i_next + 14) == 'sctree_polvect') then
                amp_type(label_count) = BLHA_AMP_SPIN_C
            end if
            label_count = label_count + 1
            i_hel = i_hel + 1
            n_entries = n_entries + 1
            n_found = n_found + 1
        end if
    end do
end subroutine

```

```

else
    call msg_fatal ("AmplitudeType present but AmpType not known!")
end if
read_flavor = .true.
else if (read_flavor .and. .not. (rd_line(1:13) == 'CouplingPower' &
    .or. rd_line(1:14) == 'CorrectionType')) then
    i_array = create_flavor_string (rd_line, n_entries)
    if (driver%include_polarizations) then
        hel_array = create_helicity_string (rd_line, n_entries)
        call check_helicity_array (hel_array, n_entries, n_in)
    else
        hel_array = 0
    end if
    if (.not. all (i_array == PROC_NOT_FOUND)) then
        do i_flv = 1, size (flavors, 2)
            flv_array = 0
            do i = 1, size (flv_array)
                if (i_array (i) == PHOTON_OFFSHELL .and. &
                    flavors (i, i_flv) == PHOTON) then
                    flv_array (i) = i_array (i)
                else
                    flv_array (i) = flavors (i, i_flv)
                end if
            end do
            if (all (i_array (1 : n_entries - 2) == flv_array (:))) then
                if (label_count > size (label)) &
                    call extend_integer_array (label, list_incr)
                label(label_count) = i_array (n_entries)
                if (label_count > size (flv_index)) &
                    call extend_integer_array (flv_index, list_incr)
                flv_index (label_count) = i_flv
                if (label_count > size (hel_index)) &
                    call extend_integer_array (hel_index, list_incr)
                hel_index (label_count) = i_hel
                if (driver%include_polarizations) then
                    helicities (label(label_count), :) = hel_array (1:n_in)
                    i_hel = i_hel + 1
                end if
                n_found = n_found + 1
                label_count = label_count + 1
                exit
            end if
        end do
        give_warning = .false.
    else
        give_warning = .true.
    end if
    read_flavor = .false.
end if
end if
end do
call crop_integer_array (amp_type, label_count-1)
if (n_found == 0) then
    call msg_fatal ("The desired process has not been found ", &

```

```

        [var_str ("by the OLP-Provider. Maybe the value of alpha_power "), &
        var_str ("or alphas_power does not correspond to the process. "), &
        var_str ("If you are using OpenLoops, you can set the option "), &
        var_str ("openloops_verbosity to a value larger than 1 to obtain "), &
        var_str ("more information")]]
else if (give_warning) then
    call msg_warning ("Some processes have not been found in the OLC file.", &
        [var_str ("This is because these processes do not fit the required "), &
        var_str ("coupling alpha_power and alphas_power. Be aware that the "), &
        var_str ("results of this calculation are not necessarily an accurate "), &
        var_str ("description of the physics of interest.")])
end if
close(unit)

contains

function create_flavor_string (s, n_entries) result (i_array)
    character(len=LEN_MAX_FLAVOR_STRING), intent(in) :: s
    integer, intent(in) :: n_entries
    integer, dimension(n_entries) :: i_array
    integer :: k, current_position
    integer :: i_entry
    k = 1; current_position = 1
    do
        if (current_position > LEN_MAX_FLAVOR_STRING) &
            call msg_fatal ("Read OLC File: Current position exceeds maximum value")
        if (s(current_position:current_position) /= " ") then
            call create_flavor (s, i_entry, current_position)
            if (i_entry /= NO_NUMBER .and. i_entry /= PROC_NOT_FOUND) then
                i_array(k) = i_entry
                k = k + 1
                if (k > n_entries) then
                    return
                else
                    call increment_current_position (s, current_position)
                end if
            else if (i_entry == PROC_NOT_FOUND) then
                i_array = PROC_NOT_FOUND
                return
            else
                call increment_current_position (s, current_position)
            end if
        else
            call increment_current_position (s, current_position)
        end if
    end do
end function create_flavor_string

function create_helicity_string (s, n_entries) result (hel_array)
    character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: s
    integer, intent(in) :: n_entries
    integer, dimension(n_entries) :: hel_array
    integer :: k, current_position
    integer :: hel

```

```

k = 1; current_position = 1
do
  if (current_position > LEN_MAX_FLAVOR_STRING) &
    call msg_fatal ("Read OLC File: Current position exceeds maximum value")
  if (s(current_position:current_position) /= " ") then
    call create_helicity (s, hel, current_position)
    if (hel >= -1 .and. hel <= 1) then
      hel_array(k) = hel
      k = k + 1
      if (k > n_entries) then
        return
      else
        call increment_current_position (s, current_position)
      end if
    else
      call increment_current_position (s, current_position)
    end if
  else
    call increment_current_position (s, current_position)
  end if
end do
end function create_helicity_string

subroutine increment_current_position (s, current_position)
  character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: s
  integer, intent(inout) :: current_position
  current_position = find_next_word_index (s, current_position)
end subroutine increment_current_position

subroutine get_next_buffer (s, current_position, buf, last_buffer_index)
  character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: s
  integer, intent(inout) :: current_position
  character(len = 10), intent(out) :: buf
  integer, intent(out) :: last_buffer_index
  integer :: i
  i = 1; buf = ""
  do
    if (s(current_position:current_position) /= " ") then
      buf(i:i) = s(current_position:current_position)
      i = i + 1; current_position = current_position + 1
    else
      exit
    end if
  end do
  last_buffer_index = i
end subroutine get_next_buffer

function is_particle_buffer (buf, i) result (valid)
  logical :: valid
  character(len = 10), intent(in) :: buf
  integer, intent(in) :: i
  valid = (buf(1 : i - 1) /= "->" .and. buf(1 : i - 1) /= "|" &
    .and. buf(1 : i - 1) /= "Process")
end function is_particle_buffer

```

```

subroutine create_flavor (s, i_particle, current_position)
  character(len=LEN_MAX_FLAVOR_STRING), intent(in) :: s
  integer, intent(out) :: i_particle
  integer, intent(inout) :: current_position
  character(len=10) :: buf
  integer :: i, last_buffer_index
  call get_next_buffer (s, current_position, buf, last_buffer_index)
  i = last_buffer_index
  if (is_particle_buffer (buf, i)) then
    call strip_helicity (buf, i)
    i_particle = read_ival (var_str (buf(1 : i - 1)))
  else if (buf(1 : i - 1) == "Process") then
    i_particle = PROC_NOT_FOUND
  else
    i_particle = NO_NUMBER
  end if
end subroutine create_flavor

subroutine create_helicity (s, helicity, current_position)
  character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: s
  integer, intent(out) :: helicity
  integer, intent(inout) :: current_position
  character(len = 10) :: buf
  integer :: i, last_buffer_index
  logical :: success
  call get_next_buffer (s, current_position, buf, last_buffer_index)
  i = last_buffer_index
  if (is_particle_buffer (buf, i)) then
    call strip_flavor (buf, i, helicity, success)
  else
    helicity = 0
  end if
end subroutine create_helicity

subroutine strip_helicity (buf, i)
  character(len = 10), intent(in) :: buf
  integer, intent(inout) :: i
  integer :: i_last
  i_last = i - 1
  if (i_last < 4) return
  if (buf(i_last - 2 : i_last) == "(1)") then
    i = i - 3
  else if (buf(i_last - 3 : i_last) == "(-1)") then
    i = i - 4
  end if
end subroutine strip_helicity

subroutine strip_flavor (buf, i, helicity, success)
  character(len = 10), intent(in) :: buf
  integer, intent(in) :: i
  integer, intent(out) :: helicity
  logical, intent(out) :: success
  integer :: i_last

```

```

i_last = i - 1
helicity = 0
if (i_last < 4) return
if (buf(i_last - 2 : i_last) == "(1)") then
    helicity = 1
    success = .true.
else if (buf(i_last - 3 : i_last) == "(-1)") then
    helicity = -1
    success = .true.
else
    success = .false.
end if
end subroutine strip_flavor

function find_next_word_index (word, i_start) result (i_next)
    character(len = LEN_MAX_FLAVOR_STRING), intent(in) :: word
    integer, intent(in) :: i_start
    integer :: i_next
    i_next = i_start + 1
    do
        if (word(i_next : i_next) /= " ") then
            exit
        else
            i_next = i_next + 1
        end if
        if (i_next > LEN_MAX_FLAVOR_STRING) &
            call msg_fatal ("Find next word: line limit exceeded")
    end do
end function find_next_word_index

subroutine check_helicity_array (hel_array, n_entries, n_in)
    integer, intent(in), dimension(:) :: hel_array
    integer, intent(in) :: n_entries, n_in
    integer :: n_particles, i
    logical :: valid
    n_particles = n_entries - 2
    !!! only allow polarisations for incoming fermions for now
    valid = all (hel_array (n_in + 1 : n_particles) == 0)
    do i = 1, n_in
        valid = valid .and. (hel_array(i) == 1 .or. hel_array(i) == -1)
    end do
    if (.not. valid) &
        call msg_fatal ("Invalid helicities encountered!")
end subroutine check_helicity_array

end subroutine blha_driver_read_contract_file

<BLHA OLP interfaces: prc blha: TBP>+≡
    procedure :: set_alpha_qed => prc_blha_set_alpha_qed

<BLHA OLP interfaces: procedures>+≡
    subroutine prc_blha_set_alpha_qed (object, model)
        class(prc_blha_t), intent(inout) :: object
        type(model_data_t), intent(in), target :: model

```

```

real(default) :: alpha

alpha = one / model%get_real (var_str ('alpha_em_i'))

select type (driver => object%driver)
class is (blha_driver_t)
  call driver%set_alpha_qed (alpha)
end select
end subroutine prc_blha_set_alpha_qed

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: set_GF => prc_blha_set_GF

<BLHA OLP interfaces: procedures>+≡
  subroutine prc_blha_set_GF (object, model)
    class(prc_blha_t), intent(inout) :: object
    type(model_data_t), intent(in), target :: model
    real(default) :: GF

    GF = model%get_real (var_str ('GF'))
    select type (driver => object%driver)
    class is (blha_driver_t)
      call driver%set_GF (GF)
    end select
  end subroutine prc_blha_set_GF

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: set_weinberg_angle => prc_blha_set_weinberg_angle

<BLHA OLP interfaces: procedures>+≡
  subroutine prc_blha_set_weinberg_angle (object, model)
    class(prc_blha_t), intent(inout) :: object
    type(model_data_t), intent(in), target :: model
    real(default) :: sw2

    sw2 = model%get_real (var_str ('sw2'))
    select type (driver => object%driver)
    class is (blha_driver_t)
      call driver%set_weinberg_angle (sw2)
    end select
  end subroutine prc_blha_set_weinberg_angle

<BLHA OLP interfaces: prc blha: TBP>+≡
  procedure :: set_electroweak_parameters => &
    prc_blha_set_electroweak_parameters

<BLHA OLP interfaces: procedures>+≡
  subroutine prc_blha_set_electroweak_parameters (object, model)
    class(prc_blha_t), intent(inout) :: object
    type(model_data_t), intent(in), target :: model
    if (count (object%ew_parameter_mask) == 0) then
      call msg_fatal ("Cannot decide EW parameter setting: No scheme set!")
    else if (count (object%ew_parameter_mask) > 1) then
      call msg_fatal ("Cannot decide EW parameter setting: More than one scheme set!")
    end if
  end subroutine prc_blha_set_electroweak_parameters

```



```

end if
if (object%ew_parameter_mask (I_ALPHA_INTERNAL)) call object%set_alpha_qed (model)
if (object%ew_parameter_mask (I_GF)) call object%set_GF (model)
if (object%ew_parameter_mask (I_SW2)) call object%set_weinberg_angle (model)
end subroutine prc_blha_set_electroweak_parameters

```

(BLHA OLP interfaces: prc blha: TBP)+≡

```

procedure :: read_contract_file => prc_blha_read_contract_file

```

(BLHA OLP interfaces: procedures)+≡

```

subroutine prc_blha_read_contract_file (object, flavors)
class(prc_blha_t), intent(inout) :: object
integer, intent(in), dimension(:,:) :: flavors
integer, dimension(:), allocatable :: amp_type, flv_index, hel_index, label
integer, dimension(:,:), allocatable :: helicities
integer :: i_proc, i_hel
allocate (helicities (N_MAX_FLAVORS, object%data%n_in))
select type (driver => object%driver)
class is (blha_driver_t)
    call driver%read_contract_file (flavors, amp_type, flv_index, &
        hel_index, label, helicities)
end select
object%n_proc = count (amp_type >= 0)
do i_proc = 1, object%n_proc
    if (amp_type (i_proc) < 0) exit
    if (hel_index(i_proc) < 0 .and. object%includes_polarization ()) &
        call msg_bug ("Object includes polarization, but helicity index is undefined.")
    i_hel = hel_index (i_proc)
    select case (amp_type (i_proc))
    case (BLHA_AMP_TREE)
        if (allocated (object%i_tree)) then
            object%i_tree(flv_index(i_proc), i_hel) = label(i_proc)
        else
            call msg_fatal ("Tree matrix element present, &
                &but neither Born nor real indices are allocated!")
        end if
    case (BLHA_AMP_COLOR_C)
        if (allocated (object%i_color_c)) then
            object%i_color_c(flv_index(i_proc), i_hel) = label(i_proc)
        else
            call msg_fatal ("Color-correlated matrix element present, &
                &but cc-indices are not allocated!")
        end if
    case (BLHA_AMP_SPIN_C)
        if (allocated (object%i_spin_c)) then
            object%i_spin_c(flv_index(i_proc), i_hel) = label(i_proc)
        else
            call msg_fatal ("Spin-correlated matrix element present, &
                &but sc-indices are not allocated!")
        end if
    case (BLHA_AMP_LOOP)
        if (allocated (object%i_virt)) then
            object%i_virt(flv_index(i_proc), i_hel) = label(i_proc)
        else

```

```

        call msg_fatal ("Loop matrix element present, &
            &but virt-indices are not allocated!")
    end if
    case default
        call msg_fatal ("Undefined amplitude type")
    end select
    if (allocated (object%i_hel)) &
        object%i_hel (i_proc, :) = helicities (label(i_proc), :)
    end do
end subroutine prc_blha_read_contract_file

```

<BLHA OLP interfaces: prc blha: TBP>+≡

```

    procedure :: print_parameter_file => prc_blha_print_parameter_file

```

<BLHA OLP interfaces: procedures>+≡

```

    subroutine prc_blha_print_parameter_file (object, i_component)
        class(prc_blha_t), intent(in) :: object
        integer, intent(in) :: i_component
        type(string_t) :: filename

        select type (def => object%def)
        class is (blha_def_t)
            filename = def%basename // '_' // str (i_component) // '.olp.parameters'
        end select
        select type (driver => object%driver)
        class is (blha_driver_t)
            call driver%blha_olp_print_parameter (char(filename)//c_null_char)
        end select
    end subroutine prc_blha_print_parameter_file

```

<BLHA OLP interfaces: prc blha: TBP>+≡

```

    procedure :: compute_amplitude => prc_blha_compute_amplitude

```

<BLHA OLP interfaces: procedures>+≡

```

    function prc_blha_compute_amplitude &
        (object, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced, &
            core_state) result (amp)
        class(prc_blha_t), intent(in) :: object
        integer, intent(in) :: j
        type(vector4_t), dimension(:), intent(in) :: p
        integer, intent(in) :: f, h, c
        real(default), intent(in) :: fac_scale, ren_scale
        real(default), intent(in), allocatable :: alpha_qcd_forced
        class(prc_core_state_t), intent(inout), allocatable, optional :: core_state
        complex(default) :: amp
        select type (core_state)
        class is (blha_state_t)
            core_state%alpha_qcd = object%qcd%alpha%get (ren_scale)
        end select
        amp = zero
    end function prc_blha_compute_amplitude

```

<BLHA OLP interfaces: prc blha: TBP>+≡

```

    procedure :: init_blha => prc_blha_init_blha

```

(BLHA OLP interfaces: procedures)+=

```

subroutine prc_blha_init_blha (object, blha_template, n_in, &
    n_particles, n_flv, n_hel)
    class(prc_blha_t), intent(inout) :: object
    type(blha_template_t), intent(in) :: blha_template
    integer, intent(in) :: n_in, n_particles, n_flv, n_hel
    object%n_particles = n_particles
    object%n_flv = n_flv
    object%n_hel = n_hel
    if (blha_template%compute_loop ()) then
        if (blha_template%include_polarizations) then
            allocate (object%i_virt (n_flv, n_hel), &
                object%i_color_c (n_flv, n_hel))
            if (blha_template%use_internal_color_correlations) then
                allocate (object%i_hel (n_flv * n_in * n_hel * 2, n_in))
            else
                allocate (object%i_hel (n_flv * n_in * n_hel, n_in))
            end if
        else
            allocate (object%i_virt (n_flv, 1), object%i_color_c (n_flv, 1))
        end if
        object%i_virt = -1
        object%i_color_c = -1
    else if (blha_template%compute_subtraction ()) then
        if (blha_template%include_polarizations) then
            allocate (object%i_tree (n_flv, n_hel), &
                object%i_color_c (n_flv, n_hel), &
                object%i_spin_c (n_flv, n_hel), &
                object%i_hel (3 * (n_flv * n_hel * n_in), n_in))
            object%i_hel = 0
        else
            allocate (object%i_tree (n_flv, 1), object%i_color_c (n_flv, 1) , &
                object%i_spin_c (n_flv, 1))
        end if
        object%i_tree = -1
        object%i_color_c = -1
        object%i_spin_c = -1
    else if (blha_template%compute_dglap ()) then
        if (blha_template%include_polarizations) then
            allocate (object%i_tree (n_flv, n_hel), &
                object%i_color_c (n_flv, n_hel), &
                object%i_hel (3 * (n_flv * n_hel * n_in), n_in))
            object%i_hel = 0
        else
            allocate (object%i_tree (n_flv, 1), object%i_color_c (n_flv, 1))
        end if
        object%i_tree = -1
        object%i_color_c = -1
    else if (blha_template%compute_real_trees () .or. blha_template%compute_born ()) then
        if (blha_template%include_polarizations) then
            allocate (object%i_tree (n_flv, n_hel))
            allocate (object%i_hel (n_flv * n_hel * n_in, n_in))
            object%i_hel = 0
        else

```

```

        allocate (object%i_tree (n_flv, 1))
    end if
    object%i_tree = -1
end if

call object%init_ew_parameters (blha_template%ew_scheme)

select type (driver => object%driver)
class is (blha_driver_t)
    driver%include_polarizations = blha_template%include_polarizations
    driver%switch_off_muon_yukawas = blha_template%switch_off_muon_yukawas
    driver%external_top_yukawa = blha_template%external_top_yukawa
end select
end subroutine prc_blha_init_blha

```

<BLHA OLP interfaces: prc blha: TBP>+≡

```

    procedure :: set_mass_and_width => prc_blha_set_mass_and_width

```

<BLHA OLP interfaces: procedures>+≡

```

subroutine prc_blha_set_mass_and_width (object, i_pdg, mass, width)
    class(prc_blha_t), intent(inout) :: object
    integer, intent(in) :: i_pdg
    real(default), intent(in) :: mass, width
    select type (driver => object%driver)
    class is (blha_driver_t)
        call driver%set_mass_and_width (i_pdg, mass, width)
    end select
end subroutine prc_blha_set_mass_and_width

```

<BLHA OLP interfaces: prc blha: TBP>+≡

```

    procedure :: set_particle_properties => prc_blha_set_particle_properties

```

<BLHA OLP interfaces: procedures>+≡

```

subroutine prc_blha_set_particle_properties (object, model)
    class(prc_blha_t), intent(inout) :: object
    class(model_data_t), intent(in), target :: model
    integer :: i, i_pdg
    type(flavor_t) :: flv
    real(default) :: mass, width
    integer :: ierr
    real(default) :: top_yukawa
    do i = 1, OLP_N_MASSIVE_PARTICLES
        i_pdg = OLP_MASSIVE_PARTICLES(i)
        if (i_pdg < 0) cycle
        call flv%init (i_pdg, model)
        mass = flv%get_mass (); width = flv%get_width ()
        select type (driver => object%driver)
        class is (blha_driver_t)
            call driver%set_mass_and_width (i_pdg, mass = mass, width = width)
            if (i_pdg == 5) call driver%blha_olp_set_parameter &
                ('yuk(5)'/c_null_char, dble(mass), 0._double, ierr)
            if (i_pdg == 6) then
                if (driver%external_top_yukawa > 0._default) then
                    top_yukawa = driver%external_top_yukawa
                end if
            end if
        end select
    end do
end subroutine prc_blha_set_particle_properties

```

```

        else
            top_yukawa = mass
        end if
        call driver%blha_olp_set_parameter &
            ('yuk(6)'//c_null_char, dble(top_yukawa), 0._double, ierr)
    end if
    if (driver%switch_off_muon_yukawas) then
        if (i_pdg == 13) call driver%blha_olp_set_parameter &
            ('yuk(13)' //c_null_char, 0._double, 0._double, ierr)
        end if
    end select
end do
end subroutine prc_blha_set_particle_properties

```

This mask adapts which electroweak parameters are supposed to set according to the chosen BLHA EWScheme. This is only implemented for the default OLP method so far.

```

<BLHA OLP interfaces: prc blha: TBP>+≡
    procedure :: init_ew_parameters => prc_blha_init_ew_parameters

<BLHA OLP interfaces: procedures>+≡
    subroutine prc_blha_init_ew_parameters (object, ew_scheme)
        class(prc_blha_t), intent(inout) :: object
        integer, intent(in) :: ew_scheme
        object%ew_parameter_mask = .false.
        select case (ew_scheme)
        case (BLHA_EW_0)
            object%ew_parameter_mask (I_ALPHA_0) = .true.
        case (BLHA_EW_GF)
            object%ew_parameter_mask (I_GF) = .true.
        case (BLHA_EW_MZ)
            object%ew_parameter_mask (I_ALPHA_MZ) = .true.
        case (BLHA_EW_INTERNAL)
            object%ew_parameter_mask (I_ALPHA_INTERNAL) = .true.
        end select
    end subroutine prc_blha_init_ew_parameters

```

Computes a virtual matrix element from an interface to an external one-loop provider. The output of `blha_olp_eval2` is an array of `dimension(4)`, corresponding to the ϵ^2 -, ϵ^1 - and ϵ^0 -poles of the virtual matrix element at position `r(1:3)` and the Born matrix element at position `r(4)`. The matrix element is rejected if its accuracy is larger than the maximal allowed accuracy. OpenLoops includes a factor of $1 / n_{\text{hel}}$ in the amplitudes, which we have to undo if polarized matrix elements are requested (GoSam does not support polarized matrix elements).

```

<BLHA OLP interfaces: prc blha: TBP>+≡
    procedure :: compute_sqme_virt => prc_blha_compute_sqme_virt

<BLHA OLP interfaces: procedures>+≡
    subroutine prc_blha_compute_sqme_virt (object, &
        i_flv, i_hel, p, ren_scale, es_scale, loop_method, sqme, bad_point)
        class(prc_blha_t), intent(in) :: object
        integer, intent(in) :: i_flv, i_hel

```

```

type(vector4_t), dimension(:), intent(in) :: p
real(default), intent(in) :: ren_scale, es_scale
integer, intent(in) :: loop_method
real(default), dimension(4), intent(out) :: sqme
logical, intent(out) :: bad_point
real(double), dimension(5 * object%n_particles) :: mom
real(double), dimension(:), allocatable :: r
real(double) :: mu_dble, es_dble
real(double) :: acc_dble
real(default) :: acc
real(default) :: alpha_s
integer :: ierr
if (object%i_virt(i_flv, i_hel) >= 0) then
  allocate (r (blha_result_array_size (object%n_particles, BLHA_AMP_LOOP)))
  if (debug_on) call msg_debug2 (D_VIRTUAL, "prc_blha_compute_sqme_virt")
  if (debug_on) call msg_debug2 (D_VIRTUAL, "i_flv", i_flv)
  if (debug_on) call msg_debug2 (D_VIRTUAL, "object%i_virt(i_flv, i_hel)", object%i_virt(i_flv, i_hel))
  if (debug2_active (D_VIRTUAL)) then
    call msg_debug2 (D_VIRTUAL, "use momenta: ")
    call vector4_write_set (p, show_mass = .true., &
      check_conservation = .true.)
  end if
  mom = object%create_momentum_array (p)
  if (vanishes (ren_scale)) &
    call msg_fatal ("prc_blha_compute_sqme_virt: ren_scale vanishes")
  mu_dble = dble (ren_scale)
  es_dble = dble (es_scale)
  alpha_s = object%qcd%alpha%get (ren_scale)
  select type (driver => object%driver)
  class is (blha_driver_t)
    if (loop_method == BLHA_MODE_OPENLOOPS) then
      call driver%blha_olp_set_parameter ('mureg'//c_null_char, es_dble, 0._double, ierr)
      if (ierr == 0) call parameter_error_message (var_str ('mureg'), &
        var_str ('prc_blha_compute_sqme_virt'))
    end if
    call driver%set_alpha_s (alpha_s)
    call driver%blha_olp_eval2 (object%i_virt(i_flv, i_hel), mom, mu_dble, r, acc_dble)
  end select
  acc = acc_dble
  sqme = r(1:4)
  bad_point = acc > object%maximum_accuracy
  if (object%includes_polarization ()) sqme = object%n_hel * sqme
else
  sqme = zero
end if
end subroutine prc_blha_compute_sqme_virt

```

Computes a tree-level matrix element from an interface to an external one-loop provider. The matrix element is rejected if its accuracy is larger than the maximal allowed accuracy. OpenLoops includes a factor of $1 / n_{hel}$ in the amplitudes, which we have to undo if polarized matrix elements are requested (GoSam does not support polarized matrix elements).

(BLHA OLP interfaces: prc blha: TBP)+≡

```

procedure :: compute_sqme => prc_blha_compute_sqme
<BLHA OLP interfaces: procedures>+=
  subroutine prc_blha_compute_sqme (object, i_flv, i_hel, p, &
    ren_scale, sqme, bad_point)
    class(prc_blha_t), intent(in) :: object
    integer, intent(in) :: i_flv, i_hel
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(out) :: sqme
    logical, intent(out) :: bad_point
    real(double), dimension(5*object%n_particles) :: mom
    real(double), dimension(OLP_RESULTS_LIMIT) :: r
    real(double) :: mu_dble, acc_dble
    real(default) :: acc, alpha_s
    if (object%i_tree(i_flv, i_hel) >= 0) then
      if (debug_on) call msg_debug2 (D_REAL, "prc_blha_compute_sqme")
      if (debug_on) call msg_debug2 (D_REAL, "i_flv", i_flv)
      if (debug2_active (D_REAL)) then
        call msg_debug2 (D_REAL, "use momenta: ")
        call vector4_write_set (p, show_mass = .true., &
          check_conservation = .true.)
      end if
      mom = object%create_momentum_array (p)
      if (vanishes (ren_scale)) &
        call msg_fatal ("prc_blha_compute_sqme: ren_scale vanishes")
      mu_dble = dble(ren_scale)
      alpha_s = object%qcd%alpha%get (ren_scale)
      select type (driver => object%driver)
      class is (blha_driver_t)
        call driver%set_alpha_s (alpha_s)
        call driver%blha_olp_eval2 (object%i_tree(i_flv, i_hel), mom, &
          mu_dble, r, acc_dble)
        sqme = r(object%sqme_tree_pos)
      end select
      acc = acc_dble
      bad_point = acc > object%maximum_accuracy
      if (object%includes_polarization ()) sqme = object%n_hel * sqme
    else
      sqme = zero
    end if
  end subroutine prc_blha_compute_sqme

```

For the color correlated matrix the standard is to compute the diagonal entries from the born amplitudes and corresponding casimirs. However, if EW corrections are activated, the thus derived entries can be computed with born amplitudes of wrong coupling powers if the flavor structure potentially induces QCD-EW interference amplitudes. For this purpose a second possibility, to compute the diagonal from the off-diagonal elements is implemented as a special case.

```

<BLHA OLP interfaces: public>+=
  public :: blha_color_c_fill_diag
<BLHA OLP interfaces: procedures>+=

```

```

subroutine blha_color_c_fill_diag (sqme_born, flavors, sqme_color_c, special_case)
  real(default), intent(in) :: sqme_born
  integer, intent(in), dimension(:) :: flavors
  logical, intent(in), optional :: special_case
  real(default), intent(inout), dimension(:, :) :: sqme_color_c
  real(default) :: sqme_line_off
  integer :: i, j
  logical :: special_c
  special_c = .false.
  if (present (special_case)) &
    special_c = special_case .and. qcd_ew_interferences (flavors)
  do i = 1, size (flavors)
    if (is_quark (flavors(i))) then
      sqme_line_off = zero
      do j = 1, size (flavors)
        if (j /= i) sqme_line_off = sqme_line_off + sqme_color_c (i, j)
      end do
      if (special_c) then
        sqme_color_c (i, i) = - sqme_line_off
      else
        sqme_color_c (i, i) = -cf * sqme_born
      end if
    else if (is_gluon (flavors(i))) then
      sqme_line_off = zero
      do j = 1, size (flavors)
        if (j /= i) sqme_line_off = sqme_line_off + sqme_color_c (i, j)
      end do
      if (special_c) then
        sqme_color_c (i, i) = - sqme_line_off
      else
        sqme_color_c (i, i) = -ca * sqme_born
      end if
    else
      sqme_color_c (i, i) = zero
    end if
  end do
end subroutine blha_color_c_fill_diag

```

(BLHA OLP interfaces: public)+≡

```
public :: blha_color_c_fill_offdiag
```

(BLHA OLP interfaces: procedures)+≡

```

subroutine blha_color_c_fill_offdiag (n, r, sqme_color_c, offset, n_flv)
  integer, intent(in) :: n
  real(default), intent(in), dimension(:) :: r
  real(default), intent(inout), dimension(:, :) :: sqme_color_c
  integer, intent(in), optional :: offset, n_flv
  integer :: i, j, pos, incr
  if (present (offset)) then
    incr = offset
  else
    incr = 0
  end if
  pos = 0

```



```

do j = 1, n
  do i = 1, j
    if (i /= j) then
      pos = (j - 1) * (j - 2) / 2 + i
      if (present (n_flv)) incr = incr + n_flv - 1
      if (present (offset)) pos = pos + incr
      sqme_color_c (i, j) = -r (pos)
      sqme_color_c (j, i) = sqme_color_c (i, j)
    end if
  end do
end do
end subroutine blha_color_c_fill_offdiag

```

Computes a color-correlated matrix element from an interface to an external one-loop provider. The output of `blha_olp_eval2` is an array of dimension($n * (n - 1) / 2$). The matrix element is rejected if its accuracy is larger than the maximal allowed accuracy. OpenLoops includes a factor of $1 / n_{\text{hel}}$ in the amplitudes, which we have to undo if polarized matrix elements are requested (GoSam does not support polarized matrix elements).

(BLHA OLP interfaces: prc blha: TBP)+≡

```

procedure :: compute_sqme_color_c_raw => prc_blha_compute_sqme_color_c_raw

```

(BLHA OLP interfaces: procedures)+≡

```

subroutine prc_blha_compute_sqme_color_c_raw &
  (object, i_flv, i_hel, p, ren_scale, rr, bad_point)
class(prc_blha_t), intent(in) :: object
integer, intent(in) :: i_flv, i_hel
type(vector4_t), intent(in), dimension(:) :: p
real(default), intent(in) :: ren_scale
real(default), intent(out), dimension(:) :: rr
logical, intent(out) :: bad_point
real(double), dimension(5 * object%n_particles) :: mom
real(double), dimension(size(rr)) :: r
real(default) :: alpha_s, acc
real(double) :: mu_dble, acc_dble
if (debug2_active (D_REAL)) then
  call msg_debug2 (D_REAL, "use momenta: ")
  call vector4_write_set (p, show_mass = .true., &
    check_conservation = .true.)
end if
if (object%i_color_c(i_flv, i_hel) >= 0) then
  mom = object%create_momentum_array (p)
  if (vanishes (ren_scale)) &
    call msg_fatal ("prc_blha_compute_sqme_color_c: ren_scale vanishes")
  mu_dble = dble(ren_scale)
  alpha_s = object%qcd%alpha%get (ren_scale)

  select type (driver => object%driver)
  class is (blha_driver_t)
    call driver%set_alpha_s (alpha_s)
    call driver%blha_olp_eval2 (object%i_color_c(i_flv, i_hel), &
      mom, mu_dble, r, acc_dble)
  end select
  rr = r

```

```

        acc = acc_dble
        bad_point = acc > object%maximum_accuracy
        if (object%includes_polarization ()) rr = object%n_hel * rr
    else
        rr = zero
    end if
end subroutine prc_blha_compute_sqme_color_c_raw

```

(BLHA OLP interfaces: prc blha: TBP)+≡

```

    procedure :: compute_sqme_color_c => prc_blha_compute_sqme_color_c

```

(BLHA OLP interfaces: procedures)+≡

```

subroutine prc_blha_compute_sqme_color_c &
    (object, i_flv, i_hel, p, ren_scale, born_color_c, bad_point, born_out)
class(prc_blha_t), intent(inout) :: object
integer, intent(in) :: i_flv, i_hel
type(vector4_t), intent(in), dimension(:) :: p
real(default), intent(in) :: ren_scale
real(default), intent(inout), dimension(:,:) :: born_color_c
real(default), intent(out), optional :: born_out
logical, intent(out) :: bad_point
real(default), dimension(:), allocatable :: r
logical :: bad_point2
real(default) :: born
integer, dimension(:), allocatable :: flavors
if (debug2_active (D_REAL)) then
    call msg_debug2 (D_REAL, "use momenta: ")
    call vector4_write_set (p, show_mass = .true., &
        check_conservation = .true.)
end if
allocate (r (blha_result_array_size &
    (size(born_color_c, dim=1), BLHA_AMP_COLOR_C)))
call object%compute_sqme_color_c_raw (i_flv, i_hel, p, ren_scale, r, bad_point)

select type (driver => object%driver)
class is (blha_driver_t)
    if (allocated (object%i_tree)) then
        call object%compute_sqme (i_flv, i_hel, p, ren_scale, born, bad_point2)
    else
        born = zero
    end if
    if (present (born_out)) born_out = born
end select
call blha_color_c_fill_offdiag (object%n_particles, r, born_color_c)
flavors = object%get_flv_state (i_flv)
call blha_color_c_fill_diag (born, flavors, born_color_c)

bad_point = bad_point .or. bad_point2
end subroutine prc_blha_compute_sqme_color_c

```

(BLHA OLP interfaces: prc blha: TBP)+≡

```

generic :: get_beam_helicities => get_beam_helicities_single
generic :: get_beam_helicities => get_beam_helicities_array

```

```

procedure :: get_beam_helicities_single => prc_blha_get_beam_helicities_single
procedure :: get_beam_helicities_array => prc_blha_get_beam_helicities_array

<BLHA OLP interfaces: procedures>+≡
function prc_blha_get_beam_helicities_single (object, i, invert_second) result (hel)
    integer, dimension(:), allocatable :: hel
    class(prc_blha_t), intent(in) :: object
    logical, intent(in), optional :: invert_second
    integer, intent(in) :: i
    logical :: inv
    inv = .false.; if (present (invert_second)) inv = invert_second
    allocate (hel (object%data%n_in))
    hel = object%i_hel (i, :)
    if (inv .and. object%data%n_in == 2) hel(2) = -hel(2)
end function prc_blha_get_beam_helicities_single

```

```

<BLHA OLP interfaces: prc blha: TBP>+≡
procedure :: includes_polarization => prc_blha_includes_polarization

```

```

<BLHA OLP interfaces: procedures>+≡
function prc_blha_includes_polarization (object) result (polarized)
    logical :: polarized
    class(prc_blha_t), intent(in) :: object
    select type (driver => object%driver)
    class is (blha_driver_t)
        polarized = driver%include_polarizations
    end select
end function prc_blha_includes_polarization

```

```

<BLHA OLP interfaces: procedures>+≡
function prc_blha_get_beam_helicities_array (object, invert_second) result (hel)
    integer, dimension(:, :), allocatable :: hel
    class(prc_blha_t), intent(in) :: object
    logical, intent(in), optional :: invert_second
    integer :: i
    allocate (hel (object%n_proc, object%data%n_in))
    do i = 1, object%n_proc
        hel(i, :) = object%get_beam_helicities (i, invert_second)
    end do
end function prc_blha_get_beam_helicities_array

```

Setup an index mapping for flavor structures and helicities that give the same matrix element. The index mapping is according to the order of flavor structures known to the `prc_core` class. Overrides `prc_core_set_equivalent_flv_hel_indices`.

```

<BLHA OLP interfaces: prc blha: TBP>+≡
procedure :: set_equivalent_flv_hel_indices => prc_blha_set_equivalent_flv_hel_indices

```

```

<BLHA OLP interfaces: procedures>+≡
subroutine prc_blha_set_equivalent_flv_hel_indices (object)
    class(prc_blha_t), intent(inout) :: object
    integer :: n_flv, n_hel
    integer :: i_flv1, i_flv2, i_hel1, i_hel2
    integer, dimension(:, :), allocatable :: amp_id, amp_id_color
    if (allocated (object%i_virt)) then

```

```

        amp_id = object%i_virt
    else
        amp_id = object%i_tree
    end if
    if (allocated (object%i_color_c)) then
        amp_id_color = object%i_color_c
    end if
    n_flv = size (amp_id, dim=1)
    n_hel = size (amp_id, dim=2)
    if (.not. allocated (object%data%eqv_flv_index)) &
        allocate (object%data%eqv_flv_index(n_flv))
    if (.not. allocated (object%data%eqv_hel_index)) &
        allocate (object%data%eqv_hel_index(n_hel))
    if (size (object%data%eqv_flv_index) /= n_flv) &
        call msg_bug ("BLHA Core: Size mismatch between eqv_flv_index and number of flavors.")
    if (size (object%data%eqv_hel_index) /= n_hel) &
        call msg_bug ("BLHA Core: Size mismatch between eqv_hel_index and number of helicities.")
    do i_flv1 = 1, n_flv
        do i_hel1 = 1, n_hel
            FLV_LOOP: do i_flv2 = 1, i_flv1
                do i_hel2 = 1, i_hel1
                    if (amp_id(i_flv2, i_hel2) == amp_id(i_flv1, i_hel1)) then
                        if (.not. allocated (amp_id_color)) then
                            object%data%eqv_flv_index(i_flv1) = i_flv2
                            object%data%eqv_hel_index(i_hel1) = i_hel2
                            exit FLV_LOOP
                        else if (amp_id_color (i_flv2, i_hel2) == &
                                amp_id_color(i_flv1, i_hel1)) then
                            object%data%eqv_flv_index(i_flv1) = i_flv2
                            object%data%eqv_hel_index(i_hel1) = i_hel2
                            exit FLV_LOOP
                        end if
                    end if
                end do
            end do
        end do FLV_LOOP
    end do
end subroutine prc_blha_set_equivalent_flv_hel_indices

```

(BLHA OLP interfaces: prc blha: TBP)+≡
 procedure(prc_blha_init_driver), deferred :: &
 init_driver

(BLHA OLP interfaces: interfaces)+≡
 abstract interface
 subroutine prc_blha_init_driver (object, os_data)
 import
 class(prc_blha_t), intent(inout) :: object
 type(os_data_t), intent(in) :: os_data
 end subroutine prc_blha_init_driver
end interface

In general, the BLHA consists of a virtual matrix element and n_{sub} subtraction terms. The subtraction terms can be pure Born matrix elements (to be used

in collinear subtraction or in internal color-correlation), color-correlated matrix elements or spin-correlated matrix elements. The numbers should be ordered in such a way that \mathcal{V}_{fin} is first, followed by the pure Born, the color-correlated and the spin-correlated matrix elements. This repeats n_{flv} times. Let ν_i be the position of the i th virtual matrix element. The next \mathcal{V}_{fin} is at position $\nu_i = \nu_{i-1} + n_{\text{sub}} + 1$. Obviously, $\nu_1 = 1$. This allows us to determine the virtual matrix element positions using the recursive function implemented below.

```

<BLHA OLP interfaces: public>+=
  public :: blha_loop_positions

<BLHA OLP interfaces: procedures>+=
  recursive function blha_loop_positions (i_flv, n_sub) result (index)
    integer :: index
    integer, intent(in) :: i_flv, n_sub
    index = 0
    if (i_flv == 1) then
      index = 1
    else
      index = blha_loop_positions (i_flv - 1, n_sub) + n_sub + 1
    end if
  end function blha_loop_positions

```

The module is split into a configuration interface which manages configuration and handles the request and contract files, a module which interfaces the OLP matrix elements and a driver.

```

<blha_config.f90>=
  <File header>

  module blha_config

    use kinds
    <Use strings>
    use io_units
    use constants
    use string_utils
    use variables, only: var_list_t
    use physics_defs, only: PHOTON, PHOTON_OFFSHELL
    use diagnostics
    use md5
    use model_data
    use flavors
    use quantum_numbers
    use pdg_arrays
    use sorting
    use lexers
    use parser
    use syntax_rules
    use ifiles

    use beam_structures, only: beam_structure_t

    <Use mpi f08>
    <Standard module head>

```

```

<BLHA config: public>

<BLHA config: parameters>

<BLHA config: types>

<BLHA config: variables>

<BLHA config: interfaces>

contains

<BLHA config: procedures>

end module blha_config

```

24.2 Configuration

Parameters to enumerate the different options in the order.

```

<BLHA config: parameters>≡
  integer, public, parameter :: &
    BLHA_CT_QCD = 1, BLHA_CT_EW = 2, BLHA_CT_OTHER = 3
  integer, public, parameter :: &
    BLHA_IRREG_CDR = 1, BLHA_IRREG_DRED = 2, BLHA_IRREG_THV = 3, &
    BLHA_IRREG_MREG = 4, BLHA_IRREG_OTHER = 5
  integer, public, parameter :: &
    BLHA_MPS_ONSHELL = 1, BLHA_MPS_OTHER = 2
  integer, public, parameter :: &
    BLHA_MODE_GOSAM = 1, BLHA_MODE_FEYNARTS = 2, BLHA_MODE_GENERIC = 3, &
    BLHA_MODE_OPENLOOPS = 4
  integer, public, parameter :: &
    BLHA_VERSION_1 = 1, BLHA_VERSION_2 = 2
  integer, public, parameter :: &
    BLHA_AMP_LOOP = 1, BLHA_AMP_COLOR_C = 2, BLHA_AMP_SPIN_C = 3, &
    BLHA_AMP_TREE = 4, BLHA_AMP_LOOPINDUCED = 5
  integer, public, parameter :: &
    BLHA_EW_INTERNAL = 0, &
    BLHA_EW_GF = 1, BLHA_EW_MZ = 2, BLHA_EW_MSBAR = 3, &
    BLHA_EW_O = 4, BLHA_EW_RUN = 5
  integer, public, parameter :: &
    BLHA_WIDTH_COMPLEX = 1, BLHA_WIDTH_FIXED = 2, &
    BLHA_WIDTH_RUNNING = 3, BLHA_WIDTH_POLE = 4, &
    BLHA_WIDTH_DEFAULT = 5

```

Those are the default pdg codes for massive particles in BLHA programs

```

<BLHA config: parameters>+≡
  integer, parameter, public :: OLP_N_MASSIVE_PARTICLES = 12
  integer, dimension(OLP_N_MASSIVE_PARTICLES), public :: &
    OLP_MASSIVE_PARTICLES = [5, -5, 6, -6, 13, -13, 15, -15, 23, 24, -24, 25]
  integer, parameter :: OLP_HEL_UNPOLARIZED = 0

```

The user might provide an extra command string for OpenLoops to apply special libraries instead of the default ones, such as signal-only amplitudes for off-shell top production. We check in this subroutine that the provided string is valid and print out the possible options to ease the user's memory.

```

<BLHA config: parameters>+=
  integer, parameter :: N_KNOWN_SPECIAL_OL_METHODS = 3

<BLHA config: procedures>=
  subroutine check_extra_cmd (extra_cmd)
    type(string_t), intent(in) :: extra_cmd
    type(string_t), dimension(N_KNOWN_SPECIAL_OL_METHODS) :: known_methods
    integer :: i
    logical :: found
    known_methods(1) = 'top'
    known_methods(2) = 'not'
    known_methods(3) = 'stop'
    if (extra_cmd == var_str("")) return
    found = .false.
    do i = 1, N_KNOWN_SPECIAL_OL_METHODS
      found = found .or. &
        (extra_cmd == var_str ('extra approx ')) // known_methods(i))
    end do
    if (.not. found) &
      call msg_fatal ("The given extra OpenLoops method is not known ", &
        [var_str ("Available commands are: "), &
        var_str ("extra approx top (only WbWb signal),"), &
        var_str ("extra approx stop (only WbWb singletop),"), &
        var_str ("extra approx not (no top in WbWb).")])
    end subroutine check_extra_cmd

```

This type contains the pdg code of the particle to be written in the process specification string and an optional additional information about the polarization of the particles. Note that the output can only be processed by OpenLoops.

```

<BLHA config: types>=
  type :: blha_particle_string_element_t
    integer :: pdg = 0
    integer :: hel = OLP_HEL_UNPOLARIZED
    logical :: polarized = .false.
  contains
    <BLHA config: blha particle string element: TBP>
  end type blha_particle_string_element_t

<BLHA config: blha particle string element: TBP>=
  generic :: init => init_default
  generic :: init => init_polarized
  procedure :: init_default => blha_particle_string_element_init_default
  procedure :: init_polarized => blha_particle_string_element_init_polarized

<BLHA config: procedures>+=
  subroutine blha_particle_string_element_init_default (blha_p, id)
    class(blha_particle_string_element_t), intent(out) :: blha_p
    integer, intent(in) :: id

```

```

        blha_p%pdg = id
    end subroutine blha_particle_string_element_init_default

<BLHA config: procedures>+≡
    subroutine blha_particle_string_element_init_polarized (blha_p, id, hel)
        class(blha_particle_string_element_t), intent(out) :: blha_p
        integer, intent(in) :: id, hel
        blha_p%polarized = .true.
        blha_p%pdg = id
        blha_p%hel = hel
    end subroutine blha_particle_string_element_init_polarized

<BLHA config: blha particle string element: TBP>+≡
    generic :: write_pdg => write_pdg_unit
    generic :: write_pdg => write_pdg_character
    procedure :: write_pdg_unit => blha_particle_string_element_write_pdg_unit
    procedure :: write_pdg_character &
        => blha_particle_string_element_write_pdg_character

<BLHA config: procedures>+≡
    subroutine blha_particle_string_element_write_pdg_unit (blha_p, unit)
        class(blha_particle_string_element_t), intent(in) :: blha_p
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, '(I3)') blha_p%pdg
    end subroutine blha_particle_string_element_write_pdg_unit

<BLHA config: procedures>+≡
    subroutine blha_particle_string_element_write_pdg_character (blha_p, c)
        class(blha_particle_string_element_t), intent(in) :: blha_p
        character(3), intent(inout) :: c
        write (c, '(I3)') blha_p%pdg
    end subroutine blha_particle_string_element_write_pdg_character

<BLHA config: blha particle string element: TBP>+≡
    generic :: write_helicity => write_helicity_unit
    generic :: write_helicity => write_helicity_character
    procedure :: write_helicity_unit &
        => blha_particle_string_element_write_helicity_unit
    procedure :: write_helicity_character &
        => blha_particle_string_element_write_helicity_character

<BLHA config: procedures>+≡
    subroutine blha_particle_string_element_write_helicity_unit (blha_p, unit)
        class(blha_particle_string_element_t), intent(in) :: blha_p
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, '(A1,I0,A1)') '(', blha_p%hel, ')'
    end subroutine blha_particle_string_element_write_helicity_unit

```



```

<BLHA config: procedures>+≡
subroutine blha_particle_string_element_write_helicity_character (blha_p, c)
  class(blha_particle_string_element_t), intent(in) :: blha_p
  character(4), intent(inout) :: c
  write (c, '(A1,I0,A1)') '(', blha_p%hel, ')')
end subroutine blha_particle_string_element_write_helicity_character

```

This type encapsulates a BLHA request.

```

<BLHA config: public>≡
public :: blha_configuration_t
public :: blha_cfg_process_node_t

<BLHA config: types>+≡
type :: blha_cfg_process_node_t
  type(blha_particle_string_element_t), dimension(:), allocatable :: pdg_in, pdg_out
  integer, dimension(:), allocatable :: fingerprint
  integer :: nsub
  integer, dimension(:), allocatable :: ids
  integer :: amplitude_type
  type(blha_cfg_process_node_t), pointer :: next => null ()
end type blha_cfg_process_node_t

type :: blha_configuration_t
  type(string_t) :: name
  class(model_data_t), pointer :: model => null ()
  type(string_t) :: md5
  integer :: version = 2
  logical :: dirty = .false.
  integer :: n_proc = 0
  real(default) :: accuracy_target
  logical :: debug_unstable = .false.
  integer :: mode = BLHA_MODE_GENERIC
  logical :: polarized = .false.
  type(blha_cfg_process_node_t), pointer :: processes => null ()
  !integer, dimension(2) :: matrix_element_square_type = BLHA_MEST_SUM
  integer :: correction_type
  type(string_t) :: correction_type_other
  integer :: irreg = BLHA_IRREG_THV
  type(string_t) :: irreg_other
  integer :: massive_particle_scheme = BLHA_MPS_ONSHELL
  type(string_t) :: massive_particle_scheme_other
  type(string_t) :: model_file
  logical :: subdivide_subprocesses = .false.
  integer :: alphas_power = -1, alpha_power = -1
  integer :: ew_scheme = BLHA_EW_GF
  integer :: width_scheme = BLHA_WIDTH_DEFAULT
  logical :: openloops_use_cms = .false.
  integer :: openloops_phs_tolerance = 0
  type(string_t) :: openloops_extra_cmd
  integer :: openloops_stability_log = 0
  integer :: n_off_photons_is = 0
  integer :: n_off_photons_fs = 0
end type blha_configuration_t

```

Translate the SINDARIN input string to the corresponding named integer.

```

<BLHA config: public>+≡
    public :: ew_scheme_string_to_int

<BLHA config: procedures>+≡
    function ew_scheme_string_to_int (ew_scheme_str) result (ew_scheme_int)
        integer :: ew_scheme_int
        type(string_t), intent(in) :: ew_scheme_str
        select case (char (ew_scheme_str))
            case ('GF', 'Gmu')
                ew_scheme_int = BLHA_EW_GF
            case ('alpha_qed', 'alpha_internal')
                ew_scheme_int = BLHA_EW_INTERNAL
            case ('alpha_mz')
                ew_scheme_int = BLHA_EW_MZ
            case ('alpha_0', 'alpha_thompson')
                ew_scheme_int = BLHA_EW_0
            case default
                call msg_fatal ("ew_scheme: " // char (ew_scheme_str) // &
                    " not supported. Try 'Gmu', 'alpha_internal', 'alpha_mz' or 'alpha_0'.")
            end select
        end function ew_scheme_string_to_int

```

Translate the SINDARIN input string to the corresponding named integer denoting the type of NLO correction.

```

<BLHA config: public>+≡
    public :: correction_type_string_to_int

<BLHA config: procedures>+≡
    function correction_type_string_to_int (correction_type_str) result (correction_type_int)
        integer :: correction_type_int
        type(string_t), intent(in) :: correction_type_str
        select case (char (correction_type_str))
            case ('QCD')
                correction_type_int = BLHA_CT_QCD
            case ('EW')
                correction_type_int = BLHA_CT_EW
            case default
                call msg_warning ("nlo_correction_type: " // char (correction_type_str) // &
                    " not supported. Try setting it to 'QCD', 'EW'.")
            end select
        end function correction_type_string_to_int

```

This types control the creation of BLHA-interface files

```

<BLHA config: public>+≡
    public :: blha_flv_state_t
    public :: blha_master_t

<BLHA config: types>+≡
    type :: blha_flv_state_t
        integer, dimension(:), allocatable :: flavors
        integer :: flv_mult
        logical :: flv_real = .false.
    end type blha_flv_state_t

```

```

type :: blha_master_t
  integer, dimension(5) :: blha_mode = BLHA_MODE_GENERIC
  logical :: compute_borns = .false.
  logical :: compute_real_trees = .false.
  logical :: compute_loops = .true.
  logical :: compute_correlations = .false.
  logical :: compute_dglap = .false.
  integer :: ew_scheme
  type(string_t), dimension(:), allocatable :: suffix
  type(blha_configuration_t), dimension(:), allocatable :: blha_cfg
  integer :: n_files = 0
  integer, dimension(:), allocatable :: i_file_to_nlo_index
contains
  <BLHA config: blha master: TBP>
end type blha_master_t

```

Master-Routines

<BLHA config: blha master: TBP>≡

```

  procedure :: set_methods => blha_master_set_methods

```

<BLHA config: procedures>+≡

```

subroutine blha_master_set_methods (master, is_nlo, var_list)
  class(blha_master_t), intent(inout) :: master
  logical, intent(in) :: is_nlo
  type(var_list_t), intent(in) :: var_list
  type(string_t) :: method, born_me_method, real_tree_me_method
  type(string_t) :: loop_me_method, correlation_me_method
  type(string_t) :: dglap_me_method
  type(string_t) :: default_method
  logical :: cmp_born, cmp_real
  logical :: cmp_loop, cmp_corr
  logical :: cmp_dglap
  if (is_nlo) then
    method = var_list%get_sval (var_str ("method"))
    born_me_method = var_list%get_sval (var_str ("born_me_method"))
    if (born_me_method == "") born_me_method = method
    real_tree_me_method = var_list%get_sval (var_str ("real_tree_me_method"))
    if (real_tree_me_method == "") real_tree_me_method = method
    loop_me_method = var_list%get_sval (var_str ("loop_me_method"))
    if (loop_me_method == "") loop_me_method = method
    correlation_me_method = var_list%get_sval (var_str ("correlation_me_method"))
    if (correlation_me_method == "") correlation_me_method = method
    dglap_me_method = var_list%get_sval (var_str ("dglap_me_method"))
    if (dglap_me_method == "") dglap_me_method = method
    cmp_born = born_me_method /= 'omega'
    cmp_real = is_nlo .and. (real_tree_me_method /= 'omega')
    cmp_loop = is_nlo .and. (loop_me_method /= 'omega')
    cmp_corr = is_nlo .and. (correlation_me_method /= 'omega')
    cmp_dglap = is_nlo .and. (dglap_me_method /= 'omega')
    call set_me_method (1, loop_me_method)
    call set_me_method (2, correlation_me_method)
    call set_me_method (3, real_tree_me_method)
    call set_me_method (4, born_me_method)
  end if
end subroutine blha_master_set_methods

```

```

        call set_me_method (5, dglap_me_method)
    else
        default_method = var_list%get_sval (var_str (" $method"))
        cmp_born = default_method /= 'omega'
        cmp_real = .false.; cmp_loop = .false.; cmp_corr = .false.
        call set_me_method (4, default_method)
    end if
    master%n_files = count ([cmp_born, cmp_real, cmp_loop, cmp_corr, cmp_dglap])
    call set_nlo_indices ()
    master%compute_borns = cmp_born
    master%compute_real_trees = cmp_real
    master%compute_loops = cmp_loop
    master%compute_correlations = cmp_corr
    master%compute_dglap = cmp_dglap
contains
    subroutine set_nlo_indices ()
        integer :: i_file
        allocate (master%i_file_to_nlo_index (master%n_files))
        master%i_file_to_nlo_index = 0
        i_file = 0
        if (cmp_loop) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 1
        end if
        if (cmp_corr) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 2
        end if
        if (cmp_real) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 3
        end if
        if (cmp_born) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 4
        end if
        if (cmp_dglap) then
            i_file = i_file + 1
            master%i_file_to_nlo_index(i_file) = 5
        end if
    end subroutine set_nlo_indices

    subroutine set_me_method (i, me_method)
        integer, intent(in) :: i
        type(string_t) :: me_method
        select case (char (me_method))
        case ('gosam')
            call master%set_gosam (i)
        case ('openloops')
            call master%set_openloops (i)
        end select
    end subroutine set_me_method
end subroutine blha_master_set_methods

```

```

<BLHA config: blha master: TBP>+≡
  procedure :: allocate_config_files => blha_master_allocate_config_files

<BLHA config: procedures>+≡
  subroutine blha_master_allocate_config_files (master)
    class(blha_master_t), intent(inout) :: master
    allocate (master%blha_cfg (master%n_files))
    allocate (master%suffix (master%n_files))
  end subroutine blha_master_allocate_config_files

<BLHA config: blha master: TBP>+≡
  procedure :: set_ew_scheme => blha_master_set_ew_scheme

<BLHA config: procedures>+≡
  subroutine blha_master_set_ew_scheme (master, ew_scheme)
    class(blha_master_t), intent(inout) :: master
    type(string_t), intent(in) :: ew_scheme
    master%ew_scheme = ew_scheme_string_to_int (ew_scheme)
  end subroutine blha_master_set_ew_scheme

<BLHA config: blha master: TBP>+≡
  procedure :: set_correction_type => blha_master_set_correction_type

<BLHA config: procedures>+≡
  subroutine blha_master_set_correction_type (master, correction_type_str)
    class(blha_master_t), intent(inout) :: master
    type(string_t), intent(in) :: correction_type_str
    master%blha_cfg(:)%correction_type = correction_type_string_to_int (correction_type_str)
  end subroutine blha_master_set_correction_type

<BLHA config: blha master: TBP>+≡
  procedure :: set_photon_characteristics => blha_master_set_photon_characteristics

<BLHA config: procedures>+≡
  subroutine blha_master_set_photon_characteristics (master, flv_born, n_in)
    class(blha_master_t), intent(inout) :: master
    integer, dimension(:, :), intent(in) :: flv_born
    integer, intent(in) :: n_in
    integer :: i_file, i, i_flv
    integer :: noff_is, noff_fs, noff_is_max, noff_fs_max
    do i_file = 1, master%n_files
      noff_is_max = 0; noff_fs_max = 0
      do i_flv = 1, size (flv_born, 2)
        noff_is = 0; noff_fs = 0
        do i = 1, n_in
          if (flv_born (i, i_flv) == PHOTON) noff_is = noff_is + 1
        end do
        noff_is_max = max (noff_is, noff_is_max)
        do i = n_in + 1, size (flv_born(:, i_flv))
          if (flv_born (i, i_flv) == PHOTON) noff_fs = noff_fs + 1
        end do
        noff_fs_max = max (noff_fs, noff_fs_max)
      end do
      if (master%blha_cfg(i_file)%correction_type == BLHA_CT_EW &
        .and. master%ew_scheme == BLHA_EW_0 &

```

```

        .and. (noff_is_max > 0 .or. noff_fs_max > 0)) then
        call msg_fatal ("For NLO EW/mixed corrections, 'alpha_0'/" &
        // "'alpha_thompson' are ", [ var_str ("inconsistent EW input " &
        // "schemes. Please use 'alpha_mz' or 'Gmu'")])
    end if
    master%blha_cfg(i_file)%n_off_photons_is = noff_is_max
    master%blha_cfg(i_file)%n_off_photons_fs = noff_fs_max
end do
end subroutine blha_master_set_photon_characteristics

```

(BLHA config: blha master: TBP)+≡

```

    procedure :: generate => blha_master_generate

```

(BLHA config: procedures)+≡

```

    subroutine blha_master_generate (master, basename, model, &
        n_in, alpha_power, alphas_power, flv_born, flv_real)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: basename
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in
        integer, intent(in) :: alpha_power, alphas_power
        integer, intent(in), dimension(:,:), allocatable :: flv_born, flv_real
        integer :: i_file
        if (master%n_files < 1) &
            call msg_fatal ("Attempting to generate OLP-files, but none are specified!")
        i_file = 1
        call master%generate_loop (basename, model, n_in, alpha_power, &
            alphas_power, flv_born, i_file)
        call master%generate_correlation (basename, model, n_in, alpha_power, &
            alphas_power, flv_born, i_file)
        call master%generate_real_tree (basename, model, n_in, alpha_power, &
            alphas_power, flv_real, i_file)
        call master%generate_born (basename, model, n_in, alpha_power, &
            alphas_power, flv_born, i_file)
        call master%generate_dglap (basename, model, n_in, alpha_power, &
            alphas_power, flv_born, i_file)
    end subroutine blha_master_generate

```

(BLHA config: blha master: TBP)+≡

```

    procedure :: generate_loop => blha_master_generate_loop

```

(BLHA config: procedures)+≡

```

    subroutine blha_master_generate_loop (master, basename, model, n_in, &
        alpha_power, alphas_power, flv_born, i_file)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: basename
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in
        integer, intent(in) :: alpha_power, alphas_power
        integer, dimension(:,:), allocatable, intent(in) :: flv_born
        integer, intent(inout) :: i_file
        type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
        integer :: i_flv
        if (master%compute_loops) then

```

```

    if (allocated (flv_born)) then
        allocate (blha_flavor (size (flv_born, 2)))
        do i_flv = 1, size (flv_born, 2)
            allocate (blha_flavor(i_flv)%flavors (size (flv_born(:,i_flv))))
            blha_flavor(i_flv)%flavors = flv_born(:,i_flv)
            blha_flavor(i_flv)%flv_mult = 2
        end do
        master%suffix(i_file) = blha_get_additional_suffix (var_str ("_LOOP"))
        call blha_init_virtual (master%blha_cfg(i_file), blha_flavor, &
            n_in, alpha_power, alphas_power, master%ew_scheme, &
            basename, model, master%blha_mode(1), master%suffix(i_file))
        i_file = i_file + 1
    else
        call msg_fatal ("BLHA Loops requested but " &
            // "Born flavor not existing")
    end if
end if
end subroutine blha_master_generate_loop

```

<BLHA config: blha master: TBP>+≡

```

    procedure :: generate_correlation => blha_master_generate_correlation

```

<BLHA config: procedures>+≡

```

    subroutine blha_master_generate_correlation (master, basename, model, n_in, &
        alpha_power, alphas_power, flv_born, i_file)
        class(blha_master_t), intent(inout) :: master
        type(string_t), intent(in) :: basename
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: n_in
        integer, intent(in) :: alpha_power, alphas_power
        integer, dimension(:,,:), allocatable, intent(in) :: flv_born
        integer, intent(inout) :: i_file
        type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
        integer :: i_flv
        if (master%compute_correlations) then
            if (allocated (flv_born)) then
                allocate (blha_flavor (size (flv_born, 2)))
                do i_flv = 1, size (flv_born, 2)
                    allocate (blha_flavor(i_flv)%flavors (size (flv_born(:,i_flv))))
                    blha_flavor(i_flv)%flavors = flv_born(:,i_flv)
                    blha_flavor(i_flv)%flv_mult = 3
                end do
                master%suffix(i_file) = blha_get_additional_suffix (var_str ("_SUB"))
                call blha_init_subtraction (master%blha_cfg(i_file), blha_flavor, &
                    n_in, alpha_power, alphas_power, master%ew_scheme, &
                    basename, model, master%blha_mode(2), master%suffix(i_file))
                i_file = i_file + 1
            else
                call msg_fatal ("BLHA Correlations requested but " &
                    // "Born flavor not existing")
            end if
        end if
    end subroutine blha_master_generate_correlation

```

```

<BLHA config: blha master: TBP>+≡
  procedure :: generate_real_tree => blha_master_generate_real_tree

<BLHA config: procedures>+≡
  subroutine blha_master_generate_real_tree (master, basename, model, n_in, &
    alpha_power, alphas_power, flv_real, i_file)
    class(blha_master_t), intent(inout) :: master
    type(string_t), intent(in) :: basename
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: n_in
    integer, intent(in) :: alpha_power, alphas_power
    integer, dimension(:,:), allocatable, intent(in) :: flv_real
    integer, intent(inout) :: i_file
    type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
    integer :: i_flv
    if (master%compute_real_trees) then
      if (allocated (flv_real)) then
        allocate (blha_flavor (size (flv_real, 2)))
        do i_flv = 1, size (flv_real, 2)
          allocate (blha_flavor(i_flv)%flavors (size (flv_real(:,i_flv))))
          blha_flavor(i_flv)%flavors = flv_real(:,i_flv)
          blha_flavor(i_flv)%flv_mult = 1
        end do
        master%suffix(i_file) = blha_get_additional_suffix (var_str ("_REAL"))
        call blha_init_real (master%blha_cfg(i_file), blha_flavor, &
          n_in, alpha_power, alphas_power, master%ew_scheme, &
          basename, model, master%blha_mode(3), master%suffix(i_file))
        i_file = i_file + 1
      else
        call msg_fatal ("BLHA Trees requested but "&
          // "Real flavor not existing")
      end if
    end if
  end subroutine blha_master_generate_real_tree

```

```

<BLHA config: blha master: TBP>+≡
  procedure :: generate_born => blha_master_generate_born

<BLHA config: procedures>+≡
  subroutine blha_master_generate_born (master, basename, model, n_in, &
    alpha_power, alphas_power, flv_born, i_file)
    class(blha_master_t), intent(inout) :: master
    type(string_t), intent(in) :: basename
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: n_in
    integer, intent(in) :: alpha_power, alphas_power
    integer, dimension(:,:), allocatable, intent(in) :: flv_born
    integer, intent(inout) :: i_file
    type(blha_flv_state_t), dimension(:), allocatable :: blha_flavor
    integer :: i_flv
    if (master%compute_borns) then
      if (allocated (flv_born)) then
        allocate (blha_flavor (size (flv_born, 2)))
        do i_flv = 1, size (flv_born, 2)
          allocate (blha_flavor(i_flv)%flavors (size (flv_born(:,i_flv))))

```



```

        blha_flavor(i_flg)%flavors = flv_born(:,i_flg)
        blha_flavor(i_flg)%flv_mult = 1
    end do
    master%suffix(i_file) = blha_get_additional_suffix (var_str ("_BORN"))
    call blha_init_born (master%blha_cfg(i_file), blha_flavor, &
        n_in, alpha_power, alphas_power, master%ew_scheme, &
        basename, model, master%blha_mode(4), master%suffix(i_file))
    i_file = i_file + 1
end if
end if
end subroutine blha_master_generate_born

```

(BLHA config: blha master: TBP)+≡

```

    procedure :: generate_dglap => blha_master_generate_dglap

```

(BLHA config: procedures)+≡

```

    subroutine blha_master_generate_dglap (master, basename, model, n_in, &
        alpha_power, alphas_power, flv_born, i_file)
    class(blha_master_t), intent(inout) :: master
    type(string_t), intent(in) :: basename
    class(model_data_t), intent(in), target :: model
    integer, intent(in) :: n_in
    integer, intent(in) :: alpha_power, alphas_power
    integer, dimension(:,:), allocatable, intent(in) :: flv_born
    integer, intent(inout) :: i_file
    type(blha_flgv_state_t), dimension(:), allocatable :: blha_flavor
    integer :: i_flgv
    if (master%compute_dglap) then
        if (allocated (flv_born)) then
            allocate (blha_flavor (size (flv_born, 2)))
            do i_flgv = 1, size (flv_born, 2)
                allocate (blha_flavor(i_flgv)%flavors (size (flv_born(:,i_flgv))))
                blha_flavor(i_flgv)%flavors = flv_born(:,i_flgv)
                blha_flavor(i_flgv)%flv_mult = 2
            end do
            master%suffix(i_file) = blha_get_additional_suffix (var_str ("_DGLAP"))
            call blha_init_dglap (master%blha_cfg(i_file), blha_flavor, &
                n_in, alpha_power, alphas_power, master%ew_scheme, &
                basename, model, master%blha_mode(5), master%suffix(i_file))
            i_file = i_file + 1
        end if
    end if
end subroutine blha_master_generate_dglap

```

(BLHA config: blha master: TBP)+≡

```

    procedure :: setup_additional_features => blha_master_setup_additional_features

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(BLHA config: procedures)+≡

```

    subroutine blha_master_setup_additional_features (master, &
        pbs_tolerance, use_cms, stability_log, extra_cmd, beam_structure)
    class(blha_master_t), intent(inout) :: master
    integer, intent(in) :: pbs_tolerance
    logical, intent(in) :: use_cms
    type(string_t), intent(in), optional :: extra_cmd

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```

integer, intent(in) :: stability_log
type(beam_structure_t), intent(in), optional :: beam_structure
integer :: i_file
logical :: polarized, throw_warning

polarized = .false.
if (present (beam_structure)) polarized = beam_structure%has_polarized_beams ()

throw_warning = .false.
if (use_cms) then
  throw_warning = throw_warning .or. (master%compute_loops &
    .and. master%blha_mode(1) /= BLHA_MODE_OPENLOOPS)
  throw_warning = throw_warning .or. (master%compute_correlations &
    .and. master%blha_mode(2) /= BLHA_MODE_OPENLOOPS)
  throw_warning = throw_warning .or. (master%compute_real_trees &
    .and. master%blha_mode(3) /= BLHA_MODE_OPENLOOPS)
  throw_warning = throw_warning .or. (master%compute_borns &
    .and. master%blha_mode(4) /= BLHA_MODE_OPENLOOPS)
  throw_warning = throw_warning .or. (master%compute_dglap &
    .and. master%blha_mode(5) /= BLHA_MODE_OPENLOOPS)
  if (throw_warning) call cms_warning ()
end if

do i_file = 1, master%n_files
  if (phs_tolerance > 0) then
    select case (master%blha_mode (master%i_file_to_nlo_index(i_file)))
    case (BLHA_MODE_GOSAM)
      if (polarized) call gosam_error_message ()
    case (BLHA_MODE_OPENLOOPS)
      master%blha_cfg(i_file)%openloops_use_cms = use_cms
      master%blha_cfg(i_file)%openloops_phs_tolerance = phs_tolerance
      master%blha_cfg(i_file)%polarized = polarized
      if (present (extra_cmd)) then
        master%blha_cfg(i_file)%openloops_extra_cmd = extra_cmd
      else
        master%blha_cfg(i_file)%openloops_extra_cmd = var_str ('')
      end if
      master%blha_cfg(i_file)%openloops_stability_log = stability_log
    end select
  end if
end do
contains
subroutine cms_warning ()
  call msg_warning ("You have set ?openloops_use_cms = true, but not all active matrix ", &
    [var_str ("element methods are set to OpenLoops. Note that other "), &
    var_str ("methods might not necessarily support the complex mass "), &
    var_str ("scheme. This can yield inconsistencies in your NLO results!")])
end subroutine cms_warning

subroutine gosam_error_message ()
  call msg_fatal ("You are trying to evaluate a process at NLO ", &
    [var_str ("which involves polarized beams using GoSam. "), &
    var_str ("This feature is not supported yet. "), &
    var_str ("Please use OpenLoops instead")])

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```

        end subroutine gosam_error_message
    end subroutine blha_master_setup_additional_features

<BLHA config: blha master: TBP>+≡
    procedure :: set_gosam => blha_master_set_gosam

<BLHA config: procedures>+≡
    subroutine blha_master_set_gosam (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
        master%blha_mode(i) = BLHA_MODE_GOSAM
    end subroutine blha_master_set_gosam

<BLHA config: blha master: TBP>+≡
    procedure :: set_openloops => blha_master_set_openloops

<BLHA config: procedures>+≡
    subroutine blha_master_set_openloops (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
        master%blha_mode(i) = BLHA_MODE_OPENLOOPS
    end subroutine blha_master_set_openloops

<BLHA config: blha master: TBP>+≡
    procedure :: set_polarization => blha_master_set_polarization

<BLHA config: procedures>+≡
    subroutine blha_master_set_polarization (master, i)
        class(blha_master_t), intent(inout) :: master
        integer, intent(in) :: i
        master%blha_cfg(i)%polarized = .true.
    end subroutine blha_master_set_polarization

<BLHA config: procedures>+≡
    subroutine blha_init_born (blha_cfg, blha_flavor, n_in, &
        ap, asp, ew_scheme, basename, model, blha_mode, suffix)
        type(blha_configuration_t), intent(inout) :: blha_cfg
        type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
        integer, intent(in) :: n_in
        integer, intent(in) :: ap, asp
        integer, intent(in) :: ew_scheme
        type(string_t), intent(in) :: basename
        type(model_data_t), intent(in), target :: model
        integer, intent(in) :: blha_mode
        type(string_t), intent(in) :: suffix
        integer, dimension(:), allocatable :: amp_type
        integer :: i

        allocate (amp_type (size (blha_flavor)))
        do i = 1, size (blha_flavor)
            amp_type(i) = BLHA_AMP_TREE
        end do
        call blha_configuration_init (blha_cfg, basename // suffix , &

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        model, blha_mode)
call blha_configuration_append_processes (blha_cfg, n_in, &
    blha_flavor, amp_type)
call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
    irreg = BLHA_IRREG_CDR, alphas_power = asp, &
    alpha_power = ap, ew_scheme = ew_scheme, &
    debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_born

subroutine blha_init_virtual (blha_cfg, blha_flavor, n_in, &
    ap, asp, ew_scheme, basename, model, blha_mode, suffix)
type(blha_configuration_t), intent(inout) :: blha_cfg
type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
integer, intent(in) :: n_in
integer, intent(in) :: ap, asp
integer, intent(in) :: ew_scheme
type(string_t), intent(in) :: basename
type(model_data_t), intent(in), target :: model
integer, intent(in) :: blha_mode
type(string_t), intent(in) :: suffix
integer, dimension(:), allocatable :: amp_type
integer :: i

allocate (amp_type (size (blha_flavor) * 2))
do i = 1, size (blha_flavor)
    amp_type(2 * i - 1) = BLHA_AMP_LOOP
    amp_type(2 * i) = BLHA_AMP_COLOR_C
end do
call blha_configuration_init (blha_cfg, basename // suffix, &
    model, blha_mode)
call blha_configuration_append_processes (blha_cfg, n_in, &
    blha_flavor, amp_type)
call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
    irreg = BLHA_IRREG_CDR, &
    alphas_power = asp, &
    alpha_power = ap, &
    ew_scheme = ew_scheme, &
    debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_virtual

subroutine blha_init_dglap (blha_cfg, blha_flavor, n_in, &
    ap, asp, ew_scheme, basename, model, blha_mode, suffix)
type(blha_configuration_t), intent(inout) :: blha_cfg
type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
integer, intent(in) :: n_in
integer, intent(in) :: ap, asp
integer, intent(in) :: ew_scheme
type(string_t), intent(in) :: basename
type(model_data_t), intent(in), target :: model
integer, intent(in) :: blha_mode
type(string_t), intent(in) :: suffix
integer, dimension(:), allocatable :: amp_type
integer :: i

```

```

allocate (amp_type (size (blha_flavor) * 2))
do i = 1, size (blha_flavor)
    amp_type(2 * i - 1) = BLHA_AMP_TREE
    amp_type(2 * i) = BLHA_AMP_COLOR_C
end do
call blha_configuration_init (blha_cfg, basename // suffix , &
    model, blha_mode)
call blha_configuration_append_processes (blha_cfg, n_in, &
    blha_flavor, amp_type)
call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
    irreg = BLHA_IRREG_CDR, &
    alphas_power = asp, &
    alpha_power = ap, &
    ew_scheme = ew_scheme, &
    debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_dglap

subroutine blha_init_subtraction (blha_cfg, blha_flavor, n_in, &
    ap, asp, ew_scheme, basename, model, blha_mode, suffix)
    type(blha_configuration_t), intent(inout) :: blha_cfg
    type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
    integer, intent(in) :: n_in
    integer, intent(in) :: ap, asp
    integer, intent(in) :: ew_scheme
    type(string_t), intent(in) :: basename
    type(model_data_t), intent(in), target :: model
    integer, intent(in) :: blha_mode
    type(string_t), intent(in) :: suffix
    integer, dimension(:), allocatable :: amp_type
    integer :: i

    allocate (amp_type (size (blha_flavor) * 3))
    do i = 1, size (blha_flavor)
        amp_type(3 * i - 2) = BLHA_AMP_TREE
        amp_type(3 * i - 1) = BLHA_AMP_COLOR_C
        amp_type(3 * i) = BLHA_AMP_SPIN_C
    end do
    call blha_configuration_init (blha_cfg, basename // suffix , &
        model, blha_mode)
    call blha_configuration_append_processes (blha_cfg, n_in, &
        blha_flavor, amp_type)
    call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
        irreg = BLHA_IRREG_CDR, &
        alphas_power = asp, &
        alpha_power = ap, &
        ew_scheme = ew_scheme, &
        debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_subtraction

subroutine blha_init_real (blha_cfg, blha_flavor, n_in, &
    ap, asp, ew_scheme, basename, model, blha_mode, suffix)
    type(blha_configuration_t), intent(inout) :: blha_cfg
    type(blha_flv_state_t), intent(in), dimension(:) :: blha_flavor
    integer, intent(in) :: n_in

```

```

integer, intent(in) :: ap, asp
integer :: ap_ew, ap_qcd
integer, intent(in) :: ew_scheme
type(string_t), intent(in) :: basename
type(model_data_t), intent(in), target :: model
integer, intent(in) :: blha_mode
type(string_t), intent(in) :: suffix
integer, dimension(:), allocatable :: amp_type
integer :: i

allocate (amp_type (size (blha_flavor)))
do i = 1, size (blha_flavor)
    amp_type(i) = BLHA_AMP_TREE
end do
select case (blha_cfg%correction_type)
case (BLHA_CT_QCD)
    ap_ew = ap
    ap_qcd = asp + 1
case (BLHA_CT_EW)
    ap_ew = ap + 1
    ap_qcd = asp
end select
call blha_configuration_init (blha_cfg, basename // suffix , &
    model, blha_mode)
call blha_configuration_append_processes (blha_cfg, n_in, &
    blha_flavor, amp_type)

call blha_configuration_set (blha_cfg, BLHA_VERSION_2, &
    irreg = BLHA_IRREG_CDR, &
    alphas_power = ap_qcd, &
    alpha_power = ap_ew, &
    ew_scheme = ew_scheme, &
    debug = blha_mode == BLHA_MODE_GOSAM)
end subroutine blha_init_real

```

```

<BLHA config: public>+≡
    public :: blha_get_additional_suffix

<BLHA config: procedures>+≡
    function blha_get_additional_suffix (base_suffix) result (suffix)
        type(string_t) :: suffix
        type(string_t), intent(in) :: base_suffix
    <blha master: blha master extend suffixes: variables>
        suffix = base_suffix
    <blha master: blha master extend suffixes: procedure>
    end function blha_get_additional_suffix

<MPI: blha master: blha master extend suffixes: variables>≡
    integer :: n_size, rank

<MPI: blha master: blha master extend suffixes: procedure>≡
    call MPI_Comm_rank (MPI_COMM_WORLD, rank)
    call MPI_Comm_size (MPI_COMM_WORLD, n_size)
    if (n_size > 1) then

```

```

        suffix = suffix // var_str ("_" ) // str (rank)
    end if

<BLHA config: blha master: TBP>+≡
    procedure :: write_olp => blha_master_write_olp

<BLHA config: procedures>+≡
    subroutine blha_master_write_olp (master, basename)
        class(blha_master_t), intent(in) :: master
        type(string_t), intent(in) :: basename
        integer :: unit
        type(string_t) :: filename
        integer :: i_file
        do i_file = 1, master%n_files
            filename = basename // master%suffix(i_file) // ".olp"
            unit = free_unit ()
            open (unit, file = char (filename), status = 'replace', action = 'write')
            call blha_configuration_write (master%blha_cfg(i_file), master%suffix(i_file), unit)
            close (unit)
        end do
    end subroutine blha_master_write_olp

<BLHA config: blha master: TBP>+≡
    procedure :: final => blha_master_final

<BLHA config: procedures>+≡
    subroutine blha_master_final (master)
        class(blha_master_t), intent(inout) :: master
        master%n_files = 0
        deallocate (master%suffix)
        deallocate (master%blha_cfg)
        deallocate (master%i_file_to_nlo_index)
    end subroutine blha_master_final

<BLHA config: public>+≡
    public :: blha_configuration_init

<BLHA config: procedures>+≡
    subroutine blha_configuration_init (cfg, name, model, mode)
        type(blha_configuration_t), intent(inout) :: cfg
        type(string_t), intent(in) :: name
        class(model_data_t), target, intent(in) :: model
        integer, intent(in), optional :: mode
        if (.not. associated (cfg%model)) then
            cfg%name = name
            cfg%model => model
        end if
        if (present (mode)) cfg%mode = mode
    end subroutine blha_configuration_init

Create an array of massive particle indices, to be used by the "MassiveParticle"-
statement of the order file.

<BLHA config: procedures>+≡
    subroutine blha_configuration_get_massive_particles &

```

```

        (cfg, massive, i_massive)
type(blha_configuration_t), intent(in) :: cfg
logical, intent(out) :: massive
integer, intent(out), dimension(:), allocatable :: i_massive
integer, parameter :: max_particles = 10
integer, dimension(max_particles) :: i_massive_tmp
integer, dimension(max_particles) :: checked
type(blha_cfg_process_node_t), pointer :: current_process
integer :: k
integer :: n_massive
n_massive = 0; k = 1
checked = 0
if (associated (cfg%processes)) then
    current_process => cfg%processes
else
    call msg_fatal ("BLHA, massive particles: " // &
        "No processes allocated!")
end if
do
    call check_pdg_list (current_process%pdg_in%pdg)
    call check_pdg_list (current_process%pdg_out%pdg)
    if (k > max_particles) &
        call msg_fatal ("BLHA, massive particles: " // &
            "Max. number of particles exceeded!")
    if (associated (current_process%next)) then
        current_process => current_process%next
    else
        exit
    end if
end do
if (n_massive > 0) then
    allocate (i_massive (n_massive))
    i_massive = i_massive_tmp (1:n_massive)
    massive = .true.
else
    massive = .false.
end if
contains
subroutine check_pdg_list (pdg_list)
    integer, dimension(:), intent(in) :: pdg_list
    integer :: i, i_pdg
    type(flavor_t) :: flv
    do i = 1, size (pdg_list)
        i_pdg = abs (pdg_list(i))
        call flv%init (i_pdg, cfg%model)
        if (flv%get_mass () > 0._default) then
            !!! Avoid duplicates in output
            if (.not. any (checked == i_pdg)) then
                i_massive_tmp(k) = i_pdg
                checked(k) = i_pdg
                k = k + 1
                n_massive = n_massive + 1
            end if
        end if
    end do
end if

```



```

        end do
    end subroutine check_pdg_list
end subroutine blha_configuration_get_massive_particles

```

(BLHA config: public)+≡

```
public :: blha_configuration_append_processes
```

(BLHA config: procedures)+≡

```

subroutine blha_configuration_append_processes (cfg, n_in, flavor, amp_type)
    type(blha_configuration_t), intent(inout) :: cfg
    integer, intent(in) :: n_in
    type(blha_flv_state_t), dimension(:), intent(in) :: flavor
    integer, dimension(:), intent(in), optional :: amp_type
    integer :: n_tot
    type(blha_cfg_process_node_t), pointer :: current_node
    integer :: i_process, i_flv
    integer, dimension(:), allocatable :: pdg_in, pdg_out
    integer, dimension(:), allocatable :: flavor_state
    integer :: proc_offset, n_proc_tot
    proc_offset = 0; n_proc_tot = 0
    do i_flv = 1, size (flavor)
        n_proc_tot = n_proc_tot + flavor(i_flv)%flv_mult
    end do
    if (.not. associated (cfg%processes)) &
        allocate (cfg%processes)
    current_node => cfg%processes
    do i_flv = 1, size (flavor)
        n_tot = size (flavor(i_flv)%flavors)
        allocate (pdg_in (n_in), pdg_out (n_tot - n_in))
        allocate (flavor_state (n_tot))
        flavor_state = flavor(i_flv)%flavors
        do i_process = 1, flavor(i_flv)%flv_mult
            pdg_in = flavor_state (1 : n_in)
            pdg_out = flavor_state (n_in + 1 : )
            if (cfg%polarized) then
                select case (cfg%mode)
                case (BLHA_MODE_OPENLOOPS)
                    call allocate_and_init_pdg_and_helicities (current_node, &
                        pdg_in, pdg_out, amp_type (proc_offset + i_process))
                case (BLHA_MODE_GOSAM)
                    !!! Nothing special for GoSam yet. This exception is already caught
                    !!! in blha_master_setup_additional_features
                end select
            else
                call allocate_and_init_pdg (current_node, pdg_in, pdg_out, &
                    amp_type (proc_offset + i_process))
            end if
            if (proc_offset + i_process /= n_proc_tot) then
                allocate (current_node%next)
                current_node => current_node%next
            end if
            if (i_process == flavor(i_flv)%flv_mult) &
                proc_offset = proc_offset + flavor(i_flv)%flv_mult
        end do
    end do

```

```

        deallocate (pdg_in, pdg_out)
        deallocate (flavor_state)
    end do

contains

    subroutine allocate_and_init_pdg (node, pdg_in, pdg_out, amp_type)
        type(blha_cfg_process_node_t), intent(inout), pointer :: node
        integer, intent(in), dimension(:), allocatable :: pdg_in, pdg_out
        integer, intent(in) :: amp_type
        allocate (node%pdg_in (size (pdg_in)))
        allocate (node%pdg_out (size (pdg_out)))
        node%pdg_in%pdg = pdg_in
        node%pdg_out%pdg = pdg_out
        node%amplitude_type = amp_type
    end subroutine allocate_and_init_pdg

    subroutine allocate_and_init_pdg_and_helicities (node, pdg_in, pdg_out, amp_type)
        type(blha_cfg_process_node_t), intent(inout), pointer :: node
        integer, intent(in), dimension(:), allocatable :: pdg_in, pdg_out
        integer, intent(in) :: amp_type
        integer :: h1, h2
        if (size (pdg_in) == 2) then
            do h1 = -1, 1, 2
                do h2 = -1, 1, 2
                    call allocate_and_init_pdg (current_node, pdg_in, pdg_out, amp_type)
                    current_node%pdg_in(1)%polarized = .true.
                    current_node%pdg_in(2)%polarized = .true.
                    current_node%pdg_in(1)%hel = h1
                    current_node%pdg_in(2)%hel = h2
                    if (h1 + h2 /= 2) then !!! not end of loop
                        allocate (current_node%next)
                        current_node => current_node%next
                    end if
                end do
            end do
        else
            do h1 = -1, 1, 2
                call allocate_and_init_pdg (current_node, pdg_in, pdg_out, amp_type)
                current_node%pdg_in(1)%polarized = .true.
                current_node%pdg_in(1)%hel = h1
                if (h1 /= 1) then !!! not end of loop
                    allocate (current_node%next)
                    current_node => current_node%next
                end if
            end do
        end if
    end subroutine allocate_and_init_pdg_and_helicities

end subroutine blha_configuration_append_processes

```

Change parameter(s).
<BLHA config: public>+≡

```

public :: blha_configuration_set
<BLHA config: procedures>+≡
subroutine blha_configuration_set (cfg, &
    version, irreg, massive_particle_scheme, &
    model_file, alphas_power, alpha_power, ew_scheme, width_scheme, &
    accuracy, debug)
type(blha_configuration_t), intent(inout) :: cfg
integer, optional, intent(in) :: version
integer, optional, intent(in) :: irreg
integer, optional, intent(in) :: massive_particle_scheme
type(string_t), optional, intent(in) :: model_file
integer, optional, intent(in) :: alphas_power, alpha_power
integer, optional, intent(in) :: ew_scheme
integer, optional, intent(in) :: width_scheme
real(default), optional, intent(in) :: accuracy
logical, optional, intent(in) :: debug
if (present (version)) &
    cfg%version = version
if (present (irreg)) &
    cfg%irreg = irreg
if (present (massive_particle_scheme)) &
    cfg%massive_particle_scheme = massive_particle_scheme
if (present (model_file)) &
    cfg%model_file = model_file
if (present (alphas_power)) &
    cfg%alphas_power = alphas_power
if (present (alpha_power)) &
    cfg%alpha_power = alpha_power
if (present (ew_scheme)) &
    cfg%ew_scheme = ew_scheme
if (present (width_scheme)) &
    cfg%width_scheme = width_scheme
if (present (accuracy)) &
    cfg%accuracy_target = accuracy
if (present (debug)) &
    cfg%debug_unstable = debug
cfg%dirty = .false.
end subroutine blha_configuration_set

<BLHA config: public>+≡
public :: blha_configuration_get_n_proc

<BLHA config: procedures>+≡
function blha_configuration_get_n_proc (cfg) result (n_proc)
type(blha_configuration_t), intent(in) :: cfg
integer :: n_proc
n_proc = cfg%n_proc
end function blha_configuration_get_n_proc

```

Write the BLHA file. Internal mode is intended for md5summing only.

Special cases of external photons in OpenLoops:

For electroweak corrections the particle ID (PID) of photons is a crucial input

for the computation of matrix elements by **OpenLoops**. According to "arXiv: 1907.13071", section 3.2, external photons are classified by the following types:

- PID = -2002: off-shell photons, that undergo $\gamma \rightarrow f\bar{f}$ splittings at NLO EW, or initial state photons from QED PDFs
- PID = 2002: on-shell photons, that do not undergo $\gamma \rightarrow f\bar{f}$ splittings at NLO EW, or initial state photons for example at photon colliders
- PID = 22: unresolved photons, representing radiated photons at NLO EW, absent at LO

For the first two types scattering amplitudes for processes with external photons at NLO EW get renormalisation factors containing photon-coupling and wave function counterterms. Logarithmic mass singularities arising due to the renormalisation of off-shell external photon wave functions are cancelled by collinear singularities of photon PDF counterterms or analogous terms in virtual contributions originating from $\gamma \rightarrow f\bar{f}$ splittings of final state photons.

The finite remainders of the renormalisation factors are thus dictated by the specific photon PID stated above. As consequence, we have to adjust the input PIDs written into the BLHA file which will be read by **OpenLoops**.

Concretely, for the case of electroweak corrections initial state photons associated with photon PDFs and final state photons (if existent at LO) are labeled as off-shell photons with PID "-2002". On-shell photons with PID "2002" are neglected for now since to include them for processes at NLO EW is non-trivial from the phenomenological point of view. Processes at NLO EW typically are studied at high energy scales for which photon-induced sub-processes in most cases can not be neglected. However, on-shell, e. g. tagged, photons are defined at low energy scales and thus the process has to be described with external photon fields and couplings at two different scales.

Another issue which has to be addressed if various photon PIDs are taken into account is that real and virtual amplitudes have to be computed at the same order in α at a specific scale for the subtraction scheme to be consistent. The complication comes by the fact that the EW coupling α of each external photon in the amplitudes will automatically be rescaled by **OpenLoops** corresponding to the specific photon type. Following eq. (3.30) of "arXiv: 1907.13071", by default the coupling of an on-shell photon will be changed to $\alpha(0)$ and that of an off-shell photon to α_{G_μ} if not chosen already at a high scale, e. g. $\alpha(M_Z)$. In order to not spoil the IR cancellation **OpenLoops** supplies to register unresolved photons with PID "22" describing a radiated photon at NLO EW for which the photon-coupling α is left unchanged at the value which is computed with the electroweak input scheme chosen by the user. This is adopted here by labeling each emitted photon as unresolved with PID "22" if no photons are present at LO.

For EW corrections the freedom to choose an electroweak input scheme is restricted, however, since the number of external photons present at LO is not conserved for the corresponding real flavor structures due to possible $\gamma \rightarrow f\bar{f}$ splittings. This forbids to choose $\alpha = \alpha(0)$ since otherwise the order in $\alpha(0)$ is not conserved in the real amplitudes corresponding to the factorizing Born process. Consequently, for FKS the NLO components are not of the same order

in $\alpha(0)$. The option `$blha_ew_scheme = "alpha_0"` is thus refused for the case if EW corrections are activated and photons are present at LO.

(BLHA config: public)+≡

public :: blha_configuration_write

(BLHA config: procedures)+≡

```
subroutine blha_configuration_write (cfg, suffix, unit, internal, no_version)
  type(blha_configuration_t), intent(in) :: cfg
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: internal, no_version
  type(string_t), intent(in) :: suffix
  integer, dimension(:), allocatable :: pdg_flv
  integer :: u
  logical :: full
  type(string_t) :: buf
  type(blha_cfg_process_node_t), pointer :: node
  integer :: i
  character(3) :: pdg_char
  character(5) :: pdg_char_extra
  character(4) :: hel_char
  character(6) :: suffix_char
  character(len=25), parameter :: pad = ""
  logical :: write_process, no_v
  no_v = .false. ; if (present (no_version)) no_v = no_version
  u = given_output_unit (unit); if (u < 0) return
  full = .true.; if (present (internal)) full = .not. internal
  if (full .and. cfg%dirty) call msg_bug ( &
    "BUG: attempted to write out a dirty BLHA configuration")
  if (full) then
    if (no_v) then
      write (u, "(A)") "# BLHA order written by WHIZARD [version]"
    else
      write (u, "(A)") "# BLHA order written by WHIZARD {Version}"
    end if
    write (u, "(A)")
  end if
  select case (cfg%mode)
    case (BLHA_MODE_GOSAM); buf = "GoSam"
    case (BLHA_MODE_OPENLOOPS); buf = "OpenLoops"
    case default; buf = "vanilla"
  end select
  write (u, "(A)") "# BLHA interface mode: " // char (buf)
  write (u, "(A)") "# process: " // char (cfg%name)
  write (u, "(A)") "# model: " // char (cfg%model%get_name ())
  select case (cfg%version)
    case (1); buf = "BLHA1"
    case (2); buf = "BLHA2"
  end select
  write (u, '(A25,A)') "InterfaceVersion " // pad, char (buf)
  select case (cfg%correction_type)
    case (BLHA_CT_QCD); buf = "QCD"
    case (BLHA_CT_EW); buf = "EW"
    case default; buf = cfg%correction_type_other
  end select
```

```

write (u,'(A25,A)') "CorrectionType" // pad, char (buf)

select case (cfg%mode)
case (BLHA_MODE_OPENLOOPS)
    buf = cfg%name // '.olc'
    write (u, '(A25,A)') "Extra AnswerFile" // pad, char (buf)
end select

select case (cfg%irreg)
case (BLHA_IRREG_CDR); buf = "CDR"
case (BLHA_IRREG_DRED); buf = "DRED"
case (BLHA_IRREG_THV); buf = "tHV"
case (BLHA_IRREG_MREG); buf = "MassReg"
case default; buf = cfg%irreg_other
end select
write (u,'(A25,A)') "IRregularisation" // pad, char (buf)
select case (cfg%massive_particle_scheme)
case (BLHA_MPS_ONSHELL); buf = "OnShell"
case default; buf = cfg%massive_particle_scheme_other
end select
if (cfg%mode == BLHA_MODE_GOSAM) &
    write (u,'(A25,A)') "MassiveParticleScheme" // pad, char (buf)
select case (cfg%version)
case (1)
    if (cfg%alphas_power >= 0) write (u,'(A25,A)') &
        "AlphasPower" // pad, int2char (cfg%alphas_power)
    if (cfg%alpha_power >= 0) write (u,'(A25,A)') &
        "AlphaPower " // pad, int2char (cfg%alpha_power)
case (2)
    if (cfg%alphas_power >= 0) write (u,'(A25,A)') &
        "CouplingPower QCD " // pad, int2char (cfg%alphas_power)
    if (cfg%alpha_power >= 0) write (u,'(A25,A)') &
        "CouplingPower QED " // pad, int2char (cfg%alpha_power)
end select
select case (cfg%mode)
case (BLHA_MODE_GOSAM)
    select case (cfg%ew_scheme)
    case (BLHA_EW_GF, BLHA_EW_INTERNAL); buf = "alphaGF"
    case (BLHA_EW_MZ); buf = "alphaMZ"
    case (BLHA_EW_MSBAR); buf = "alphaMSbar"
    case (BLHA_EW_0); buf = "alpha0"
    case (BLHA_EW_RUN); buf = "alphaRUN"
    end select
    write (u, '(A25, A)') "EWScheme " // pad, char (buf)
case (BLHA_MODE_OPENLOOPS)
    select case (cfg%ew_scheme)
    case (BLHA_EW_0); buf = "alpha0"
    case (BLHA_EW_GF); buf = "Gmu"
    case (BLHA_EW_MZ, BLHA_EW_INTERNAL); buf = "alphaMZ"
    case default
        call msg_fatal ("OpenLoops input: Only supported EW schemes &
            & are 'alpha0', 'Gmu', and 'alphaMZ'")
    end select
    write (u, '(A25, A)') "ewscheme " // pad, char (buf)

```

```

end select
select case (cfg%mode)
case (BLHA_MODE_GOSAM)
    write (u, '(A25)', advance='no') "MassiveParticles " // pad
    do i = 1, size (OLP_MASSIVE_PARTICLES)
        if (OLP_MASSIVE_PARTICLES(i) > 0) &
            write (u, '(I2,I1)', advance='no') OLP_MASSIVE_PARTICLES(i)
    end do
    write (u,*)
case (BLHA_MODE_OPENLOOPS)
    if (cfg%openloops_use_cms) then
        write (u, '(A25,I1)') "extra use_cms " // pad, 1
    else
        write (u, '(A25,I1)') "extra use_cms " // pad, 0
    end if
    write (u, '(A25,I1)') "extra me_cache " // pad, 0
    !!! Turn off calculation of 1/eps & 1/eps^2 poles in one-loop calculation
    !!! Not needed in FKS (or any numerical NLO subtraction scheme)
    write (u, '(A25,I1)') "extra IR_on " // pad, 0
    if (cfg%openloops_phs_tolerance > 0) then
        write (u, '(A25,A4,I0)') "extra psp_tolerance " // pad, "10e-", &
            cfg%openloops_phs_tolerance
    end if
    call check_extra_cmd (cfg%openloops_extra_cmd)
    write (u, '(A)') char (cfg%openloops_extra_cmd)
    if (cfg%openloops_stability_log > 0) &
        write (u, '(A25,I1)') "extra stability_log " // pad, &
            cfg%openloops_stability_log
end select
if (full) then
    write (u, "(A)")
    write (u, "(A)") "# Process definitions"
    write (u, "(A)")
end if
if (cfg%debug_unstable) &
    write (u, '(A25,A)') "DebugUnstable " // pad, "True"
write (u, *)
node => cfg%processes
do while (associated (node))
    write_process = .true.
    allocate (pdg_flv (size (node%pdg_in) + size (node%pdg_out)))
    do i = 1, size (node%pdg_in)
        pdg_flv (i) = node%pdg_in(i)%pdg
    end do
    do i = 1, size (node%pdg_out)
        pdg_flv (i + size (node%pdg_in)) = node%pdg_out(i)%pdg
    end do
    suffix_char = char (suffix)
    if (cfg%correction_type == BLHA_CT_EW .and. cfg%alphas_power > 0) then
        if ((suffix_char (1:5) == "_BORN" .and. .not. query_coupling_powers &
            (pdg_flv, cfg%alpha_power, cfg%alphas_power)) .or. &
            ((suffix_char (1:4) == "_SUB" .or. suffix_char (1:5) == "_LOOP" .or. &
            suffix_char (1:6) == "_DGLAP") .and. (.not. (query_coupling_powers &
            (pdg_flv, cfg%alpha_power, cfg%alphas_power) .or. query_coupling_powers &

```

```

        (pdg_flg, cfg%alpha_power + 1, cfg%alphas_power - 1)) .or. &
        all (is_gluon (pdg_flg)))))) then
        deallocate (pdg_flg)
        node => node%next
        cycle
    end if
end if
select case (node%amplitude_type)
    case (BLHA_AMP_LOOP); buf = "Loop"
    case (BLHA_AMP_COLOR_C); buf = "ccTree"
    case (BLHA_AMP_SPIN_C)
        if (cfg%mode == BLHA_MODE_OPENLOOPS) then
            buf = "sctree_polvect"
        else
            buf = "scTree"
        end if
    case (BLHA_AMP_TREE); buf = "Tree"
    case (BLHA_AMP_LOOPINDUCED); buf = "LoopInduced"
end select
if (write_process) then
    write (u, '(A25, A)') "AmplitudeType " // pad, char (buf)
    buf = ""
    if (cfg%correction_type == BLHA_CT_EW .and. cfg%alphas_power > 0 .and. &
        (suffix_char (1:4) == "_SUB" .or. suffix_char (1:5) == "_LOOP" &
        .or. suffix_char (1:6) == "_DGLAP")) then
        if (query_coupling_powers (pdg_flg, cfg%alpha_power, cfg%alphas_power)) then
            write (u, '(A25,A)') "CorrectionType" // pad, "EW"
            select case (cfg%version)
                case (1)
                    if (cfg%alphas_power >= 0) write (u, '(A25,A)') &
                        "AlphasPower" // pad, int2char (cfg%alphas_power)
                    if (cfg%alpha_power >= 0) write (u, '(A25,A)') &
                        "AlphaPower " // pad, int2char (cfg%alpha_power)
                case (2)
                    if (cfg%alphas_power >= 0) write (u, '(A25,A)') &
                        "CouplingPower QCD " // pad, int2char (cfg%alphas_power)
                    if (cfg%alpha_power >= 0) write (u, '(A25,A)') &
                        "CouplingPower QED " // pad, int2char (cfg%alpha_power)
            end select
        else if (query_coupling_powers &
            (pdg_flg, cfg%alpha_power + 1, cfg%alphas_power - 1)) then
            write (u, '(A25,A)') "CorrectionType" // pad, "QCD"
            select case (cfg%version)
                case (1)
                    if (cfg%alphas_power >= 0) write (u, '(A25,A)') &
                        "AlphasPower" // pad, int2char (cfg%alphas_power - 1)
                    if (cfg%alpha_power >= 0) write (u, '(A25,A)') &
                        "AlphaPower " // pad, int2char (cfg%alpha_power + 1)
                case (2)
                    if (cfg%alphas_power >= 0) write (u, '(A25,A)') &
                        "CouplingPower QCD " // pad, int2char (cfg%alphas_power - 1)
                    if (cfg%alpha_power >= 0) write (u, '(A25,A)') &
                        "CouplingPower QED " // pad, int2char (cfg%alpha_power + 1)
            end select
        end if
    end if
end if
end select

```



```

        end if
    end if
    do i = 1, size (node%pdg_in)
        if (cfg%correction_type == BLHA_CT_EW .and. node%pdg_in(i)%pdg == PHOTON &
            .and. cfg%n_off_photons_is > 0) then
            if (cfg%ew_scheme == BLHA_EW_0) then
                call msg_fatal ("ew_scheme: 'alpha_0' or 'alpha_thompson' " &
                    // "in combination", [ var_str ("with off-shell external photons " &
                    // "is not consistent with FKS.")])
            end if
            write (pdg_char_extra, '(I5)') PHOTON_OFFSHELL
            buf = (buf // pdg_char_extra) // " "
        else
            call node%pdg_in(i)%write_pdg (pdg_char)
            if (node%pdg_in(i)%polarized) then
                call node%pdg_in(i)%write_helicity (hel_char)
                buf = (buf // pdg_char // hel_char) // " "
            else
                buf = (buf // pdg_char) // " "
            end if
        end if
    end do
    buf = buf // "-> "
    do i = 1, size (node%pdg_out)
        if (cfg%correction_type == BLHA_CT_EW .and. node%pdg_out(i)%pdg == PHOTON &
            .and. cfg%n_off_photons_fs > 0) then
            if (cfg%ew_scheme == BLHA_EW_0) then
                call msg_fatal ("ew_scheme: 'alpha_0' or 'alpha_thompson' " &
                    // "in combination with off-shell external photons " &
                    // "is not consistent with FKS. Try a different one.")
            end if
            write (pdg_char_extra, '(I5)') PHOTON_OFFSHELL
            buf = (buf // pdg_char_extra) // " "
        else
            call node%pdg_out(i)%write_pdg (pdg_char)
            buf = (buf // pdg_char) // " "
        end if
    end do
    write (u, "(A)") char (trim (buf))
    write (u, *)
end if
deallocate (pdg_flv)
node => node%next
end do
end subroutine blha_configuration_write

```

24.2.1 Unit tests

Test module, followed by the corresponding implementation module.

(blha_ut.f90)≡
⟨File header⟩

```

module blha_ut
  use unit_tests
  use blha_util

  <Standard module head>

  <BLHA: public tests>

  contains

  <BLHA: test driver>

end module blha_ut

```

<blha_util.f90>≡
 <File header>

```

module blha_util

  <Use strings>
  use format_utils, only: write_separator
  use variables, only: var_list_t
  use os_interface
  use models
  use blha_config

```

```

  <Standard module head>

  <BLHA: test declarations>

  contains

  <BLHA: test procedures>

  <BLHA: tests>

end module blha_util

```

API: driver for the unit tests below.

```

<BLHA: public tests>≡
  public :: blha_test

<BLHA: test driver>≡
  subroutine blha_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    call test(blha_1, "blha_1", "Test the creation of BLHA-OLP files", u, results)
    call test(blha_2, "blha_2", "Test the creation of BLHA-OLP files for "&
      &"multiple flavor structures", u, results)
    call test(blha_3, "blha_3", "Test helicity-information in OpenLoops OLP files", &
      u, results)
  end subroutine blha_test

```

(BLHA: test procedures)≡

```

subroutine setup_and_write_blha_configuration (u, single, polarized)
  integer, intent(in) :: u
  logical, intent(in), optional :: single
  logical, intent(in), optional :: polarized
  logical :: polrzd, singl
  type(blha_master_t) :: blha_master
  integer :: i
  integer :: n_in, n_out
  integer :: alpha_power, alphas_power
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(string_t) :: proc_id, method, correction_type
  type(os_data_t) :: os_data
  type(model_list_t) :: model_list
  type(var_list_t) :: var_list
  type(model_t), pointer :: model => null ()
  integer :: openloops_phs_tolerance

  polrzd = .false.; if (present (polarized)) polrzd = polarized
  singl = .true.; if (present (single)) singl = single

  if (singl) then
    write (u, "(A)") "* Process: e+ e- -> W+ W- b b~"
    n_in = 2; n_out = 4
    alpha_power = 4; alphas_power = 0
    allocate (flv_born (n_in + n_out, 1))
    allocate (flv_real (n_in + n_out + 1, 1))
    flv_born(1,1) = 11; flv_born(2,1) = -11
    flv_born(3,1) = 24; flv_born(4,1) = -24
    flv_born(5,1) = 5; flv_born(6,1) = -5
    flv_real(1:6,1) = flv_born(:,1)
    flv_real(7,1) = 21
  else
    write (u, "(A)") "* Process: e+ e- -> u:d:s U:D:S"
    n_in = 2; n_out = 2
    alpha_power = 2; alphas_power = 0
    allocate (flv_born (n_in + n_out, 3))
    allocate (flv_real (n_in + n_out + 1, 3))
    flv_born(1,:) = 11; flv_born(2,:) = -11
    flv_born(3,1) = 1; flv_born(4,1) = -1
    flv_born(3,2) = 2; flv_born(4,2) = -2
    flv_born(3,3) = 3; flv_born(4,3) = -3
    flv_real(1:4,:) = flv_born
    flv_real(5,:) = 21
  end if
  proc_id = var_str ("BLHA_Test")

  call syntax_model_file_init ()
  call os_data%init ()
  call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), os_data, model)

  write (u, "(A)") "* BLHA matrix elements assumed for all process components"
  write (u, "(A)") "* Mode: GoSam"

```

```

method = var_str ("gosam")
correction_type = var_str ("QCD")
call var_list%append_string (var_str ("$born_me_method"), method)
call var_list%append_string (var_str ("$real_tree_me_method"), method)
call var_list%append_string (var_str ("$loop_me_method"), method)
call var_list%append_string (var_str ("$correlation_me_method"), method)
call blha_master%set_ew_scheme (var_str ("GF"))
call blha_master%set_methods (.true., var_list)
call blha_master%allocate_config_files ()
call blha_master%set_correction_type (correction_type)
call blha_master%generate (proc_id, model, n_in, &
    alpha_power, alphas_power, flv_born, flv_real)

call test_output (u)

call blha_master%final ()
call var_list%final ()
write (u, "(A)") "* Switch to OpenLoops"
openloops_phs_tolerance = 7

method = var_str ("openloops")
correction_type = var_str ("QCD")
call var_list%append_string (var_str ("$born_me_method"), method)
call var_list%append_string (var_str ("$real_tree_me_method"), method)
call var_list%append_string (var_str ("$loop_me_method"), method)
call var_list%append_string (var_str ("$correlation_me_method"), method)
call blha_master%set_methods (.true., var_list)
call blha_master%allocate_config_files ()
call blha_master%set_correction_type (correction_type)
call blha_master%generate (proc_id, model, n_in, &
    alpha_power, alphas_power, flv_born, flv_real)

if (polrzd) then
    do i = 1, 4
        call blha_master%set_polarization (i)
    end do
end if
call blha_master%setup_additional_features &
    (openloops_phs_tolerance, .false., 0)

call test_output (u)

contains

subroutine test_output (u)
    integer, intent(in) :: u
    do i = 1, 4
        call write_separator (u)
        call write_component_type (i, u)
        call write_separator (u)
        call blha_configuration_write &
            (blha_master%blha_cfg(i), blha_master%suffix(i), u, no_version = .true.)
    end do

```

```

end subroutine test_output

subroutine write_component_type (i, u)
  integer, intent(in) :: i, u
  type(string_t) :: message, component_type
  message = var_str ("OLP-File content for ")
  select case (i)
  case (1)
    component_type = var_str ("loop")
  case (2)
    component_type = var_str ("subtraction")
  case (3)
    component_type = var_str ("real")
  case (4)
    component_type = var_str ("born")
  end select
  message = message // component_type // " matrix elements"
  write (u, "(A)") char (message)
end subroutine write_component_type

end subroutine setup_and_write_blha_configuration

<BLHA: test declarations>≡
public :: blha_1

<BLHA: tests>≡
subroutine blha_1 (u)
  integer, intent(in) :: u
  write (u, "(A)") "* Test output: blha_1"
  write (u, "(A)") "* Purpose: Test the creation of olp-files for single "&
    &"and unpolarized flavor structures"
  write (u, "(A)")
  call setup_and_write_blha_configuration (u, single = .true., polarized = .false.)
end subroutine blha_1

<BLHA: test declarations>+≡
public :: blha_2

<BLHA: tests>+≡
subroutine blha_2 (u)
  integer, intent(in) :: u
  write (u, "(A)") "* Test output: blha_2"
  write (u, "(A)") "* Purpose: Test the creation of olp-files for multiple "&
    &"and unpolarized flavor structures"
  write (u, "(A)")
  call setup_and_write_blha_configuration (u, single = .false., polarized = .false.)
end subroutine blha_2

<BLHA: test declarations>+≡
public :: blha_3

<BLHA: tests>+≡
subroutine blha_3 (u)
  integer, intent(in) :: u

```

```
write (u, "(A)") "* Test output: blha_3"
write (u, "(A)") "* Purpose: Test the creation of olp-files for single "&
      &"and polarized flavor structures"
write (u, "(A)")
      call setup_and_write_blha_configuration (u, single = .true., polarized = .true.)
end subroutine blha_3
```

Chapter 25

GoSam Interface

The code in this chapter makes amplitudes accessible to **WHIZARD** that are generated and computed by the GoSam package.

These are the modules:

loop_archive Provide some useful extra functionality.

prc_gosam The actual interface, following the **WHIZARD** conventions for matrix-element generator methods.

No internal dependencies

Figure 25.1: Module dependencies in `src/gosam`.

25.1 Gosam Interface

```
<prc_gosam.f90>≡  
  <File header>  
  
  module prc_gosam  
  
    use, intrinsic :: iso_c_binding !NODEP!  
    use, intrinsic :: iso_fortran_env  
  
    use kinds  
    <Use strings>  
    use io_units  
    use constants  
    use numeric_utils  
    use system_defs, only: TAB  
    use system_dependencies  
    use file_utils  
    use string_utils  
    use physics_defs  
    use diagnostics  
    use os_interface  
    use lorentz  
    use interactions  
    use pdg_arrays  
    use sm_qcd  
    use flavors  
    use model_data  
    use variables  
  
    use process_constants  
    use prclib_interfaces  
    use process_libraries  
    use prc_core_def  
    use prc_core  
  
    use blha_config  
    use blha_olp_interfaces  
  
    <Standard module head>  
  
    <prc gosam: constants>  
  
    <prc gosam: public>  
  
    <prc gosam: types>  
  
    <prc gosam: interfaces>  
  
    contains  
  
    <prc gosam: procedures>  
  
  end module prc_gosam
```

```

<prc gosam: types>≡
  type, extends (prc_blha_writer_t) :: gosam_writer_t
    type(string_t) :: gosam_dir
    type(string_t) :: golem_dir
    type(string_t) :: samurai_dir
    type(string_t) :: ninja_dir
    type(string_t) :: form_dir
    type(string_t) :: qgraf_dir
    type(string_t) :: filter_lo, filter_nlo
    type(string_t) :: symmetries
    integer :: form_threads
    integer :: form_workspace
    type(string_t) :: fc
  contains
  <prc gosam: gosam writer: TBP>
  end type gosam_writer_t

```

```

<prc gosam: public>≡
  public :: gosam_def_t

```

```

<prc gosam: types>+≡
  type, extends (blha_def_t) :: gosam_def_t
    logical :: execute_olp = .true.
  contains
  <prc gosam: gosam def: TBP>
  end type gosam_def_t

```

```

<prc gosam: types>+≡
  type, extends (blha_driver_t) :: gosam_driver_t
    type(string_t) :: gosam_dir
    type(string_t) :: olp_file
    type(string_t) :: olc_file
    type(string_t) :: olp_dir
    type(string_t) :: olp_lib
  contains
  <prc gosam: gosam driver: TBP>
  end type gosam_driver_t

```

```

<prc gosam: public>+≡
  public :: prc_gosam_t

```

```

<prc gosam: types>+≡
  type, extends (prc_blha_t) :: prc_gosam_t
    logical :: initialized = .false.
  contains
  <prc gosam: prc gosam: TBP>
  end type prc_gosam_t

```

```

<prc gosam: types>+≡
  type, extends (blha_state_t) :: gosam_state_t
  contains

```

```

    <prc gosam: gosam state: TBP>
    end type gosam_state_t

    <prc gosam: gosam def: TBP>≡
    procedure :: init => gosam_def_init

    <prc gosam: procedures>≡
    subroutine gosam_def_init (object, basename, model_name, &
        prt_in, prt_out, nlo_type, restrictions, var_list)
    class(gosam_def_t), intent(inout) :: object
    type(string_t), intent(in) :: basename
    type(string_t), intent(in) :: model_name
    type(string_t), dimension(:), intent(in) :: prt_in, prt_out
    integer, intent(in) :: nlo_type
    type(string_t), intent(in), optional :: restrictions
    type(var_list_t), intent(in) :: var_list
    object%basename = basename
    allocate (gosam_writer_t :: object%writer)
    select case (nlo_type)
    case (BORN)
        object%suffix = '_BORN'
    case (NLO_REAL)
        object%suffix = '_REAL'
    case (NLO_VIRTUAL)
        object%suffix = '_LOOP'
    case (NLO_SUBTRACTION)
        object%suffix = '_SUB'
    end select
    select type (writer => object%writer)
    type is (gosam_writer_t)
        call writer%init (model_name, prt_in, prt_out, restrictions)
        writer%filter_lo = var_list%get_sval (var_str ("gosam_filter_lo"))
        writer%filter_nlo = var_list%get_sval (var_str ("gosam_filter_nlo"))
        writer%symmetries = &
            var_list%get_sval (var_str ("gosam_symmetries"))
        writer%form_threads = &
            var_list%get_ival (var_str ("form_threads"))
        writer%form_workspace = &
            var_list%get_ival (var_str ("form_workspace"))
        writer%fc = &
            var_list%get_sval (var_str ("gosam_fc"))
    end select
    end subroutine gosam_def_init

    <prc gosam: gosam writer: TBP>≡
    procedure :: write_config => gosam_writer_write_config

    <prc gosam: procedures>+≡
    subroutine gosam_writer_write_config (gosam_writer)
    class(gosam_writer_t), intent(in) :: gosam_writer
    integer :: unit
    unit = free_unit ()
    open (unit, file = "golem.in", status = "replace", action = "write")
    call gosam_writer%generate_configuration_file (unit)

```

```

        close(unit)
    end subroutine gosam_writer_write_config

    <prc gosam: gosam def: TBP>+≡
        procedure, nopass :: type_string => gosam_def_type_string

    <prc gosam: procedures>+≡
        function gosam_def_type_string () result (string)
            type(string_t) :: string
            string = "gosam"
        end function gosam_def_type_string

    <prc gosam: gosam def: TBP>+≡
        procedure :: write => gosam_def_write

    <prc gosam: procedures>+≡
        subroutine gosam_def_write (object, unit)
            class(gosam_def_t), intent(in) :: object
            integer, intent(in) :: unit
            select type (writer => object%writer)
                type is (gosam_writer_t)
                    call writer%write (unit)
            end select
        end subroutine gosam_def_write

    <prc gosam: gosam def: TBP>+≡
        procedure :: read => gosam_def_read

    <prc gosam: procedures>+≡
        subroutine gosam_def_read (object, unit)
            class(gosam_def_t), intent(out) :: object
            integer, intent(in) :: unit
        end subroutine gosam_def_read

    <prc gosam: gosam def: TBP>+≡
        procedure :: allocate_driver => gosam_def_allocate_driver

    <prc gosam: procedures>+≡
        subroutine gosam_def_allocate_driver (object, driver, basename)
            class(gosam_def_t), intent(in) :: object
            class(prc_core_driver_t), intent(out), allocatable :: driver
            type(string_t), intent(in) :: basename
            if (.not. allocated (driver)) allocate (gosam_driver_t :: driver)
        end subroutine gosam_def_allocate_driver

    <prc gosam: gosam writer: TBP>+≡
        procedure, nopass :: type_name => gosam_writer_type_name

    <prc gosam: procedures>+≡
        function gosam_writer_type_name () result (string)
            type(string_t) :: string
            string = "gosam"
        end function gosam_writer_type_name

```

```

<prc gosam: gosam writer: TBP>+≡
    procedure :: init => gosam_writer_init

<prc gosam: procedures>+≡
    pure subroutine gosam_writer_init (writer, model_name, prt_in, prt_out, restrictions)
        class(gosam_writer_t), intent(inout) :: writer
        type(string_t), intent(in) :: model_name
        type(string_t), dimension(:), intent(in) :: prt_in, prt_out
        type(string_t), intent(in), optional :: restrictions
        writer%gosam_dir = GOSAM_DIR
        writer%golem_dir = GOLEM_DIR
        writer%samurai_dir = SAMURAI_DIR
        writer%ninja_dir = NINJA_DIR
        writer%form_dir = FORM_DIR
        writer%qgraf_dir = QGRAF_DIR
        call writer%base_init (model_name, prt_in, prt_out)
    end subroutine gosam_writer_init

<prc gosam: gosam driver: TBP>≡
    procedure, nopass :: type_name => gosam_driver_type_name

<prc gosam: procedures>+≡
    function gosam_driver_type_name () result (string)
        type(string_t) :: string
        string = "gosam"
    end function gosam_driver_type_name

<prc gosam: gosam driver: TBP>+≡
    procedure :: init_gosam => gosam_driver_init_gosam

<prc gosam: procedures>+≡
    subroutine gosam_driver_init_gosam (object, os_data, olp_file, &
                                         olc_file, olp_dir, olp_lib)
        class(gosam_driver_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        type(string_t), intent(in) :: olp_file, olc_file, olp_dir, olp_lib
        object%gosam_dir = GOSAM_DIR
        object%olp_file = olp_file
        object%contract_file = olc_file
        object%olp_dir = olp_dir
        object%olp_lib = olp_lib
    end subroutine gosam_driver_init_gosam

<prc gosam: gosam driver: TBP>+≡
    procedure :: init_dlaccess_to_library => gosam_driver_init_dlaccess_to_library

<prc gosam: procedures>+≡
    subroutine gosam_driver_init_dlaccess_to_library &
        (object, os_data, dlaccess, success)
        class(gosam_driver_t), intent(in) :: object
        type(os_data_t), intent(in) :: os_data
        type(dlaccess_t), intent(out) :: dlaccess
        logical, intent(out) :: success
        type(string_t) :: libname, msg_buffer

```

```

libname = object%olp_dir // './.libs/libgolem_olp.' // &
os_data%shrlib_ext
msg_buffer = "One-Loop-Provider: Using Gosam"
call msg_message (char(msg_buffer))
msg_buffer = "Loading library: " // libname
call msg_message (char(msg_buffer))
call dlaccess_init (dlaccess, var_str("."), libname, os_data)
success = .not. dlaccess_has_error (dlaccess)
end subroutine gosam_driver_init_dlaccess_to_library

```

(prc gosam: gosam writer: TBP)+≡

```

procedure :: generate_configuration_file => &
    gosam_writer_generate_configuration_file

```

(prc gosam: procedures)+≡

```

subroutine gosam_writer_generate_configuration_file &
    (object, unit)
    class(gosam_writer_t), intent(in) :: object
    integer, intent(in) :: unit
    type(string_t) :: fc_bin
    type(string_t) :: form_bin, qgraf_bin, haggies_bin
    type(string_t) :: fcflags_golem, ldflags_golem
    type(string_t) :: fcflags_samurai, ldflags_samurai
    type(string_t) :: fcflags_ninja, ldflags_ninja
    type(string_t) :: ldflags_avh_olo, ldflags_qcdloop
    fc_bin = DEFAULT_FC
    form_bin = object%form_dir // '/bin/tform'
    qgraf_bin = object%qgraf_dir // '/bin/qgraf'
    if (object%gosam_dir /= "") then
        haggies_bin = '/usr/bin/java -jar ' // object%gosam_dir // &
            '/share/golem/haggies/haggies.jar'
    else
        call msg_fatal ("generate_configuration_file: At least " // &
            "the GoSam Directory has to be specified!")
    end if
    if (object%golem_dir /= "") then
        fcflags_golem = "-I" // object%golem_dir // "/include/golem95"
        ldflags_golem = "-L" // object%golem_dir // "/lib -lgolem"
    end if
    if (object%samurai_dir /= "") then
        fcflags_samurai = "-I" // object%samurai_dir // "/include/samurai"
        ldflags_samurai = "-L" // object%samurai_dir // "/lib -lsamurai"
        ldflags_avh_olo = "-L" // object%samurai_dir // "/lib -lavh_olo"
        ldflags_qcdloop = "-L" // object%samurai_dir // "/lib -lqcdloop"
    end if
    if (object%ninja_dir /= "") then
        fcflags_ninja = "-I" // object%ninja_dir // "/include/ninja " &
            // "-I" // object%ninja_dir // "/include"
        ldflags_ninja = "-L" // object%ninja_dir // "/lib -lninja"
    end if
    write (unit, "(A)") "#+avh_olo.ldflags=" &
        // char (ldflags_avh_olo)
    write (unit, "(A)") "reduction_programs=golem95, samurai, ninja"
    write (unit, "(A)") "extensions=autotools"

```

```

write (unit, "(A)") "#+qcdloop.ldflags=" &
    // char (ldflags_qcdloop)
write (unit, "(A)") "#+zzz.extensions=qcdloop, avh_olo"
write (unit, "(A)") "#fc.bin=" // char (fc_bin)
write (unit, "(A)") "form.bin=" // char (form_bin)
write (unit, "(A)") "qgraf.bin=" // char (qgraf_bin)
write (unit, "(A)") "#golem95.fcflags=" // char (fcflags_golem)
write (unit, "(A)") "#golem95.ldflags=" // char (ldflags_golem)
write (unit, "(A)") "haggies.bin=" // char (haggies_bin)
write (unit, "(A)") "#samurai.fcflags=" // char (fcflags_samurai)
write (unit, "(A)") "#samurai.ldflags=" // char (ldflags_samurai)
write (unit, "(A)") "#ninja.fcflags=" // char (fcflags_ninja)
write (unit, "(A)") "#ninja.ldflags=" // char (ldflags_ninja)
!!! This might collide with the mass-setup in the order-file
!!! write (unit, "(A)") "zero=mU,mD,mC,mS,mB"
!!! This is covered by the BLHA2 interface
write (unit, "(A)") "PSP_check=False"
if (char (object%filter_lo) /= "") &
    write (unit, "(A)") "filter.lo=" // char (object%filter_lo)
if (char (object%filter_nlo) /= "") &
    write (unit, "(A)") "filter.nlo=" // char (object%filter_nlo)
if (char (object%symmetries) /= "") &
    write (unit, "(A)") "symmetries=" // char (object%symmetries)
write (unit, "(A,IO)") "form.threads=", object%form_threads
write (unit, "(A,IO)") "form.workspace=", object%form_workspace
if (char (object%fc) /= "") &
    write (unit, "(A)") "fc.bin=" // char (object%fc)
end subroutine gosam_writer_generate_configuration_file

```

We have to assure that all files necessary for the configure process in the GoSam code are ready. This is done with a stamp mechanism.

```

<prc gosam: gosam driver: TBP>+≡
    procedure :: write_makefile => gosam_driver_write_makefile

<prc gosam: procedures>+≡
    subroutine gosam_driver_write_makefile (object, unit, libname)
        class(gosam_driver_t), intent(in) :: object
        integer, intent(in) :: unit
        type(string_t), intent(in) :: libname
        write (unit, "(2A)") "OLP_FILE = ", char (object%olp_file)
        write (unit, "(2A)") "OLP_DIR = ", char (object%olp_dir)
        write (unit, "(A)")
        write (unit, "(A)") "all: $(OLP_DIR)/config.log"
        write (unit, "(2A)") TAB, "make -C $(OLP_DIR) install"
        write (unit, "(A)")
        write (unit, "(3A)") "$(OLP_DIR)/config.log: "
        write (unit, "(4A)") TAB, char (object%gosam_dir // "/bin/gosam.py "), &
            "--olp $(OLP_FILE) --destination=$(OLP_DIR)", &
            " -f -z"
        write (unit, "(3A)") TAB, "cd $(OLP_DIR); ./autogen.sh --prefix=", &
            "$(dir $(abspath $(lastword $(MAKEFILE_LIST))))"
    end subroutine gosam_driver_write_makefile

<prc gosam: gosam driver: TBP>+≡
    procedure :: set_alpha_s => gosam_driver_set_alpha_s

```

```

<prc gosam: procedures>+≡
  subroutine gosam_driver_set_alpha_s (driver, alpha_s)
    class(gosam_driver_t), intent(in) :: driver
    real(default), intent(in) :: alpha_s
    integer :: ierr
    call driver%blha_olp_set_parameter &
      (c_char_'alphaS'//c_null_char, &
       dble (alpha_s), 0._double, ierr)
  end subroutine gosam_driver_set_alpha_s

<prc gosam: gosam driver: TBP>+≡
  procedure :: set_alpha_qed => gosam_driver_set_alpha_qed

<prc gosam: procedures>+≡
  subroutine gosam_driver_set_alpha_qed (driver, alpha)
    class(gosam_driver_t), intent(inout) :: driver
    real(default), intent(in) :: alpha
    integer :: ierr
    call driver%blha_olp_set_parameter &
      (c_char_'alpha'//c_null_char, &
       dble (alpha), 0._double, ierr)
    if (ierr == 0) call ew_parameter_error_message (var_str ('alpha'))
  end subroutine gosam_driver_set_alpha_qed

<prc gosam: gosam driver: TBP>+≡
  procedure :: set_GF => gosam_driver_set_GF

<prc gosam: procedures>+≡
  subroutine gosam_driver_set_GF (driver, GF)
    class(gosam_driver_t), intent(inout) :: driver
    real(default), intent(in) :: GF
    integer :: ierr
    call driver%blha_olp_set_parameter &
      (c_char_'GF'//c_null_char, &
       dble(GF), 0._double, ierr)
    if (ierr == 0) call ew_parameter_error_message (var_str ('GF'))
  end subroutine gosam_driver_set_GF

<prc gosam: gosam driver: TBP>+≡
  procedure :: set_weinberg_angle => gosam_driver_set_weinberg_angle

<prc gosam: procedures>+≡
  subroutine gosam_driver_set_weinberg_angle (driver, sw2)
    class(gosam_driver_t), intent(inout) :: driver
    real(default), intent(in) :: sw2
    integer :: ierr
    call driver%blha_olp_set_parameter &
      (c_char_'sw2'//c_null_char, &
       dble(sw2), 0._double, ierr)
    if (ierr == 0) call ew_parameter_error_message (var_str ('sw2'))
  end subroutine gosam_driver_set_weinberg_angle

<prc gosam: gosam driver: TBP>+≡
  procedure :: print_alpha_s => gosam_driver_print_alpha_s

```



```

<prc gosam: procedures>+≡
  subroutine gosam_driver_print_alpha_s (object)
    class(gosam_driver_t), intent(in) :: object
    call object%blha_olp_print_parameter (c_char_'alphaS'//c_null_char)
  end subroutine gosam_driver_print_alpha_s

<prc gosam: prc gosam: TBP>≡
  procedure :: prepare_library => prc_gosam_prepare_library

<prc gosam: procedures>+≡
  subroutine prc_gosam_prepare_library (object, os_data, libname)
    class(prc_gosam_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: libname
    select type (writer => object%def%writer)
      type is (gosam_writer_t)
        call writer%write_config ()
      end select
    call object%create_olp_library (libname)
    call object%load_driver (os_data)
  end subroutine prc_gosam_prepare_library

<prc gosam: prc gosam: TBP>+≡
  procedure :: prepare_external_code => &
    prc_gosam_prepare_external_code

<prc gosam: procedures>+≡
  subroutine prc_gosam_prepare_external_code &
    (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
    class(prc_gosam_t), intent(inout) :: core
    integer, intent(in), dimension(:, :), allocatable :: flv_states
    type(var_list_t), intent(in) :: var_list
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: libname
    type(model_data_t), intent(in), target :: model
    integer, intent(in) :: i_core
    logical, intent(in) :: is_nlo
    core%sqme_tree_pos = 4
    call core%prepare_library (os_data, libname)
    call core%start ()
    call core%read_contract_file (flv_states)
    call core%set_particle_properties (model)
    call core%set_electroweak_parameters (model)
    call core%print_parameter_file (i_core)
  end subroutine prc_gosam_prepare_external_code

<prc gosam: prc gosam: TBP>+≡
  procedure :: write_makefile => prc_gosam_write_makefile

<prc gosam: procedures>+≡
  subroutine prc_gosam_write_makefile (object, unit, libname)
    class(prc_gosam_t), intent(in) :: object
    integer, intent(in) :: unit
    type(string_t), intent(in) :: libname

```

```

        select type (driver => object%driver)
        type is (gosam_driver_t)
            call driver%write_makefile (unit, libname)
        end select
    end subroutine prc_gosam_write_makefile

<prc gosam: prc gosam: TBP>+≡
    procedure :: execute_makefile => prc_gosam_execute_makefile

<prc gosam: procedures>+≡
    subroutine prc_gosam_execute_makefile (object, libname)
        class(prc_gosam_t), intent(in) :: object
        type(string_t), intent(in) :: libname
        select type (driver => object%driver)
        type is (gosam_driver_t)
            call os_system_call ("make -f " // &
                libname // "_gosam.makefile")
        end select
    end subroutine prc_gosam_execute_makefile

<prc gosam: prc gosam: TBP>+≡
    procedure :: create_olp_library => prc_gosam_create_olp_library

<prc gosam: procedures>+≡
    subroutine prc_gosam_create_olp_library (object, libname)
        class(prc_gosam_t), intent(inout) :: object
        type(string_t), intent(in) :: libname
        integer :: unit
        select type (driver => object%driver)
        type is (gosam_driver_t)
            unit = free_unit ()
            open (unit, file = char (libname // "_gosam.makefile"), &
                status = "replace", action= "write")
            call object%write_makefile (unit, libname)
            close (unit)
            call object%execute_makefile (libname)
        end select
    end subroutine prc_gosam_create_olp_library

<prc gosam: prc gosam: TBP>+≡
    procedure :: load_driver => prc_gosam_load_driver

<prc gosam: procedures>+≡
    subroutine prc_gosam_load_driver (object, os_data)
        class(prc_gosam_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        logical :: dl_success

        select type (driver => object%driver)
        type is (gosam_driver_t)
            call driver%load (os_data, dl_success)
            if (.not. dl_success) &
                call msg_fatal ("GoSam Libraries could not be loaded")
        end select
    end subroutine

```

```

end subroutine prc_gosam_load_driver

<prc gosam: prc gosam: TBP>+≡
  procedure :: start => prc_gosam_start

<prc gosam: procedures>+≡
  subroutine prc_gosam_start (object)
    class(prc_gosam_t), intent(inout) :: object
    integer :: ierr
    if (object%includes_polarization()) &
      call msg_fatal ('GoSam does not support polarized beams!')
    select type (driver => object%driver)
    type is (gosam_driver_t)
      call driver%blha_olp_start (string_f2c (driver%contract_file), ierr)
    end select
  end subroutine prc_gosam_start

<prc gosam: prc gosam: TBP>+≡
  procedure :: write => prc_gosam_write

<prc gosam: procedures>+≡
  subroutine prc_gosam_write (object, unit)
    class(prc_gosam_t), intent(in) :: object
    integer, intent(in), optional :: unit
    call msg_message (unit = unit, string = "GOSAM")
  end subroutine prc_gosam_write

<prc gosam: prc gosam: TBP>+≡
  procedure :: write_name => prc_gosam_write_name

<prc gosam: procedures>+≡
  subroutine prc_gosam_write_name (object, unit)
    class(prc_gosam_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Core: GoSam"
  end subroutine prc_gosam_write_name

<prc gosam: prc gosam: TBP>+≡
  procedure :: init_driver => prc_gosam_init_driver

<prc gosam: procedures>+≡
  subroutine prc_gosam_init_driver (object, os_data)
    class(prc_gosam_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
    type(string_t) :: olp_file, olc_file, olp_dir
    type(string_t) :: suffix

    select type (def => object%def)
    type is (gosam_def_t)
      suffix = def%suffix
      olp_file = def%basename // suffix // '.olp'
      olc_file = def%basename // suffix // '.olc'

```

```

        olp_dir = def%basename // suffix // '_olp_modules'
class default
    call msg_bug ("prc_gosam_init_driver: core_def should be of gosam-type")
end select

select type(driver => object%driver)
type is (gosam_driver_t)
    driver%nlo_suffix = suffix
    call driver%init_gosam (os_data, olp_file, olc_file, olp_dir, &
        var_str ("libgolem_olp"))
end select
end subroutine prc_gosam_init_driver

```

```

<prc gosam: prc gosam: TBP>+≡
    procedure :: set_initialized => prc_gosam_set_initialized

<prc gosam: procedures>+≡
    subroutine prc_gosam_set_initialized (prc_gosam)
        class(prc_gosam_t), intent(inout) :: prc_gosam
        prc_gosam%initialized = .true.
    end subroutine prc_gosam_set_initialized

```

The BLHA-interface conventions require the quantity $S_{ij} = \langle M_{i,+} | T_i T_j | M_{i,-} \rangle$ to be produced, where i is the position of the splitting gluon. However, $\tilde{M} = \langle M_{i,-} | M_{i,+} \rangle$ is needed. This can be obtained using color conservation, $\sum_j T_j |M\rangle = 0$, so that

$$\sum_{j \neq i} S_{ij} = -\langle M_{i,+} | T_i^2 | M_{i,-} \rangle = -C_A \langle M_{i,+} | M_{i,-} \rangle = -C_A \tilde{M}^*$$

According to BLHA conventions, the real part of S_{ij} is located at positions $2i + 2nj$ in the output array, where n denotes the number of external particles and the enumeration of particles starts at zero. The subsequent position, i.e. $2i + 2nj + 1$ is designated to the imaginary part of S_{ij} . Note that, since the first array position is 1, the implemented position association deviates from the above one in the addition of 1.

```

<prc gosam: procedures>+≡
<prc gosam: prc gosam: TBP>+≡
    procedure :: compute_sqme_spin_c => prc_gosam_compute_sqme_spin_c

<prc gosam: procedures>+≡
    subroutine prc_gosam_compute_sqme_spin_c (object, &
        i_flg, i_hel, em, p, ren_scale, me_sc, bad_point)
        class(prc_gosam_t), intent(inout) :: object
        integer, intent(in) :: i_flg, i_hel
        integer, intent(in) :: em
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), intent(in) :: ren_scale
        complex(default), intent(out) :: me_sc
        logical, intent(out) :: bad_point
        real(double), dimension(5*object%n_particles) :: mom
        real(double), dimension(OLP_RESULTS_LIMIT) :: r
        real(double) :: ren_scale_dble
    end subroutine

```

```

integer :: i, igm1, n
integer :: pos_real, pos_imag
real(double) :: acc_dble
real(default) :: acc, alpha_s
if (object%i_spin_c(i_flv, i_hel) >= 0) then
  me_sc = cmplx (zero ,zero, kind=default)
  mom = object%create_momentum_array (p)
  if (vanishes (ren_scale)) &
    call msg_fatal ("prc_gosam_compute_sqme_spin_c: ren_scale vanishes")
  alpha_s = object%qcd%alpha%get (ren_scale)
  ren_scale_dble = dble (ren_scale)
  select type (driver => object%driver)
  type is (gosam_driver_t)
    call driver%set_alpha_s (alpha_s)
    call driver%blha_olp_eval2 (object%i_spin_c(i_flv, i_hel), &
      mom, ren_scale_dble, r, acc_dble)
  end select
  igm1 = em - 1
  n = size(p)
  do i = 0, n - 1
    pos_real = 2 * igm1 + 2 * n * i + 1
    pos_imag = pos_real + 1
    me_sc = me_sc + cmplx (r(pos_real), r(pos_imag), default)
  end do

  me_sc = - conjg(me_sc) / CA

  acc = acc_dble
  if (acc > object%maximum_accuracy) bad_point = .true.
else
  r = 0._double
end if
end subroutine prc_gosam_compute_sqme_spin_c

```

<prc gosam: prc gosam: TBP>+≡

```

procedure :: allocate_workspace => prc_gosam_allocate_workspace

```

<prc gosam: procedures>+≡

```

subroutine prc_gosam_allocate_workspace (object, core_state)
  class(prc_gosam_t), intent(in) :: object
  class(prc_core_state_t), intent(inout), allocatable :: core_state
  allocate (gosam_state_t :: core_state)
end subroutine prc_gosam_allocate_workspace

```

<prc gosam: gosam state: TBP>≡

```

procedure :: write => gosam_state_write

```

<prc gosam: procedures>+≡

```

subroutine gosam_state_write (object, unit)
  class(gosam_state_t), intent(in) :: object
  integer, intent(in), optional :: unit
  call msg_warning (unit = unit, string = "gosam_state_write: What to write?")
end subroutine gosam_state_write

```

```

<prc gosam: prc gosam: TBP>+≡
  procedure :: set_particle_properties => prc_gosam_set_particle_properties

<prc gosam: procedures>+≡
  subroutine prc_gosam_set_particle_properties (object, model)
    class(prc_gosam_t), intent(inout) :: object
    class(model_data_t), intent(in), target :: model
    integer :: i, i_pdg
    type(flavor_t) :: flv
    real(default) :: mass, width
    integer :: ierr
    real(default) :: top_yukawa
    do i = 1, OLP_N_MASSIVE_PARTICLES
      i_pdg = OLP_MASSIVE_PARTICLES(i)
      if (i_pdg < 0) cycle
      call flv%init (i_pdg, model)
      mass = flv%get_mass (); width = flv%get_width ()
      select type (driver => object%driver)
      class is (blha_driver_t)
        if (i_pdg == 13) then
          call driver%set_mass_and_width (i_pdg, mass = mass)
        else
          call driver%set_mass_and_width (i_pdg, mass = mass, width = width)
        end if
        if (i_pdg == 5) call driver%blha_olp_set_parameter &
          ('yuk(5)'//c_null_char, dble(mass), 0._double, ierr)
        if (i_pdg == 6) then
          if (driver%external_top_yukawa > 0._default) then
            top_yukawa = driver%external_top_yukawa
          else
            top_yukawa = mass
          end if
          call driver%blha_olp_set_parameter &
            ('yuk(6)'//c_null_char, dble(top_yukawa), 0._double, ierr)
        end if
        if (driver%switch_off_muon_yukawas) then
          if (i_pdg == 13) call driver%blha_olp_set_parameter &
            ('yuk(13)' //c_null_char, 0._double, 0._double, ierr)
        end if
      end select
    end do
  end subroutine prc_gosam_set_particle_properties

```

Chapter 26

OpenLoops Interface

The interface to OpenLoops.

No internal dependencies

Figure 26.1: Module dependencies in `src/openloops`.


```

⟨prc_openloops.f90⟩≡
  ⟨File header⟩

  module prc_openloops

    use, intrinsic :: iso_c_binding !NODEP!

    use kinds
    use io_units
  ⟨Use strings⟩
    use string_utils, only: str
    use constants
    use numeric_utils
    use diagnostics
  ⟨Use debug⟩
    use system_dependencies
    use physics_defs
    use variables
    use os_interface
    use lorentz
    use interactions
    use sm_qcd
    use sm_physics, only: top_width_sm_lo, top_width_sm_qcd_nlo_jk
    use model_data

    use prclib_interfaces
    use prc_core_def
    use prc_core

    use blha_config
    use blha_olp_interfaces
  ⟨Use mpi f08⟩

  ⟨Standard module head⟩

  ⟨prc openloops: public⟩

  ⟨prc openloops: parameters⟩

  ⟨prc openloops: types⟩

  ⟨prc openloops: interfaces⟩

  contains

  ⟨prc openloops: procedures⟩

  end module prc_openloops

  ⟨prc openloops: parameters⟩≡
    real(default), parameter :: openloops_default_bmass = 0._default
    real(default), parameter :: openloops_default_topmass = 172._default
    real(default), parameter :: openloops_default_topwidth = 0._default
    real(default), parameter :: openloops_default_wmass = 80.399_default
    real(default), parameter :: openloops_default_wwidth = 0._default

```

```

real(default), parameter :: openloops_default_zmass = 91.1876_default
real(default), parameter :: openloops_default_zwidth = 0._default
real(default), parameter :: openloops_default_higgsmass = 125._default
real(default), parameter :: openloops_default_higgswidth = 0._default

integer :: N_EXTERNAL = 0

<prc openloops: interfaces>≡
  abstract interface
    subroutine ol_evaluate_scpowheg (id, pp, emitter, res, resmunu) bind(C)
      import
      integer(kind = c_int), value :: id, emitter
      real(kind = c_double), intent(in) :: pp(5 * N_EXTERNAL)
      real(kind = c_double), intent(out) :: res, resmunu(16)
    end subroutine ol_evaluate_scpowheg
  end interface

<prc openloops: interfaces>+≡
  abstract interface
    subroutine ol_getparameter_double (variable_name, value) bind(C)
      import
      character(kind = c_char, len = 1), intent(in) :: variable_name
      real(kind = c_double), intent(out) :: value
    end subroutine ol_getparameter_double
  end interface

<prc openloops: types>≡
  type, extends (prc_blha_writer_t) :: openloops_writer_t
  contains
  <prc openloops: openloops writer: TBP>
  end type openloops_writer_t

<prc openloops: public>≡
  public :: openloops_def_t

<prc openloops: types>+≡
  type, extends (blha_def_t) :: openloops_def_t
    integer :: verbosity
  contains
  <prc openloops: openloops def: TBP>
  end type openloops_def_t

<prc openloops: types>+≡
  type, extends (blha_driver_t) :: openloops_driver_t
    integer :: n_external = 0
    type(string_t) :: olp_file
    procedure(ol_evaluate_scpowheg), nopass, pointer :: &
      evaluate_spin_correlations_powheg => null ()
    procedure(ol_getparameter_double), nopass, pointer :: &
      get_parameter_double => null ()
  contains
  <prc openloops: openloops driver: TBP>

```

```

end type openloops_driver_t

<prc openloops: types>+≡
type :: openloops_threshold_data_t
  logical :: nlo = .true.
  real(default) :: alpha_ew
  real(default) :: sinthw
  real(default) :: m_b, m_W
  real(default) :: vtb
contains
<prc openloops: openloops threshold data: TBP>
end type openloops_threshold_data_t

<prc openloops: openloops threshold data: TBP>≡
procedure :: compute_top_width => &
  openloops_threshold_data_compute_top_width

<prc openloops: procedures>≡
function openloops_threshold_data_compute_top_width &
  (data, mtop, alpha_s) result (wtop)
  real(default) :: wtop
  class(openloops_threshold_data_t), intent(in) :: data
  real(default), intent(in) :: mtop, alpha_s
  if (data%nlo) then
    wtop = top_width_sm_qcd_nlo_jk (data%alpha_ew, data%sinthw, &
      data%vtb, mtop, data%m_W, data%m_b, alpha_s)
  else
    wtop = top_width_sm_lo (data%alpha_ew, data%sinthw, data%vtb, &
      mtop, data%m_W, data%m_b)
  end if
end function openloops_threshold_data_compute_top_width

<prc openloops: public>+≡
public :: openloops_state_t

<prc openloops: types>+≡
type, extends (blha_state_t) :: openloops_state_t
  type(openloops_threshold_data_t), allocatable :: threshold_data
contains
<prc openloops: openloops state: TBP>
end type openloops_state_t

<prc openloops: openloops state: TBP>≡
procedure :: init_threshold => openloops_state_init_threshold

<prc openloops: procedures>+≡
subroutine openloops_state_init_threshold (object, model)
  class(openloops_state_t), intent(inout) :: object
  type(model_data_t), intent(in) :: model
  if (model%get_name () == "SM_tt_threshold") then
    allocate (object%threshold_data)
    associate (data => object%threshold_data)
      data%nlo = btest (int (model%get_real (var_str ('offshell_strategy'))), 0)
    end associate
  end if
end subroutine openloops_state_init_threshold

```

```

        data%alpha_ew = one / model%get_real (var_str ('alpha_em_i'))
        data%sinthw = model%get_real (var_str ('sw'))
        data%m_b = model%get_real (var_str ('mb'))
        data%m_W = model%get_real (var_str ('mW'))
        data%vtb = model%get_real (var_str ('Vtb'))
    end associate
end if
end subroutine openloops_state_init_threshold

<prc openloops: public>+≡
    public :: prc_openloops_t

<prc openloops: types>+≡
    type, extends (prc_blha_t) :: prc_openloops_t
    contains
    <prc openloops: prc openloops: TBP>
    end type prc_openloops_t

<prc openloops: openloops writer: TBP>≡
    procedure, nopass :: type_name => openloops_writer_type_name

<prc openloops: procedures>+≡
    function openloops_writer_type_name () result (string)
        type(string_t) :: string
        string = "openloops"
    end function openloops_writer_type_name

<prc openloops: openloops def: TBP>≡
    procedure :: init => openloops_def_init

<prc openloops: procedures>+≡
    subroutine openloops_def_init (object, basename, model_name, &
        prt_in, prt_out, nlo_type, restrictions, var_list)
        class(openloops_def_t), intent(inout) :: object
        type(string_t), intent(in) :: basename, model_name
        type(string_t), dimension(:), intent(in) :: prt_in, prt_out
        integer, intent(in) :: nlo_type
        type(string_t), intent(in), optional :: restrictions
        type(var_list_t), intent(in) :: var_list
    <prc openloops: openloops def init: variables>
        object%basename = basename
        allocate (openloops_writer_t :: object%writer)
        select case (nlo_type)
        case (BORN)
            object%suffix = '_BORN'
        case (NLO_REAL)
            object%suffix = '_REAL'
        case (NLO_VIRTUAL)
            object%suffix = '_LOOP'
        case (NLO_SUBTRACTION, NLO_MISMATCH)
            object%suffix = '_SUB'
        case (NLO_DGLAP)
            object%suffix = '_DGLAP'
        end select

```

```

<prc openloops: openloops def init: suffix>
  select type (writer => object%writer)
  class is (prc_blha_writer_t)
    call writer%init (model_name, prt_in, prt_out, restrictions)
  end select
  object%verbosity = var_list%get_ival (var_str ("openloops_verbosity"))
end subroutine openloops_def_init

```

Add additional suffix for each rank of the communicator, such that the filenames do not clash.

```

<MPI: prc openloops: openloops def init: variables>≡
  integer :: n_size, rank

```

```

<MPI: prc openloops: openloops def init: suffix>≡
  call MPI_comm_rank (MPI_COMM_WORLD, rank)
  call MPI_Comm_size (MPI_COMM_WORLD, n_size)
  if (n_size > 1) then
    object%suffix = object%suffix // var_str ("-") // str (rank)
  end if

```

```

<prc openloops: openloops def: TBP>+≡
  procedure, nopass :: type_string => openloops_def_type_string

```

```

<prc openloops: procedures>+≡
  function openloops_def_type_string () result (string)
    type(string_t) :: string
    string = "openloops"
  end function openloops_def_type_string

```

```

<prc openloops: openloops def: TBP>+≡
  procedure :: write => openloops_def_write

```

```

<prc openloops: procedures>+≡
  subroutine openloops_def_write (object, unit)
    class(openloops_def_t), intent(in) :: object
    integer, intent(in) :: unit
    select type (writer => object%writer)
    type is (openloops_writer_t)
      call writer%write (unit)
    end select
  end subroutine openloops_def_write

```

```

<prc openloops: openloops driver: TBP>≡
  procedure :: init_dlaccess_to_library => openloops_driver_init_dlaccess_to_library

```

```

<prc openloops: procedures>+≡
  subroutine openloops_driver_init_dlaccess_to_library &
    (object, os_data, dlaccess, success)
    class(openloops_driver_t), intent(in) :: object
    type(os_data_t), intent(in) :: os_data
    type(dlaccess_t), intent(out) :: dlaccess
    logical, intent(out) :: success
    type(string_t) :: ol_library, msg_buffer
    ol_library = OPENLOOPS_DIR // '/lib/libopenloops.' // &

```

```

        os_data%shrlib_ext
msg_buffer = "One-Loop-Provider: Using OpenLoops"
call msg_message (char(msg_buffer))
msg_buffer = "Loading library: " // ol_library
call msg_message (char(msg_buffer))
if (os_file_exist (ol_library)) then
    call dlaccess_init (dlaccess, var_str (""), ol_library, os_data)
else
    call msg_fatal ("Link OpenLoops: library not found")
end if
success = .not. dlaccess_has_error (dlaccess)
end subroutine openloops_driver_init_dlaccess_to_library

```

```

<prc openloops: openloops driver: TBP>+≡
    procedure :: set_alpha_s => openloops_driver_set_alpha_s
<prc openloops: procedures>+≡
    subroutine openloops_driver_set_alpha_s (driver, alpha_s)
        class(openloops_driver_t), intent(in) :: driver
        real(default), intent(in) :: alpha_s
        integer :: ierr
        if (associated (driver%blha_olp_set_parameter)) then
            call driver%blha_olp_set_parameter &
                (c_char_'alphas'//c_null_char, &
                 dble (alpha_s), 0._double, ierr)
        else
            call msg_fatal ("blha_olp_set_parameter not associated!")
        end if
        if (ierr == 0) call parameter_error_message (var_str ('alphas'), &
            var_str ('openloops_driver_set_alpha_s'))
    end subroutine openloops_driver_set_alpha_s

```

```

<prc openloops: openloops driver: TBP>+≡
    procedure :: set_alpha_qed => openloops_driver_set_alpha_qed
<prc openloops: procedures>+≡
    subroutine openloops_driver_set_alpha_qed (driver, alpha)
        class(openloops_driver_t), intent(inout) :: driver
        real(default), intent(in) :: alpha
        integer :: ierr
        call driver%blha_olp_set_parameter &
            (c_char_'alpha_qed'//c_null_char, &
             dble (alpha), 0._double, ierr)
        if (ierr == 0) call ew_parameter_error_message (var_str ('alpha_qed'))
    end subroutine openloops_driver_set_alpha_qed

```

```

<prc openloops: openloops driver: TBP>+≡
    procedure :: set_GF => openloops_driver_set_GF
<prc openloops: procedures>+≡
    subroutine openloops_driver_set_GF (driver, GF)
        class(openloops_driver_t), intent(inout) :: driver
        real(default), intent(in) :: GF
        integer :: ierr

```

```

        call driver%blha_olp_set_parameter &
            (c_char_'Gmu'//c_null_char, &
             dble(GF), 0._double, ierr)
        if (ierr == 0) call ew_parameter_error_message (var_str ('Gmu'))
    end subroutine openloops_driver_set_GF

<prc openloops: openloops driver: TBP>+≡
    procedure :: set_weinberg_angle => openloops_driver_set_weinberg_angle

<prc openloops: procedures>+≡
    subroutine openloops_driver_set_weinberg_angle (driver, sw2)
        class(openloops_driver_t), intent(inout) :: driver
        real(default), intent(in) :: sw2
        integer :: ierr
        call driver%blha_olp_set_parameter &
            (c_char_'sw2'//c_null_char, &
             dble(sw2), 0._double, ierr)
        if (ierr == 0) call ew_parameter_error_message (var_str ('sw2'))
    end subroutine openloops_driver_set_weinberg_angle

<prc openloops: openloops driver: TBP>+≡
    procedure :: print_alpha_s => openloops_driver_print_alpha_s

<prc openloops: procedures>+≡
    subroutine openloops_driver_print_alpha_s (object)
        class(openloops_driver_t), intent(in) :: object
        call object%blha_olp_print_parameter (c_char_'alphas'//c_null_char)
    end subroutine openloops_driver_print_alpha_s

<prc openloops: openloops driver: TBP>+≡
    procedure, nopass :: type_name => openloops_driver_type_name

<prc openloops: procedures>+≡
    function openloops_driver_type_name () result (type)
        type(string_t) :: type
        type = "OpenLoops"
    end function openloops_driver_type_name

<prc openloops: openloops driver: TBP>+≡
    procedure :: load_procedures => openloops_driver_load_procedures

<prc openloops: procedures>+≡
    subroutine openloops_driver_load_procedures (object, os_data, success)
        class(openloops_driver_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        logical, intent(out) :: success
        type(dlaccess_t) :: dlaccess
        type(c_funptr) :: c_fptr
        logical :: init_success

        call object%init_dlaccess_to_library (os_data, dlaccess, init_success)

        c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("ol_evaluate_scpowheg"))
        call c_f_procpointer (c_fptr, object%evaluate_spin_correlations_powheg)

```

```

call check_for_error (var_str ("ol_evaluate_scpowheg"))
c_fptr = dlaccess_get_c_funptr (dlaccess, var_str ("ol_getparameter_double"))
call c_f_procpointer (c_fptr, object%get_parameter_double)
call check_for_error (var_str ("ol_getparameter_double"))
success = .true.

contains
  subroutine check_for_error (function_name)
    type(string_t), intent(in) :: function_name
    if (dlaccess_has_error (dlaccess)) &
      call msg_fatal (char ("Loading of " // function_name // " failed!"))
  end subroutine check_for_error
end subroutine openloops_driver_load_procedures

<prc openloops: openloops def: TBP>+≡
  procedure :: read => openloops_def_read

<prc openloops: procedures>+≡
  subroutine openloops_def_read (object, unit)
    class(openloops_def_t), intent(out) :: object
    integer, intent(in) :: unit
  end subroutine openloops_def_read

<prc openloops: openloops def: TBP>+≡
  procedure :: allocate_driver => openloops_def_allocate_driver

<prc openloops: procedures>+≡
  subroutine openloops_def_allocate_driver (object, driver, basename)
    class(openloops_def_t), intent(in) :: object
    class(prc_core_driver_t), intent(out), allocatable :: driver
    type(string_t), intent(in) :: basename
    if (.not. allocated (driver)) allocate (openloops_driver_t :: driver)
  end subroutine openloops_def_allocate_driver

<prc openloops: openloops state: TBP>+≡
  procedure :: write => openloops_state_write

<prc openloops: procedures>+≡
  subroutine openloops_state_write (object, unit)
    class(openloops_state_t), intent(in) :: object
    integer, intent(in), optional :: unit
  end subroutine openloops_state_write

<prc openloops: prc openloops: TBP>≡
  procedure :: allocate_workspace => prc_openloops_allocate_workspace

<prc openloops: procedures>+≡
  subroutine prc_openloops_allocate_workspace (object, core_state)
    class(prc_openloops_t), intent(in) :: object
    class(prc_core_state_t), intent(inout), allocatable :: core_state
    allocate (openloops_state_t :: core_state)
  end subroutine prc_openloops_allocate_workspace

```



```

<prc openloops: prc openloops: TBP>+≡
    procedure :: init_driver => prc_openloops_init_driver

<prc openloops: procedures>+≡
    subroutine prc_openloops_init_driver (object, os_data)
        class(prc_openloops_t), intent(inout) :: object
        type(os_data_t), intent(in) :: os_data
        type(string_t) :: olp_file, olc_file
        type(string_t) :: suffix

        select type (def => object%def)
        type is (openloops_def_t)
            suffix = def%suffix
            olp_file = def%basename // suffix // '.olp'
            olc_file = def%basename // suffix // '.olc'
        class default
            call msg_bug ("prc_openloops_init_driver: core_def should be openloops-type")
        end select

        select type (driver => object%driver)
        type is (openloops_driver_t)
            driver%olp_file = olp_file
            driver%contract_file = olc_file
            driver%nlo_suffix = suffix
        end select
    end subroutine prc_openloops_init_driver

<prc openloops: prc openloops: TBP>+≡
    procedure :: write => prc_openloops_write

<prc openloops: procedures>+≡
    subroutine prc_openloops_write (object, unit)
        class(prc_openloops_t), intent(in) :: object
        integer, intent(in), optional :: unit
        call msg_message (unit = unit, string = "OpenLoops")
    end subroutine prc_openloops_write

<prc openloops: prc openloops: TBP>+≡
    procedure :: write_name => prc_openloops_write_name

<prc openloops: procedures>+≡
    subroutine prc_openloops_write_name (object, unit)
        class(prc_openloops_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Core: OpenLoops"
    end subroutine prc_openloops_write_name

<prc openloops: prc openloops: TBP>+≡
    procedure :: prepare_library => prc_openloops_prepare_library

```

```

<prc openloops: procedures>+≡
  subroutine prc_openloops_prepare_library (object, os_data, model)
    class(prc_openloops_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
    type(model_data_t), intent(in), target :: model
    call object%load_driver (os_data)
    call object%reset_parameters ()
    call object%set_particle_properties (model)
    select type(def => object%def)
      type is (openloops_def_t)
        call object%set_verbosity (def%verbosity)
    end select
  end subroutine prc_openloops_prepare_library

<prc openloops: prc openloops: TBP>+≡
  procedure :: load_driver => prc_openloops_load_driver

<prc openloops: procedures>+≡
  subroutine prc_openloops_load_driver (object, os_data)
    class(prc_openloops_t), intent(inout) :: object
    type(os_data_t), intent(in) :: os_data
    logical :: success
    select type (driver => object%driver)
      type is (openloops_driver_t)
        call driver%load (os_data, success)
        call driver%load_procedures (os_data, success)
    end select
  end subroutine prc_openloops_load_driver

<prc openloops: prc openloops: TBP>+≡
  procedure :: start => prc_openloops_start

<prc openloops: procedures>+≡
  subroutine prc_openloops_start (object)
    class(prc_openloops_t), intent(inout) :: object
    integer :: ierr
    select type (driver => object%driver)
      type is (openloops_driver_t)
        call driver%blha_olp_start (char (driver%olp_file)//c_null_char, ierr)
    end select
  end subroutine prc_openloops_start

<prc openloops: prc openloops: TBP>+≡
  procedure :: set_n_external => prc_openloops_set_n_external

<prc openloops: procedures>+≡
  subroutine prc_openloops_set_n_external (object, n)
    class(prc_openloops_t), intent(inout) :: object
    integer, intent(in) :: n
    N_EXTERNAL = n
  end subroutine prc_openloops_set_n_external

<prc openloops: prc openloops: TBP>+≡
  procedure :: reset_parameters => prc_openloops_reset_parameters

```

```

<prc openloops: procedures>+≡
  subroutine prc_openloops_reset_parameters (object)
    class(prc_openloops_t), intent(inout) :: object
    integer :: ierr
    select type (driver => object%driver)
    type is (openloops_driver_t)
      call driver%blha_olp_set_parameter ('mass(5)'/c_null_char, &
        dble(openloops_default_bmass), 0._double, ierr)
      call driver%blha_olp_set_parameter ('mass(6)'/c_null_char, &
        dble(openloops_default_topmass), 0._double, ierr)
      call driver%blha_olp_set_parameter ('width(6)'/c_null_char, &
        dble(openloops_default_topwidth), 0._double, ierr)
      call driver%blha_olp_set_parameter ('mass(23)'/c_null_char, &
        dble(openloops_default_zmass), 0._double, ierr)
      call driver%blha_olp_set_parameter ('width(23)'/c_null_char, &
        dble(openloops_default_zwidth), 0._double, ierr)
      call driver%blha_olp_set_parameter ('mass(24)'/c_null_char, &
        dble(openloops_default_wmass), 0._double, ierr)
      call driver%blha_olp_set_parameter ('width(24)'/c_null_char, &
        dble(openloops_default_wwidth), 0._double, ierr)
      call driver%blha_olp_set_parameter ('mass(25)'/c_null_char, &
        dble(openloops_default_higsmass), 0._double, ierr)
      call driver%blha_olp_set_parameter ('width(25)'/c_null_char, &
        dble(openloops_default_higgswidth), 0._double, ierr)
    end select
  end subroutine prc_openloops_reset_parameters

```

Set the verbosity level for openloops. The different levels are as follows:

- 0 minimal output (startup message et.al.)
- 1 show which libraries are loaded
- 2 show debug information of the library loader, but not during run time
- 3 show debug information during run time
- 4 output for each call of `set_parameters`.

```

<prc openloops: prc openloops: TBP>+≡
  procedure :: set_verbosity => prc_openloops_set_verbosity

<prc openloops: procedures>+≡
  subroutine prc_openloops_set_verbosity (object, verbose)
    class(prc_openloops_t), intent(inout) :: object
    integer, intent(in) :: verbose
    integer :: ierr
    select type (driver => object%driver)
    type is (openloops_driver_t)
      call driver%blha_olp_set_parameter ('verbose'/c_null_char, &
        dble(verbose), 0._double, ierr)
    end select
  end subroutine prc_openloops_set_verbosity

```

```

<prc openloops: prc openloops: TBP>+=
  procedure :: prepare_external_code => &
    prc_openloops_prepare_external_code

<prc openloops: procedures>+=
  subroutine prc_openloops_prepare_external_code &
    (core, flv_states, var_list, os_data, libname, model, i_core, is_nlo)
    class(prc_openloops_t), intent(inout) :: core
    integer, intent(in), dimension(:,:), allocatable :: flv_states
    type(var_list_t), intent(in) :: var_list
    type(os_data_t), intent(in) :: os_data
    type(string_t), intent(in) :: libname
    type(model_data_t), intent(in), target :: model
    integer, intent(in) :: i_core
    logical, intent(in) :: is_nlo
    integer :: ierr
    core%sqme_tree_pos = 1
    call core%set_n_external (core%data%get_n_tot ())
    call core%prepare_library (os_data, model)
    call core%start ()
    call core%set_electroweak_parameters (model)
    select type (driver => core%driver)
    type is (openloops_driver_t)
      !!! We have to set the external vector boson wavefunction to the MadGraph convention
      !!! in order to be consistent with our calculation of the spin correlated contributions.
      call driver%blha_olp_set_parameter ('wf_v_select'//c_null_char, &
        3._double, 0._double, ierr)
      if (ierr == 0) call parameter_error_message (var_str ('wf_v_select'), &
        var_str ('prc_openloops_prepare_external_code'))
    end select
    call core%read_contract_file (flv_states)
    call core%print_parameter_file (i_core)
  end subroutine prc_openloops_prepare_external_code

```

Computes a spin-correlated matrix element from an interface to an external one-loop provider. The output of `blha_olp_eval2` is an array of `dimension(16)`. The current interface does not give out an accuracy, so that `bad_point` is always `.false..` OpenLoops includes a factor of $1 / n_{\text{hel}}$ in the amplitudes, which we have to undo if polarized matrix elements are requested.

```

<prc openloops: prc openloops: TBP>+=
  procedure :: compute_sqme_spin_c => prc_openloops_compute_sqme_spin_c

<prc openloops: procedures>+=
  subroutine prc_openloops_compute_sqme_spin_c (object, &
    i_flv, i_hel, em, p, ren_scale, sqme_spin_c, bad_point)
    class(prc_openloops_t), intent(inout) :: object
    integer, intent(in) :: i_flv, i_hel
    integer, intent(in) :: em
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale
    real(default), intent(out), dimension(6) :: sqme_spin_c
    logical, intent(out) :: bad_point
    real(default), dimension(16) :: sqme_spin_c_tmp
    real(double), dimension(5*N_EXTERNAL) :: mom

```

```

real(double) :: res
real(double), dimension(16) :: res_munu
real(default) :: alpha_s
if (object%i_spin_c(i_flv, i_hel) >= 0) then
  mom = object%create_momentum_array (p)
  if (vanishes (ren_scale)) call msg_fatal &
    ("prc_openloops_compute_sqme_spin_c: ren_scale vanishes")
  alpha_s = object%qcd%alpha%get (ren_scale)
  select type (driver => object%driver)
  type is (openloops_driver_t)
    call driver%set_alpha_s (alpha_s)
    call driver%evaluate_spin_correlations_powheg &
      (object%i_spin_c(i_flv, i_hel), mom, em, res, res_munu)
  end select
  sqme_spin_c_tmp = res_munu
  bad_point = .false.
  if (object%includes_polarization ()) &
    sqme_spin_c_tmp = object%n_hel * sqme_spin_c_tmp
  if (debug_on) then
    if (sum(sqme_spin_c_tmp) == 0) then
      call msg_debug(D_SUBTRACTION,'Spin-correlated matrix elements provided by OpenLoops a
    end if
  end if
else
  sqme_spin_c_tmp = zero
end if
!!! Using symmetry of the 4x4 matrix of spin correlated squared Born MEs and
!!! the fact that we multiply only with vectors with E=0. We thus store the
!!! upper triangle of the lower 3x3 matrix as columns in a 1-dim array
sqme_spin_c(1:2) = sqme_spin_c_tmp(6:7)
sqme_spin_c(3) = sqme_spin_c_tmp(11)
sqme_spin_c(4) = sqme_spin_c_tmp(8)
sqme_spin_c(5) = sqme_spin_c_tmp(12)
sqme_spin_c(6) = sqme_spin_c_tmp(16)
end subroutine prc_openloops_compute_sqme_spin_c

```

<prc openloops: prc openloops: TBP>+≡

```

procedure :: get_alpha_qed => prc_openloops_get_alpha_qed

```

<prc openloops: procedures>+≡

```

function prc_openloops_get_alpha_qed (object) result (alpha_qed)
  class(prc_openloops_t), intent(in) :: object
  real(double) :: value
  real(default) :: alpha_qed
  select type (driver => object%driver)
  type is (openloops_driver_t)
    call driver%get_parameter_double ('alpha_qed'//c_null_char, value)
    alpha_qed = value
    return
  end select
  call msg_fatal ("prc_openloops_get_alpha_qed: called by wrong driver, only supported for OpenL
end function prc_openloops_get_alpha_qed

```

Chapter 27

FKS Subtraction Scheme

The code in this chapter implements the FKS subtraction scheme for use with WHIZARD.

These are the modules:

fks_regions Given a process definition, identify singular regions in the associated phase space.

virtual Handle the virtual correction matrix element.

real_subtraction Handle the real-subtraction matrix element.

nlo_data Manage the subtraction objects.

This chapter deals with next-to-leading order contributions to cross sections. Basically, there are three major issues to be addressed: The creation of the $N + 1$ -particle flavor structure, the construction of the $N + 1$ -particle phase space and the actual calculation of the real- and virtual-subtracted matrix elements. The first is dealt with using the `auto_components` class, and it will be shown that the second and third issue are connected in FKS subtraction.

27.1 Brief outline of FKS subtraction

In the current state, this discussion is only concerned with lepton collisions. For hadron collisions, renormalization of parton distributions has to be taken into account. Further, for QCD corrections, initial-state radiation is necessarily present.

The aim is to calculate the next-to-leading order cross section according to

$$d\sigma_{\text{NLO}} = \mathcal{B} + \mathcal{V} + \mathcal{R}d\Phi_{\text{rad}}.$$

Analytically, the divergences, in terms of poles in the complex quantity $\varepsilon = 2 - d/2$, cancel. However, this is in general only valid in an arbitrary, complex number of dimensions. This is, roughly, the content of the KLN-theorem. WHIZARD, as any other numerical program, is confined to four dimensions. We will assume that the KLN-theorem is valid and that there exist subtraction terms \mathcal{C} such that

$$d\sigma_{\text{NLO}} = \mathcal{B} + \underbrace{\mathcal{V} + \mathcal{C}}_{\text{finite}} + \underbrace{\mathcal{R} - \mathcal{C}}_{\text{finite}},$$

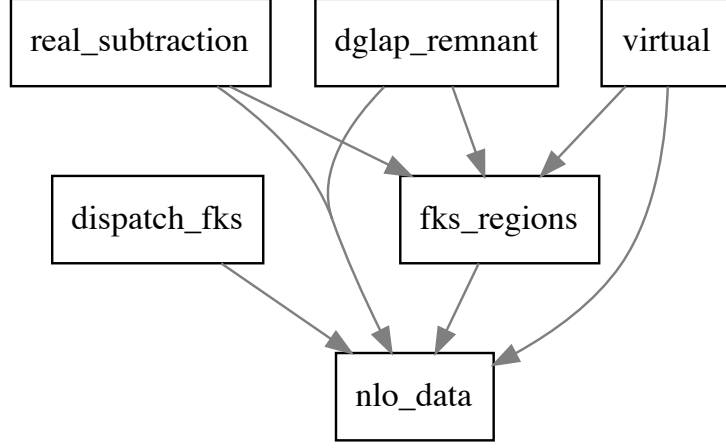


Figure 27.1: Module dependencies in `src/fks`.

i.e. the subtraction terms correspond to the divergent limits of the real and virtual matrix element.

Because \mathcal{C} subtracts the divergences of \mathcal{R} as well as those of \mathcal{V} , it suffices to consider one of them, so we focus on \mathcal{R} . For this purpose, \mathcal{R} is rewritten as

$$\mathcal{R} = \frac{1}{\xi^2} \frac{1}{1-y} (\xi^2(1-y)\mathcal{R}) = \frac{1}{\xi^2} \frac{1}{1-y} \tilde{\mathcal{R}},$$

with $\xi = (2k_{\text{rad}}^0)/\sqrt{s}$ and $y = \cos\theta$, where k_{rad}^0 denotes the energy of the radiated parton and θ is the angle between emitter and radiated parton. $\tilde{\mathcal{R}}$ is finite, therefore the whole singularity structure is contained in the prefactor $\xi^{-2}(1-y)^{-1}$. Combined with the d -dimensional phase space element,

$$\frac{d^{d-1}k}{2k^0(2\pi)^{d-1}} = \frac{s^{1-\varepsilon}}{(4\pi)^{d-1}} \xi^{1-2\varepsilon} (1-y^2)^{-\varepsilon} d\xi dy d\Omega^{d-2},$$

this yields

$$d\Phi_{\text{rad}}\mathcal{R} = dy(1-y)^{-1-\varepsilon} d\xi \xi^{-1-2\varepsilon} \tilde{\mathcal{R}}.$$

This can further be rewritten in terms of plus-distributions,

$$\begin{aligned} \xi^{-1-2\varepsilon} &= -\frac{1}{2\varepsilon} \delta(\xi) + \left(\frac{1}{\xi}\right)_+ - 2\varepsilon \left(\frac{\log \xi}{\xi}\right)_+ + \mathcal{O}(\varepsilon^2), \\ (1-y)^{-1-\varepsilon} &= -\frac{2^{-\varepsilon}}{\varepsilon} \delta(1-y) + \left(\frac{1}{1-y}\right)_+ - \varepsilon \left(\frac{1}{1-y}\right)_+ \log(1-y) + \mathcal{O}(\varepsilon^2), \end{aligned}$$

(imagine that all this is written inside of integrals, which are spared for ease of

notation) such that

$$d\Phi_{\text{rad}}\mathcal{R} = -\frac{1}{2\varepsilon}dy(1-y)^{-1-\varepsilon}\tilde{R}(0,y) - d\xi \left[\frac{2^{-\varepsilon}}{\varepsilon} \left(\frac{1}{\xi} \right)_+ - 2 \left(\frac{\log \xi}{\xi} \right)_+ \right] \tilde{R}(\xi,1) \\ + dyd\xi \left(\frac{1}{\xi} \right)_+ \left(\frac{1}{1-y} \right)_+ \tilde{R}(\xi,y) + \mathcal{O}(\varepsilon).$$

The summand in the second line is of order $\mathcal{O}(1)$ and is the only one to reproduce $\mathcal{R}(\xi,y)$. It thus constitutes the sum of the real matrix element and the corresponding counterterms. The first summand consequently consists of the subtraction terms to the virtual matrix elements. Above formula thus allows to calculate all quantities to render the matrix elements finite.

alr	flst_alr	emitter	ftuple_list
1	[-11,11,2,-2,21,21]	3	(3,5), (3,6), (4,5), (4,6), (5,6)
2	[-11,11,2,-2,21,21]	4	(3,5), (3,6), (4,5), (4,6), (5,6)
3	[-11,11,2,-2,21,21]	5	(3,5), (3,6), (4,5), (4,6), (5,6)
4	[-11,11,2,-2,2,-2]	5	(3,4), (3,6), (4,5), (5,6)

Table 27.1: List of singular regions. The particles are represented by their PDG codes. The third column contains the emitter for the specific singular region. For the process involving an additional gluon, the gluon can either be emitted from one of the quarks or from the first gluon. Each emitter yields the same list of fundamental tuples, five in total. The last singular region corresponds to the process where the gluon splits up into two quarks. As the matrix element for this process has no information on which quarks originate from a gluon splitting, there are ftuples for all the quark pairs and not just those involving the emitter.

27.2 Identifying singular regions

In the FKS subtraction scheme, the phase space is decomposed into disjoint singular regions, such that

$$\sum_i \mathcal{S}_i + \sum_{ij} \mathcal{S}_{ij} = 1. \quad (27.1)$$

The quantities \mathcal{S}_i and \mathcal{S}_{ij} are functions of phase space corresponding to a pair of particles indices which can make up a divergent phase space region. We call such an index pair a fundamental tuple. For example, the process $e^+ e^- \rightarrow u \bar{u} g$ has two singular regions, (3, 5) and (4, 5), indicating that the gluon can be soft or collinear with respect to either the quark or the anti-quark. Therefore, the functions \mathcal{S}_{ij} have to be chosen in such a way that their contribution makes up most of (27.1) in phase-space configurations where (final-state) particle j is collinear to particle i or/and particle j is soft. The functions \mathcal{S}_i is the corresponding quantity for initial-state divergences.

As a singular region we understand the collection of real flavor structures associated with an emitter and a list of all possible fundamental tuples. As an example, consider the process $e^+ e^- \rightarrow u \bar{u} g$. At next-to-leading order, processes with an additionally radiated particle have to be considered. In this case, these are $e^+ e^- \rightarrow u \bar{u}, g g$, and $e^+ e^- \rightarrow u \bar{u} u \bar{u}$ (or the same process with any other quark). Table 27.1 sums up all possible singular regions for this problem.

Thus, during the preparation of a NLO-calculation, the possible singular regions have to be identified. `fkf_regions.f90` deals with this issue.

alr	ftuple	emitter	flst_alr
1	(3, 5)	5	[-11,11,-2,21,2,21]
2	(4, 5)	5	[-11,11,2,21,-2,21]
3	(3, 6)	5	[-11,11,-2,21,2,21]
4	(4, 6)	5	[-11,11,2,21,-2,21]
5	(5, 6)	5	[-11,11,2,-2,21,21]
6	(5, 6)	5	[-11,11,2,-2,2,-2]

Table 27.2: Initial list of singular regions

27.3 FKS Regions

```

⟨fks_regions.f90⟩≡
  ⟨File header⟩

  module fks_regions

    ⟨Use kinds⟩
    use format_utils, only: write_separator
    use numeric_utils
    use string_utils, only: str
    use io_units
    use os_interface
    ⟨Use strings⟩
    ⟨Use debug⟩
    use constants
    use permutations
    use diagnostics
    use flavors
    use process_constants
    use lorentz
    use pdg_arrays
    use models
    use physics_defs
    use resonances, only: resonance_contributors_t, resonance_history_t
    use phs_fks, only: phs_identifier_t, check_for_phs_identifier

    use nlo_data

    ⟨Standard module head⟩

    ⟨fks regions: public⟩

    ⟨fks regions: parameters⟩

    ⟨fks regions: types⟩

    ⟨fks regions: interfaces⟩

    contains

    ⟨fks regions: procedures⟩

    end module fks_regions

```

There are three fundamental splitting types: $q \rightarrow qq$, $g \rightarrow gg$ and $g \rightarrow qq$ for FSR and additionally $q \rightarrow gq$ for ISR which is different from $q \rightarrow qq$ by which particle enters the hard process.

```

⟨fks regions: parameters⟩≡
  integer, parameter :: UNDEFINED_SPLITTING = 0
  integer, parameter :: F_TO_FV = 1
  integer, parameter :: V_TO_VV = 2
  integer, parameter :: V_TO_FF = 3
  integer, parameter :: F_TO_VF = 4

```

We group the indices of the emitting and the radiated particle in the `ftuple`-object.

```

<fks regions: public>≡
  public :: ftuple_t

<fks regions: types>≡
  type :: ftuple_t
    integer, dimension(2) :: ireg = [-1,-1]
    integer :: i_res = 0
    integer :: splitting_type
    logical :: pseudo_isr = .false.
    logical :: qcd_split = .false.
  contains
    <fks regions: ftuple: TBP>
  end type ftuple_t

<fks regions: interfaces>≡
  interface assignment(=)
    module procedure ftuple_assign
  end interface

  interface operator(==)
    module procedure ftuple_equal
  end interface

  interface operator(>)
    module procedure ftuple_greater
  end interface

  interface operator(<)
    module procedure ftuple_less
  end interface

<fks regions: procedures>≡
  pure subroutine ftuple_assign (ftuple_out, ftuple_in)
    type(ftuple_t), intent(out) :: ftuple_out
    type(ftuple_t), intent(in) :: ftuple_in
    ftuple_out%ireg = ftuple_in%ireg
    ftuple_out%i_res = ftuple_in%i_res
    ftuple_out%splitting_type = ftuple_in%splitting_type
    ftuple_out%pseudo_isr = ftuple_in%pseudo_isr
    ftuple_out%qcd_split = ftuple_in%qcd_split
  end subroutine ftuple_assign

<fks regions: procedures>+≡
  elemental function ftuple_equal (f1, f2) result (value)
    logical :: value
    type(ftuple_t), intent(in) :: f1, f2
    value = all (f1%ireg == f2%ireg) .and. f1%i_res == f2%i_res &
      .and. f1%splitting_type == f2%splitting_type &
      .and. (f1%pseudo_isr .eqv. f2%pseudo_isr) &

```

```

        .and. (f1%qcd_split .eqv. f2%qcd_split)
    end function ftuple_equal

```

```

<fks regions: procedures>+=
    elemental function ftuple_equal_ireg (f1, f2) result (value)
        logical :: value
        type(ftuple_t), intent(in) :: f1, f2
        value = all (f1%ireg == f2%ireg)
    end function ftuple_equal_ireg

```

```

<fks regions: procedures>+=
    elemental function ftuple_greater (f1, f2) result (greater)
        logical :: greater
        type(ftuple_t), intent(in) :: f1, f2
        if (f1%ireg(1) == f2%ireg(1)) then
            greater = f1%ireg(2) > f2%ireg(2)
        else
            greater = f1%ireg(1) > f2%ireg(1)
        end if
    end function ftuple_greater

```

```

<fks regions: procedures>+=
    elemental function ftuple_less (f1, f2) result (less)
        logical :: less
        type(ftuple_t), intent(in) :: f1, f2
        if (f1%ireg(1) == f2%ireg(1)) then
            less = f1%ireg(2) < f2%ireg(2)
        else
            less = f1%ireg(1) < f2%ireg(1)
        end if
    end function ftuple_less

```

```

<fks regions: procedures>+=
    subroutine ftuple_sort_array (ftuple_array, equivalences)
        type(ftuple_t), intent(inout), dimension(:), allocatable :: ftuple_array
        logical, intent(inout), dimension(:,:), allocatable :: equivalences
        type(ftuple_t) :: ftuple_tmp
        logical, dimension(:), allocatable :: eq_tmp
        integer :: i1, i2, n
        n = size (ftuple_array)
        allocate (eq_tmp (n))
        do i1 = 2, n
            i2 = i1
            do while (ftuple_array(i2 - 1) > ftuple_array(i2))
                ftuple_tmp = ftuple_array(i2 - 1)
                eq_tmp = equivalences(i2, :)
                ftuple_array(i2 - 1) = ftuple_array(i2)
                ftuple_array(i2) = ftuple_tmp
                equivalences(i2 - 1, :) = equivalences(i2, :)
                equivalences(i2, :) = eq_tmp
                i2 = i2 - 1
            end while
            if (i2 == 1) exit
        end do
    end subroutine ftuple_sort_array

```

```

        end do
    end do
end subroutine ftuple_sort_array

```

(fks regions: ftuple: TBP)≡

```

procedure :: write => ftuple_write

```

(fks regions: procedures)+≡

```

subroutine ftuple_write (ftuple, unit, newline)
    class(ftuple_t), intent(in) :: ftuple
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: newline
    integer :: u
    logical :: nl
    u = given_output_unit (unit); if (u < 0) return
    nl = .true.; if (present(newline)) nl = newline
    if (all (ftuple%ireg > -1)) then
        if (ftuple%i_res > 0) then
            if (nl) then
                write (u, "(A1,I1,A1,I1,A1,I1,A1)" &
                    '(', ftuple%ireg(1), ',', ftuple%ireg(2), ';', ftuple%i_res, ')')
            else
                write (u, "(A1,I1,A1,I1,A1,I1,A1)", advance = "no") &
                    '(', ftuple%ireg(1), ',', ftuple%ireg(2), ';', ftuple%i_res, ')')
            end if
        else
            if (nl) then
                write (u, "(A1,I1,A1,I1,A1)" &
                    '(', ftuple%ireg(1), ',', ftuple%ireg(2), ')')
            else
                write (u, "(A1,I1,A1,I1,A1)", advance = "no") &
                    '(', ftuple%ireg(1), ',', ftuple%ireg(2), ')')
            end if
        end if
    else
        write (u, "(A)") "(Empty)"
    end if
end subroutine ftuple_write

```

(fks regions: procedures)+≡

```

function ftuple_string (ftuples, latex)
    type(string_t) :: ftuple_string
    type(ftuple_t), intent(in), dimension(:) :: ftuples
    logical, intent(in) :: latex
    integer :: i, nreg
    if (latex) then
        ftuple_string = var_str ("$\left\{" )
    else
        ftuple_string = var_str ("{" )
    end if
    nreg = size(ftuples)
    do i = 1, nreg
        if (ftuples(i)%i_res == 0) then

```

```

        ftuple_string = ftuple_string // var_str "(" // &
        str (ftuples(i)%ireg(1)) // var_str "," // &
        str (ftuples(i)%ireg(2)) // var_str ")"
    else
        ftuple_string = ftuple_string // var_str "(" // &
        str (ftuples(i)%ireg(1)) // var_str "," // &
        str (ftuples(i)%ireg(2)) // var_str ";" // &
        str (ftuples(i)%i_res) // var_str ")"
    end if
    if (ftuples(i)%pseudo_isr) ftuple_string = ftuple_string // var_str "*"
    if (i < nreg) ftuple_string = ftuple_string // var_str ","
end do
if (latex) then
    ftuple_string = ftuple_string // var_str "\right\}"
else
    ftuple_string = ftuple_string // var_str "}"
end if
end function ftuple_string

```

<fks regions: ftuple: TBP>+≡

```

procedure :: get => ftuple_get

```

<fks regions: procedures>+≡

```

subroutine ftuple_get (ftuple, pos1, pos2)
    class(ftuple_t), intent(in) :: ftuple
    integer, intent(out) :: pos1, pos2
    pos1 = ftuple%ireg(1)
    pos2 = ftuple%ireg(2)
end subroutine ftuple_get

```

<fks regions: ftuple: TBP>+≡

```

procedure :: set => ftuple_set

```

<fks regions: procedures>+≡

```

subroutine ftuple_set (ftuple, pos1, pos2)
    class(ftuple_t), intent(inout) :: ftuple
    integer, intent(in) :: pos1, pos2
    ftuple%ireg(1) = pos1
    ftuple%ireg(2) = pos2
end subroutine ftuple_set

```

Determines the splitting type for FSR. There are three different types of splittings relevant here: $g \rightarrow gg$ tagged V_TO_VV, $g \rightarrow qq$ tagged V_TO_FF and $q \rightarrow qq$ tagged F_TO_FV. For FSR, there is no need to differentiate between $q \rightarrow qq$ and $q \rightarrow gq$ splittings.

<fks regions: ftuple: TBP>+≡

```

procedure :: determine_splitting_type_fsr => ftuple_determine_splitting_type_fsr

```

<fks regions: procedures>+≡

```

subroutine ftuple_determine_splitting_type_fsr (ftuple, flv, i, j)
    class(ftuple_t), intent(inout) :: ftuple
    type(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: i, j
    associate (flst => flv%flst)

```

```

      if (is_vector (flst(i)) .and. is_vector (flst(j))) then
        ftuple%splitting_type = V_TO_VV
      else if (flst(i)+flst(j) == 0 &
        .and. is_fermion (flst(i))) then
        ftuple%splitting_type = V_TO_FF
      else if (is_fermion(flst(i)) .and. is_massless_vector (flst(j)) &
        .or. is_fermion(flst(j)) .and. is_massless_vector (flst(i))) then
        ftuple%splitting_type = F_TO_FV
      else
        ftuple%splitting_type = UNDEFINED_SPLITTING
      end if
    end associate
  end subroutine ftuple_determine_splitting_type_fsr

```

Determines the splitting type for ISR. There are four different types of splittings relevant here: $g \rightarrow gg$ tagged V_TO_VV, $g \rightarrow qq$ tagged V_TO_FF, $q \rightarrow qq$ tagged F_TO_FV and $q \rightarrow gq$ tagged F_TO_VF. The latter two need to be considered separately for ISR as they differ with respect to which particle enters the hard process. A splitting F_TO_FV may lead to soft divergences while F_TO_VF does not.

We also want to emphasize that the splitting type naming convention for ISR names the splittings considering backwards evolution. So in the splitting V_TO_FF, it is the *gluon* that enters the hard process!

Special treatment here is required if emitter 0 is assigned. This is the case only when a gluon was radiated from any of the IS particles. In this case, both splittings are soft divergent so we can equivalently choose 1 or 2 as the emitter here even if both have different flavors.

```

<fks regions: ftuple: TBP>+=
  procedure :: determine_splitting_type_isr => ftuple_determine_splitting_type_isr

<fks regions: procedures>+=
  subroutine ftuple_determine_splitting_type_isr (ftuple, flv, i, j)
    class(ftuple_t), intent(inout) :: ftuple
    type(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: i, j
    integer :: em
    em = i; if (i == 0) em = 1
    associate (flst => flv%flst)
      if (is_vector (flst(em)) .and. is_vector (flst(j))) then
        ftuple%splitting_type = V_TO_VV
      else if (is_massless_vector(flst(em)) .and. is_fermion(flst(j))) then
        ftuple%splitting_type = F_TO_VF
      else if (is_fermion(flst(em)) .and. is_massless_vector(flst(j))) then
        ftuple%splitting_type = F_TO_FV
      else if (is_fermion(flst(em)) .and. is_fermion(flst(j))) then
        ftuple%splitting_type = V_TO_FF
      else
        ftuple%splitting_type = UNDEFINED_SPLITTING
      end if
    end associate
  end subroutine ftuple_determine_splitting_type_isr

```



```

(fks regions: ftuple: TBP)+≡
  procedure :: determine_sub_correction_type => ftuple_determine_sub_correction_type

(fks regions: procedures)+≡
  subroutine ftuple_determine_sub_correction_type (ftuple, flv_born, flv_real, i, j)
    class(ftuple_t), intent(inout) :: ftuple
    type(flv_structure_t), intent(in) :: flv_born, flv_real
    type(flv_structure_t) :: flv_test_qcd
    integer, intent(in) :: i, j
    integer :: em
    em = i; if (i == 0) em = 1
    select case (ftuple%splitting_type)
    case (V_T0_VV)
      ftuple%qcd_split = is_gluon (flv_real%flst(em)) .and. is_gluon (flv_real%flst(j))
    case (F_T0_VF)
      ftuple%qcd_split = is_gluon (flv_real%flst(em))
    case (F_T0_FV)
      if (i == 0) then
        ftuple%qcd_split = is_gluon (flv_real%flst(j))
      else
        ftuple%qcd_split = is_gluon (flv_real%flst(i)) .or. is_gluon (flv_real%flst(j))
      end if
    case (V_T0_FF)
      if (any ([i, j] <= flv_real%n_in)) then
        flv_test_qcd = flv_real%insert_particle_isr (i, j, GLUON)
      else
        flv_test_qcd = flv_real%insert_particle_fsr (i, j, GLUON)
      end if
      ftuple%qcd_split = flv_test_qcd .equiv. flv_born
    case (UNDEFINED_SPLITTING)
      ftuple%qcd_split = .false.
    end select
  end subroutine ftuple_determine_sub_correction_type

```

Two debug functions to check the consistency of ftuples

```

(fks regions: ftuple: TBP)+≡
  procedure :: has_negative_elements => ftuple_has_negative_elements
  procedure :: has_identical_elements => ftuple_has_identical_elements

(fks regions: procedures)+≡
  elemental function ftuple_has_negative_elements (ftuple) result (value)
    logical :: value
    class(ftuple_t), intent(in) :: ftuple
    value = any (ftuple%ireg < 0)
  end function ftuple_has_negative_elements

  elemental function ftuple_has_identical_elements (ftuple) result (value)
    logical :: value
    class(ftuple_t), intent(in) :: ftuple
    value = ftuple%ireg(1) == ftuple%ireg(2)
  end function ftuple_has_identical_elements

```

Each singular region can have a different number of emitter-radiation pairs.
This is coped with using the linked list `ftuple_list`.

```

<fks regions: types>+≡
type :: ftuple_list_t
integer :: index = 0
type(ftuple_t) :: ftuple
type(ftuple_list_t), pointer :: next => null ()
type(ftuple_list_t), pointer :: prev => null ()
type(ftuple_list_t), pointer :: equiv => null ()
contains
  <fks regions: ftuple list: TBP>
end type ftuple_list_t

<fks regions: ftuple list: TBP>≡
procedure :: write => ftuple_list_write

<fks regions: procedures>+≡
subroutine ftuple_list_write (list, unit, verbose)
  class(ftuple_list_t), intent(in), target :: list
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  type(ftuple_list_t), pointer :: current
  logical :: verb
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  verb = .false.; if (present (verbose)) verb = verbose
  select type (list)
    type is (ftuple_list_t)
      current => list
      do
        call current%ftuple%write (unit = u, newline = .false.)
        if (verb .and. associated (current%equiv)) write (u, '(A)', advance = "no") ""
        if (associated (current%next)) then
          current => current%next
        else
          exit
        end if
      end do
      write (u, *) ""
    end select
end subroutine ftuple_list_write

<fks regions: ftuple list: TBP>+≡
procedure :: append => ftuple_list_append

<fks regions: procedures>+≡
subroutine ftuple_list_append (list, ftuple)
  class(ftuple_list_t), intent(inout), target :: list
  type(ftuple_t), intent(in) :: ftuple
  type(ftuple_list_t), pointer :: current

  select type (list)
    type is (ftuple_list_t)
      if (list%index == 0) then
        nullify (list%next)
        list%index = 1

```

```

        list%ftuple = ftuple
    else
        current => list
    do
        if (associated (current%next)) then
            current => current%next
        else
            allocate (current%next)
            nullify (current%next%next)
            nullify (current%next%equiv)
            current%next%prev => current
            current%next%index = current%index + 1
            current%next%ftuple = ftuple
            exit
        end if
    end do
end if
end select
end subroutine ftuple_list_append

```

<fks regions: ftuple list: TBP>+≡

```

procedure :: get_n_tuples => ftuple_list_get_n_tuples

```

<fks regions: procedures>+≡

```

impure elemental function ftuple_list_get_n_tuples (list) result(n_tuples)
    integer :: n_tuples
    class(ftuple_list_t), intent(in), target :: list
    type(ftuple_list_t), pointer :: current
    n_tuples = 0
    select type (list)
    type is (ftuple_list_t)
        current => list
        if (current%index > 0) then
            n_tuples = 1
            do
                if (associated (current%next)) then
                    current => current%next
                    n_tuples = n_tuples + 1
                else
                    exit
                end if
            end do
        end if
    end select
end function ftuple_list_get_n_tuples

```

<fks regions: ftuple list: TBP>+≡

```

procedure :: get_entry => ftuple_list_get_entry

```

<fks regions: procedures>+≡

```

function ftuple_list_get_entry (list, index) result (entry)
    type(ftuple_list_t), pointer :: entry
    class(ftuple_list_t), intent(in), target :: list
    integer, intent(in) :: index

```

```

type(ftuple_list_t), pointer :: current
integer :: i
entry => null()
select type (list)
type is (ftuple_list_t)
    current => list
    if (index == 1) then
        entry => current
    else
        do i = 1, index - 1
            current => current%next
        end do
        entry => current
    end if
end select
end function ftuple_list_get_entry

```

```

⟨fks regions: ftuple list: TBP⟩+≡
    procedure :: get_ftuple => ftuple_list_get_ftuple

⟨fks regions: procedures⟩+≡
    function ftuple_list_get_ftuple (list, index) result (ftuple)
        type(ftuple_t) :: ftuple
        class(ftuple_list_t), intent(in), target :: list
        integer, intent(in) :: index
        type(ftuple_list_t), pointer :: entry
        entry => list%get_entry (index)
        ftuple = entry%ftuple
    end function ftuple_list_get_ftuple

```

```

⟨fks regions: ftuple list: TBP⟩+≡
    procedure :: set_equiv => ftuple_list_set_equiv

⟨fks regions: procedures⟩+≡
    subroutine ftuple_list_set_equiv (list, i1, i2)
        class(ftuple_list_t), intent(in) :: list
        integer, intent(in) :: i1, i2
        type(ftuple_list_t), pointer :: list1, list2 => null ()
        select type (list)
        type is (ftuple_list_t)
            if (list%get_ftuple (i1) > list%get_ftuple (i2)) then
                list1 => list%get_entry (i2)
                list2 => list%get_entry (i1)
            else
                list1 => list%get_entry (i1)
                list2 => list%get_entry (i2)
            end if
        do
            if (associated (list1%equiv)) then
                list1 => list1%equiv
            else
                exit
            end if
        end do
    end subroutine

```

```

        list1%equiv => list2
    end select
end subroutine ftuple_list_set_equiv

```

<fks regions: ftuple list: TBP>+≡

```

    procedure :: check_equiv => ftuple_list_check_equiv

```

<fks regions: procedures>+≡

```

function ftuple_list_check_equiv(list, i1, i2) result(eq)
    class(ftuple_list_t), intent(in) :: list
    integer, intent(in) :: i1, i2
    logical :: eq
    type(ftuple_list_t), pointer :: current
    eq = .false.
    select type (list)
    type is (ftuple_list_t)
        current => list%get_entry (i1)
        do
            if (associated (current%equiv)) then
                current => current%equiv
                if (current%index == i2) then
                    eq = .true.
                    exit
                end if
            else
                exit
            end if
        end do
    end select
end function ftuple_list_check_equiv

```

<fks regions: ftuple list: TBP>+≡

```

    procedure :: to_array => ftuple_list_to_array

```

<fks regions: procedures>+≡

```

subroutine ftuple_list_to_array (ftuple_list, ftuple_array, equivalences, ordered)
    class(ftuple_list_t), intent(in), target :: ftuple_list
    type(ftuple_t), intent(out), dimension(:), allocatable :: ftuple_array
    logical, intent(out), dimension(:,:), allocatable :: equivalences
    logical, intent(in) :: ordered
    integer :: i_tuple, n
    type(ftuple_list_t), pointer :: current => null ()
    integer :: i1, i2
    type(ftuple_t) :: ftuple_tmp
    logical, dimension(:), allocatable :: eq_tmp
    n = ftuple_list%get_n_tuples ()
    allocate (ftuple_array (n), equivalences (n, n))
    equivalences = .false.
    select type (ftuple_list)
    type is (ftuple_list_t)
        current => ftuple_list
        i_tuple = 1
        do
            ftuple_array(i_tuple) = current%ftuple

```

```

        if (associated (current%equiv)) then
            i1 = current%index
            i2 = current%equiv%index
            equivalences (i1, i2) = .true.
        end if
        if (associated (current%next)) then
            current => current%next
            i_tuple = i_tuple + 1
        else
            exit
        end if
    end do
end select
if (ordered) call ftuple_sort_array (ftuple_array, equivalences)
end subroutine ftuple_list_to_array

```

```

<fks regions: procedures>+=
subroutine print_equivalence_matrix (ftuple_array, equivalences)
    type(ftuple_t), intent(in), dimension(:) :: ftuple_array
    logical, intent(in), dimension(:, :) :: equivalences
    integer :: i, i1, i2
    print *, 'Equivalence matrix: '
    do i = 1, size (ftuple_array)
        call ftuple_array(i)%get(i1,i2)
        print *, 'i: ', i, '(', i1, i2, '): ', equivalences(i,:)
    end do
end subroutine print_equivalence_matrix

```

Class for working with the flavor specification arrays.

```

<fks regions: public>+=
public :: flv_structure_t

<fks regions: types>+=
type :: flv_structure_t
    integer, dimension(:), allocatable :: flst
    integer, dimension(:), allocatable :: tag
    integer :: nlegs = 0
    integer :: n_in = 0
    logical, dimension(:), allocatable :: massive
    logical, dimension(:), allocatable :: colored
    real(default), dimension(:), allocatable :: charge
    real(default) :: prt_symm_fs = 1._default
    integer :: eqv_index = 0
contains
    <fks regions: flv structure: TBP>
end type flv_structure_t

```

Returns `true` if the two particles at position `i` and `j` in the flavor array can originate from the same splitting. For this purpose, the function first checks whether the splitting is allowed at all. If this is the case, the emitter is removed from the flavor array. If the resulting array is equivalent to the Born flavor structure `flv.born`, the pair is accepted as a valid splitting.

We first check whether the splitting is possible. The array `flv_orig` contains all particles which share a vertex with the particles at position `i` and `j`. If any of these particles belongs to the initial state, a PDG-ID flip is necessary to correctly recognize the vertex. If its size is equal to zero, no splitting is possible and the subroutine is exited. Otherwise, we loop over all possible underlying Born flavor structures and check if any of them equals the actual underlying Born flavor structure. For a quark emitting a gluon, `flv_orig` contains the PDG code of the anti-quark. To be on the safe side, a second array is created, which contains both the positively and negatively signed PDG codes. Then, the original tuple (i, j) is removed from the real flavor structure and the particles in `flv_orig2` are inserted. If the resulting Born configuration is equal to the underlying Born configuration, up to a permutation of final-state particles, the tuple (i, j) is accepted as valid.

```

<fks regions: flv structure: TBP>≡
  procedure :: valid_pair => flv_structure_valid_pair

<fks regions: procedures>+≡
  function flv_structure_valid_pair &
    (flv, i, j, flv_ref, model) result (valid)
    logical :: valid
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: i, j
    type(flv_structure_t), intent(in) :: flv_ref
    type(model_t), intent(in) :: model
    integer :: k, n_orig
    type(flv_structure_t) :: flv_test
    integer, dimension(:), allocatable :: flv_orig
    valid = .false.
    if (all ([i, j] <= flv%n_in)) return
    if (i <= flv%n_in .and. is_fermion(flv%flst(i))) then
      call model%match_vertex (-flv%flst(i), flv%flst(j), flv_orig)
    else if (j <= flv%n_in .and. is_fermion(flv%flst(j))) then
      call model%match_vertex (flv%flst(i), -flv%flst(j), flv_orig)
    else
      call model%match_vertex (flv%flst(i), flv%flst(j), flv_orig)
    end if
    n_orig = size (flv_orig)
    if (n_orig == 0) then
      return
    else
      do k = 1, n_orig
        if (any ([i, j] <= flv%n_in)) then
          flv_test = flv%insert_particle_isr (i, j, flv_orig(k))
        else
          flv_test = flv%insert_particle_fsr (i, j, flv_orig(k))
        end if
        valid = flv_ref .equiv. flv_test
        call flv_test%final ()
        if (valid) return
      end do
    end if
    deallocate (flv_orig)
  end function flv_structure_valid_pair

```

This function checks whether two flavor arrays are the same up to a permutation of the final-state particles

```

(fks regions: procedures)+≡
function flv_structure_equivalent (flv1, flv2, with_tag) result(equiv)
  logical :: equiv
  type(flv_structure_t), intent(in) :: flv1, flv2
  logical, intent(in) :: with_tag
  type(flavor_permutation_t) :: perm
  integer :: n
  n = size (flv1%flst)
  equiv = .true.
  if (n /= size (flv2%flst)) then
    call msg_fatal &
      ('flv_structure_equivalent: flavor arrays do not have equal lengths')
  else if (flv1%n_in /= flv2%n_in) then
    call msg_fatal &
      ('flv_structure_equivalent: flavor arrays do not have equal n_in')
  else
    call perm%init (flv1, flv2, flv1%n_in, flv1%nlegs, with_tag)
    equiv = perm%test (flv2, flv1, with_tag)
    call perm%final ()
  end if
end function flv_structure_equivalent

```

```

(fks regions: procedures)+≡
function flv_structure_equivalent_no_tag (flv1, flv2) result(equiv)
  logical :: equiv
  type(flv_structure_t), intent(in) :: flv1, flv2
  equiv = flv_structure_equivalent (flv1, flv2, .false.)
end function flv_structure_equivalent_no_tag

function flv_structure_equivalent_with_tag (flv1, flv2) result(equiv)
  logical :: equiv
  type(flv_structure_t), intent(in) :: flv1, flv2
  equiv = flv_structure_equivalent (flv1, flv2, .true.)
end function flv_structure_equivalent_with_tag

```

```

(fks regions: procedures)+≡
pure subroutine flv_structure_assign_flv (flv_out, flv_in)
  type(flv_structure_t), intent(out) :: flv_out
  type(flv_structure_t), intent(in) :: flv_in
  flv_out%nlegs = flv_in%nlegs
  flv_out%n_in = flv_in%n_in
  flv_out%prt_symm_fs = flv_in%prt_symm_fs
  if (allocated (flv_in%flst)) then
    allocate (flv_out%flst (size (flv_in%flst)))
    flv_out%flst = flv_in%flst
  end if
  if (allocated (flv_in%tag)) then
    allocate (flv_out%tag (size (flv_in%tag)))

```



```

        flv_out%tag = flv_in%tag
    end if
    if (allocated (flv_in%massive)) then
        allocate (flv_out%massive (size (flv_in%massive)))
        flv_out%massive = flv_in%massive
    end if
    if (allocated (flv_in%colored)) then
        allocate (flv_out%colored (size (flv_in%colored)))
        flv_out%colored = flv_in%colored
    end if
end subroutine flv_structure_assign_flv

```

(fks regions: procedures)+≡

```

pure subroutine flv_structure_assign_integer (flv_out, iarray)
    type(flv_structure_t), intent(out) :: flv_out
    integer, intent(in), dimension(:) :: iarray
    integer :: i
    flv_out%nlegs = size (iarray)
    allocate (flv_out%flst (flv_out%nlegs))
    allocate (flv_out%tag (flv_out%nlegs))
    flv_out%flst = iarray
    flv_out%tag = [(i, i = 1, flv_out%nlegs)]
end subroutine flv_structure_assign_integer

```

Returns a new flavor array with the particle at position index removed.

(fks regions: flv structure: TBP)+≡

```

procedure :: remove_particle => flv_structure_remove_particle

```

(fks regions: procedures)+≡

```

function flv_structure_remove_particle (flv, index) result(flv_new)
    type(flv_structure_t) :: flv_new
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in) :: index
    integer :: n1, n2
    integer :: i, removed_tag
    n1 = size (flv%flst); n2 = n1 - 1
    allocate (flv_new%flst (n2), flv_new%tag (n2))
    flv_new%nlegs = n2
    flv_new%n_in = flv%n_in
    removed_tag = flv%tag(index)
    if (index == 1) then
        flv_new%flst(1 : n2) = flv%flst(2 : n1)
        flv_new%tag(1 : n2) = flv%tag(2 : n1)
    else if (index == n1) then
        flv_new%flst(1 : n2) = flv%flst(1 : n2)
        flv_new%tag(1 : n2) = flv%tag(1 : n2)
    else
        flv_new%flst(1 : index - 1) = flv%flst(1 : index - 1)
        flv_new%flst(index : n2) = flv%flst(index + 1 : n1)
        flv_new%tag(1 : index - 1) = flv%tag(1 : index - 1)
        flv_new%tag(index : n2) = flv%tag(index + 1 : n1)
    end if
    do i = 1, n2
        if (flv_new%tag(i) > removed_tag) &

```

```

        flv_new%tag(i) = flv_new%tag(i) - 1
    end do
    call flv_new%compute_prt_symm_fs (flv_new%n_in)
end function flv_structure_remove_particle

```

Removes the particles at position i1 and i2 and inserts a new particle of matching flavor at position i1.

```

⟨fks regions: flv structure: TBP⟩+≡
    procedure :: insert_particle_fsr => flv_structure_insert_particle_fsr

⟨fks regions: procedures⟩+≡
    function flv_structure_insert_particle_fsr (flv, i1, i2, flv_add) result (flv_new)
        type(flv_structure_t) :: flv_new
        class(flv_structure_t), intent(in) :: flv
        integer, intent(in) :: i1, i2, flv_add
        if (flv%flst(i1) + flv_add == 0 .or. flv%flst(i2) + flv_add == 0) then
            flv_new = flv%insert_particle (i1, i2, -flv_add)
        else
            flv_new = flv%insert_particle (i1, i2, flv_add)
        end if
    end function flv_structure_insert_particle_fsr

```

Same as `insert_particle_fsr` but for ISR, the two particles are not exchangeable.

```

⟨fks regions: flv structure: TBP⟩+≡
    procedure :: insert_particle_isr => flv_structure_insert_particle_isr

⟨fks regions: procedures⟩+≡
    function flv_structure_insert_particle_isr (flv, i_in, i_out, flv_add) result (flv_new)
        type(flv_structure_t) :: flv_new
        class(flv_structure_t), intent(in) :: flv
        integer, intent(in) :: i_in, i_out, flv_add
        if (flv%flst(i_in) + flv_add == 0) then
            flv_new = flv%insert_particle (i_in, i_out, -flv_add)
        else
            flv_new = flv%insert_particle (i_in, i_out, flv_add)
        end if
    end function flv_structure_insert_particle_isr

```

Removes the particles at position i1 and i2 and inserts a new particle at position i1.

```

⟨fks regions: flv structure: TBP⟩+≡
    procedure :: insert_particle => flv_structure_insert_particle

⟨fks regions: procedures⟩+≡
    function flv_structure_insert_particle (flv, i1, i2, particle) result (flv_new)
        type(flv_structure_t) :: flv_new
        class(flv_structure_t), intent(in) :: flv
        integer, intent(in) :: i1, i2, particle
        type(flv_structure_t) :: flv_tmp
        integer :: n1, n2
        integer :: new_tag
        n1 = size (flv%flst); n2 = n1 - 1
        allocate (flv_new%flst (n2), flv_new%tag (n2))

```

```

flv_new%nlegs = n2
flv_new%n_in = flv%n_in
new_tag = maxval(flval%tag) + 1
if (i1 < i2) then
  flv_tmp = flv%remove_particle (i1)
  flv_tmp = flv_tmp%remove_particle (i2 - 1)
else if (i2 < i1) then
  flv_tmp = flv%remove_particle(i2)
  flv_tmp = flv_tmp%remove_particle(i1 - 1)
else
  call msg_fatal ("flv_structure_insert_particle: Indices are identical!")
end if
if (i1 == 1) then
  flv_new%flst(1) = particle
  flv_new%flst(2 : n2) = flv_tmp%flst(1 : n2 - 1)
  flv_new%tag(1) = new_tag
  flv_new%tag(2 : n2) = flv_tmp%tag(1 : n2 - 1)
else if (i1 == n1 .or. i1 == n2) then
  flv_new%flst(1 : n2 - 1) = flv_tmp%flst(1 : n2 - 1)
  flv_new%flst(n2) = particle
  flv_new%tag(1 : n2 - 1) = flv_tmp%tag(1 : n2 - 1)
  flv_new%tag(n2) = new_tag
else
  flv_new%flst(1 : i1 - 1) = flv_tmp%flst(1 : i1 - 1)
  flv_new%flst(i1) = particle
  flv_new%flst(i1 + 1 : n2) = flv_tmp%flst(i1 : n2 - 1)
  flv_new%tag(1 : i1 - 1) = flv_tmp%tag(1 : i1 - 1)
  flv_new%tag(i1) = new_tag
  flv_new%tag(i1 + 1 : n2) = flv_tmp%tag(i1 : n2 - 1)
end if
call flv_new%compute_prt_symm_fs (flv_new%n_in)
end function flv_structure_insert_particle

```

Counts the number of occurrences of a particle in a flavor array

```

<fks regions: flv structure: TBP>+≡
  procedure :: count_particle => flv_structure_count_particle

<fks regions: procedures>+≡
  function flv_structure_count_particle (flv, part) result (n)
    class(flval_structure_t), intent(in) :: flv
    integer, intent(in) :: part
    integer :: n
    n = count (flv%flst == part)
  end function flv_structure_count_particle

```

Initializer for flavor structures

```

<fks regions: flv structure: TBP>+≡
  procedure :: init => flv_structure_init

<fks regions: procedures>+≡
  subroutine flv_structure_init (flv, aval, n_in, tags)
    class(flval_structure_t), intent(inout) :: flv
    integer, intent(in), dimension(:) :: aval
    integer, intent(in) :: n_in

```

```

integer, intent(in), dimension(:), optional :: tags
integer :: i, n
integer, dimension(:), allocatable :: aval_unique
integer, dimension(:), allocatable :: mult
n = size (aval)
allocate (flv%flst (n), flv%tag (n))
flv%flst = aval
if (present (tags)) then
    flv%tag = tags
else
    do i = 1, n
        flv%tag(i) = i
    end do
end if
flv%nlegs = n
flv%n_in = n_in
call flv%compute_prt_symm_fs (flv%n_in)
end subroutine flv_structure_init

```

<fks regions: flv structure: TBP>+≡

```

procedure :: compute_prt_symm_fs => flv_structure_compute_prt_symm_fs

```

<fks regions: procedures>+≡

```

subroutine flv_structure_compute_prt_symm_fs (flv, n_in)
    class(flv_structure_t), intent(inout) :: flv
    integer, intent(in) :: n_in
    integer, dimension(:), allocatable :: flst_unique
    integer, dimension(:), allocatable :: mult
    integer :: i
    flst_unique = remove_duplicates_from_int_array (flv%flst(n_in + 1 :))
    allocate (mult(size (flst_unique)))
    do i = 1, size (flst_unique)
        mult(i) = count (flv%flst(n_in + 1 :) == flst_unique(i))
    end do
    flv%prt_symm_fs = one / product (gamma (real (mult + 1, default)))
end subroutine flv_structure_compute_prt_symm_fs

```

<fks regions: flv structure: TBP>+≡

```

procedure :: write => flv_structure_write

```

<fks regions: procedures>+≡

```

subroutine flv_structure_write (flv, unit)
    class(flv_structure_t), intent(in) :: flv
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, '(A)') char (flv%to_string ())
end subroutine flv_structure_write

```

<fks regions: flv structure: TBP>+≡

```

procedure :: to_string => flv_structure_to_string

```

```

(fks regions: procedures)+≡
function flv_structure_to_string (flv) result (flv_string)
  type(string_t) :: flv_string
  class(flv_structure_t), intent(in) :: flv
  integer :: i, n
  if (allocated (flv%flst)) then
    flv_string = var_str ("["
    n = size (flv%flst)
    do i = 1, n - 1
      flv_string = flv_string // str (flv%flst(i)) // var_str(",")
    end do
    flv_string = flv_string // str (flv%flst(n)) // var_str("]")
  else
    flv_string = var_str ("[not allocated]")
  end if
end function flv_structure_to_string

```

Creates the underlying Born flavor structure for a given real flavor structure if the particle at position `emitter` is removed

```

(fks regions: flv structure: TBP)+≡
procedure :: create_uborn => flv_structure_create_uborn

(fks regions: procedures)+≡
function flv_structure_create_uborn (flv, emitter, nlo_correction_type) result(flv_uborn)
  type(flv_structure_t) :: flv_uborn
  class(flv_structure_t), intent(in) :: flv
  type(string_t), intent(in) :: nlo_correction_type
  integer, intent(in) :: emitter
  integer n_legs
  integer :: f1, f2
  integer :: gauge_boson

  n_legs = size(flv%flst)
  allocate (flv_uborn%flst (n_legs - 1), flv_uborn%tag (n_legs - 1))
  gauge_boson = determine_gauge_boson_to_be_inserted ()

  if (emitter > flv%n_in) then
    f1 = flv%flst(n_legs); f2 = flv%flst(n_legs - 1)
    if (is_massless_vector (f1)) then
      !!! Emitted particle is a gluon or photon => just remove it
      flv_uborn = flv%remove_particle(n_legs)
    else if (is_fermion (f1) .and. is_fermion (f2) .and. f1 + f2 == 0) then
      !!! Emission type is a gauge boson splitting into two fermions
      flv_uborn = flv%insert_particle(n_legs - 1, n_legs, gauge_boson)
    else
      call msg_error ("Create underlying Born: Unsupported splitting type.")
      call msg_error (char (str (flv%flst)))
      call msg_fatal ("FKS - FAIL")
    end if
  else if (emitter > 0) then
    f1 = flv%flst(n_legs); f2 = flv%flst(emitter)
    if (is_massless_vector (f1)) then
      flv_uborn = flv%remove_particle(n_legs)
    else if (is_fermion (f1) .and. is_massless_vector (f2)) then

```

```

        flv_uborn = flv%insert_particle (emitter, n_legs, -f1)
    else if (is_fermion (f1) .and. is_fermion (f2) .and. f1 == f2) then
        flv_uborn = flv%insert_particle(emitter, n_legs, gauge_boson)
    end if
else
    flv_uborn = flv%remove_particle (n_legs)
end if

contains
    integer function determine_gauge_boson_to_be_inserted ()
        select case (char (nlo_correction_type))
            case ("QCD")
                determine_gauge_boson_to_be_inserted = GLUON
            case ("EW")
                determine_gauge_boson_to_be_inserted = PHOTON
            case ("Full")
                call msg_fatal ("NLO correction type 'Full' not yet implemented!")
            case default
                call msg_fatal ("Invalid NLO correction type! Valid inputs are: QCD, EW and Full (default)")
            end select
        end function determine_gauge_boson_to_be_inserted

    end function flv_structure_create_uborn

<fks regions: flv structure: TBP>+≡
    procedure :: init_mass_color_and_charge => flv_structure_init_mass_color_and_charge

<fks regions: procedures>+≡
    subroutine flv_structure_init_mass_color_and_charge (flv, model)
        class(fl_v_structure_t), intent(inout) :: flv
        type(model_t), intent(in) :: model
        integer :: i
        type(flavor_t) :: flavor
        allocate (flv%massive (flv%nlegs), flv%colored(flv%nlegs), flv%charge(flv%nlegs))
        do i = 1, flv%nlegs
            call flavor%init (flv%flst(i), model)
            flv%massive(i) = flavor%get_mass () > 0
            flv%colored(i) = &
                is_quark (flv%flst(i)) .or. is_gluon (flv%flst(i))
            flv%charge(i) = flavor%get_charge ()
        end do
    end subroutine flv_structure_init_mass_color_and_charge

<fks regions: flv structure: TBP>+≡
    procedure :: get_last_two => flv_structure_get_last_two

<fks regions: procedures>+≡
    function flv_structure_get_last_two (flv, n) result (flst_last)
        integer, dimension(2) :: flst_last
        class(fl_v_structure_t), intent(in) :: flv
        integer, intent(in) :: n
        flst_last = [flv%flst(n - 1), flv%flst(n)]
    end function flv_structure_get_last_two

```

```

<fks regions: flv structure: TBP>+≡
  procedure :: final => flv_structure_final

<fks regions: procedures>+≡
  subroutine flv_structure_final (flv)
    class(fl_v_structure_t), intent(inout) :: flv
    if (allocated (flv%flst)) deallocate (flv%flst)
    if (allocated (flv%tag)) deallocate (flv%tag)
    if (allocated (flv%massive)) deallocate (flv%massive)
    if (allocated (flv%colored)) deallocate (flv%colored)
    if (allocated (flv%charge)) deallocate (flv%charge)
  end subroutine flv_structure_final

<fks regions: public>+≡
  public :: flavor_permutation_t

<fks regions: types>+≡
  type :: flavor_permutation_t
    integer, dimension(:,,:), allocatable :: perms
  contains
    <fks regions: flavor permutation: TBP>
  end type flavor_permutation_t

<fks regions: flavor permutation: TBP>≡
  procedure :: init => flavor_permutation_init

<fks regions: procedures>+≡
  subroutine flavor_permutation_init (perm, flv_in, flv_ref, n_first, n_last, with_tag)
    class(flavor_permutation_t), intent(out) :: perm
    type(fl_v_structure_t), intent(in) :: flv_in, flv_ref
    integer, intent(in) :: n_first, n_last
    logical, intent(in) :: with_tag
    integer :: flv1, flv2, tmp
    integer :: tag1, tag2
    integer :: i, j, j_min, i_perm
    integer, dimension(:,,:), allocatable :: perm_list_tmp
    type(fl_v_structure_t) :: flv_copy
    logical :: condition
    logical, dimension(:), allocatable :: already_correct
    flv_copy = flv_in
    allocate (perm_list_tmp (factorial (n_last - n_first - 1), 2))
    allocate (already_correct (flv_in%nlegs))
    already_correct = flv_in%flst == flv_ref%flst
    if (with_tag) &
      already_correct = already_correct .and. (flv_in%tag == flv_ref%tag)
    j_min = n_first + 1
    i_perm = 0
    do i = n_first + 1, n_last
      flv1 = flv_ref%flst(i)
      tag1 = flv_ref%tag(i)
      do j = j_min, n_last
        if (already_correct(i) .or. already_correct(j)) cycle
        flv2 = flv_copy%flst(j)
        tag2 = flv_copy%tag(j)
        condition = (flv1 == flv2) .and. i /= j

```

```

        if (with_tag) condition = condition .and. (tag1 == tag2)
        if (condition) then
            i_perm = i_perm + 1
            tmp = flv_copy%flst(i)
            flv_copy%flst(i) = flv2
            flv_copy%flst(j) = tmp
            tmp = flv_copy%tag(i)
            flv_copy%tag(i) = tag2
            flv_copy%tag(j) = tmp
            perm_list_tmp (i_perm, 1) = i
            perm_list_tmp (i_perm, 2) = j
            exit
        end if
    end do
    j_min = j_min + 1
end do
allocate (perm%perms (i_perm, 2))
perm%perms = perm_list_tmp (1 : i_perm, :)
deallocate (perm_list_tmp)
call flv_copy%final ()
end subroutine flavor_permutation_init

```

<fks regions: flavor permutation: TBP>+≡

```

    procedure :: write => flavor_permutation_write

```

<fks regions: procedures>+≡

```

    subroutine flavor_permutation_write (perm, unit)
        class(flavor_permutation_t), intent(in) :: perm
        integer, intent(in), optional :: unit
        integer :: i, n, u
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(A)") "Flavor permutation list: "
        n = size (perm%perms, dim = 1)
        if (n > 0) then
            do i = 1, n
                write (u, "(A1,I1,1X,I1,A1)", advance = "no") "[", perm%perms(i,1), perm%perms(i,2), "]"
                if (i < n) write (u, "(A4)", advance = "no") " // "
            end do
            write (u, "(A)") ""
        else
            write (u, "(A)") "[Empty]"
        end if
    end subroutine flavor_permutation_write

```

<fks regions: flavor permutation: TBP>+≡

```

    procedure :: reset => flavor_permutation_final
    procedure :: final => flavor_permutation_final

```

<fks regions: procedures>+≡

```

    subroutine flavor_permutation_final (perm)
        class(flavor_permutation_t), intent(inout) :: perm
        if (allocated (perm%perms)) deallocate (perm%perms)
    end subroutine flavor_permutation_final

```



```

(fks regions: flavor permutation: TBP)+≡
generic :: apply => apply_permutation, &
    apply_flavor, apply_integer, apply_ftuple
procedure :: apply_permutation => flavor_permutation_apply_permutation
procedure :: apply_flavor => flavor_permutation_apply_flavor
procedure :: apply_integer => flavor_permutation_apply_integer
procedure :: apply_ftuple => flavor_permutation_apply_ftuple

(fks regions: procedures)+≡
elemental function flavor_permutation_apply_permutation (perm_1, perm_2) &
    result (perm_out)
    type(flavor_permutation_t) :: perm_out
    class(flavor_permutation_t), intent(in) :: perm_1
    type(flavor_permutation_t), intent(in) :: perm_2
    integer :: n1, n2
    n1 = size (perm_1%perms, dim = 1)
    n2 = size (perm_2%perms, dim = 1)
    allocate (perm_out%perms (n1 + n2, 2))
    perm_out%perms (1 : n1, :) = perm_1%perms
    perm_out%perms (n1 + 1: n1 + n2, :) = perm_2%perms
end function flavor_permutation_apply_permutation

(fks regions: procedures)+≡
elemental function flavor_permutation_apply_flavor (perm, flv_in, invert) &
    result (flv_out)
    type(flv_structure_t) :: flv_out
    class(flavor_permutation_t), intent(in) :: perm
    type(flv_structure_t), intent(in) :: flv_in
    logical, intent(in), optional :: invert
    integer :: i, i1, i2
    integer :: p1, p2, incr
    integer :: flv_tmp, tag_tmp
    logical :: inv
    inv = .false.; if (present(invert)) inv = invert
    flv_out = flv_in
    if (inv) then
        p1 = 1
        p2 = size (perm%perms, dim = 1)
        incr = 1
    else
        p1 = size (perm%perms, dim = 1)
        p2 = 1
        incr = -1
    end if
    do i = p1, p2, incr
        i1 = perm%perms(i,1)
        i2 = perm%perms(i,2)
        flv_tmp = flv_out%flst(i1)
        tag_tmp = flv_out%tag(i1)
        flv_out%flst(i1) = flv_out%flst(i2)
        flv_out%flst(i2) = flv_tmp
        flv_out%tag(i1) = flv_out%tag(i2)
        flv_out%tag(i2) = tag_tmp
    end do

```

```

end function flavor_permutation_apply_flavor

⟨fks regions: procedures⟩+=
elemental function flavor_permutation_apply_integer (perm, i_in) result (i_out)
  integer :: i_out
  class(flavor_permutation_t), intent(in) :: perm
  integer, intent(in) :: i_in
  integer :: i, i1, i2
  i_out = i_in
  do i = size (perm%perms(:,1)), 1, -1
    i1 = perm%perms(i,1)
    i2 = perm%perms(i,2)
    if (i_out == i1) then
      i_out = i2
    else if (i_out == i2) then
      i_out = i1
    end if
  end do
end function flavor_permutation_apply_integer

⟨fks regions: procedures⟩+=
elemental function flavor_permutation_apply_ftuple (perm, f_in) result (f_out)
  type(ftuple_t) :: f_out
  class(flavor_permutation_t), intent(in) :: perm
  type(ftuple_t), intent(in) :: f_in
  integer :: i, i1, i2
  f_out = f_in
  do i = size (perm%perms, dim = 1), 1, -1
    i1 = perm%perms(i,1)
    i2 = perm%perms(i,2)
    if (f_out%ireg(1) == i1) then
      f_out%ireg(1) = i2
    else if (f_out%ireg(1) == i2) then
      f_out%ireg(1) = i1
    end if
    if (f_out%ireg(2) == i1) then
      f_out%ireg(2) = i2
    else if (f_out%ireg(2) == i2) then
      f_out%ireg(2) = i1
    end if
  end do
  if (f_out%ireg(1) > f_out%ireg(2)) f_out%ireg = f_out%ireg([2,1])
end function flavor_permutation_apply_ftuple

⟨fks regions: flavor permutation: TBP⟩+=
procedure :: test => flavor_permutation_test

⟨fks regions: procedures⟩+=
function flavor_permutation_test (perm, flv1, flv2, with_tag) result (valid)
  logical :: valid
  class(flavor_permutation_t), intent(in) :: perm
  type(flv_structure_t), intent(in) :: flv1, flv2
  logical, intent(in) :: with_tag

```

```

type(flv_structure_t) :: flv_test
flv_test = perm%apply (flv2, invert = .true.)
valid = all (flv_test%flst == flv1%flst)
if (with_tag) valid = valid .and. all (flv_test%tag == flv1%tag)
call flv_test%final ()
end function flavor_permutation_test

```

A singular region is a partition of phase space which is associated with an individual emitter and, if relevant, resonance. It is associated with an α_r - and resonance-index, with a real flavor structure and its underlying Born flavor structure. To compute the FKS weights, it is relevant to know all the other particle indices which can result in a divergent phase space configuration, which are collected in the **ftuples**-array.

Some singular regions might behave physically identical. E.g. a real flavor structure associated with three-jet production is $[11, -11, 2, -2, 21, 21]$. Here, there are two possible **ftuples** which contribute to the same $u \rightarrow ug$ splitting, namely (3,5) and (3,6). The resulting singular regions will be identical. To avoid this, one singular region is associated with the multiplicity factor **mult**. When computing the subtraction terms for each singular region, the result is then simply multiplied by this factor.

The **double_fsr**-flag indicates whether the singular region should also be supplied by a symmetry factor, explained below.

```

<fks regions: public>+≡
public :: singular_region_t

<fks regions: types>+≡
type :: singular_region_t
integer :: alr
integer :: i_res
type(flv_structure_t) :: flst_real
type(flv_structure_t) :: flst_uborn
integer :: mult
integer :: emitter
integer :: nregions
integer :: real_index
type(ftuple_t), dimension(:), allocatable :: ftuples
integer :: uborn_index
logical :: double_fsr = .false.
logical :: soft_divergence = .false.
logical :: coll_divergence = .false.
type(string_t) :: nlo_correction_type
integer, dimension(:), allocatable :: i_reg_to_i_con
logical :: pseudo_isr = .false.
logical :: sc_required = .false.
integer :: eqv_index = 0
contains
<fks regions: singular region: TBP>
end type singular_region_t

```

```

<fks regions: singular region: TBP>≡
procedure :: init => singular_region_init

```

```

<fks regions: procedures>+=
subroutine singular_region_init (sregion, alr, mult, i_res, &
    flst_real, flst_uborn, flv_born, emitter, ftuples, equivalences, &
    nlo_correction_type)
    class(singular_region_t), intent(out) :: sregion
    integer, intent(in) :: alr, mult, i_res
    type(flv_structure_t), intent(in) :: flst_real
    type(flv_structure_t), intent(in) :: flst_uborn
    type(flv_structure_t), dimension(:), intent(in) :: flv_born
    integer, intent(in) :: emitter
    type(ftuple_t), intent(inout), dimension(:) :: ftuples
    logical, intent(inout), dimension(:,:) :: equivalences
    type(string_t), intent(in) :: nlo_correction_type
    integer :: i
    call debug_input_values ()
    sregion%alr = alr
    sregion%mult = mult
    sregion%i_res = i_res
    sregion%flst_real = flst_real
    sregion%flst_uborn = flst_uborn
    sregion%emitter = emitter
    sregion%nlo_correction_type = nlo_correction_type
    sregion%nregions = size (ftuples)
    allocate (sregion%ftuples (sregion%nregions))
    sregion%ftuples = ftuples
    do i = 1, size(flv_born)
        if (flv_born (i) .equiv. sregion%flst_uborn) then
            sregion%uborn_index = i
            exit
        end if
    end do
    sregion%sc_required = any (sregion%flst_uborn%flst == GLUON) .or. &
        any (sregion%flst_uborn%flst == PHOTON)
contains
    subroutine debug_input_values()
        if (debug_on) call msg_debug2 (D_SUBTRACTION, "singular_region_init")
        if (debug2_active (D_SUBTRACTION)) then
            print *, 'alr = ', alr
            print *, 'mult = ', mult
            print *, 'i_res = ', i_res
            call flst_real%write ()
            call flst_uborn%write ()
            print *, 'emitter = ', emitter
            call print_equivalence_matrix (ftuples, equivalences)
        end if
    end subroutine debug_input_values
end subroutine singular_region_init

```

```

<fks regions: singular region: TBP>+=
procedure :: write => singular_region_write

```

```

<fks regions: procedures>+=
subroutine singular_region_write (sregion, unit, maxnregions)
    class(singular_region_t), intent(in) :: sregion

```

```

integer, intent(in), optional :: unit
integer, intent(in), optional :: maxnregions
character(len=7), parameter :: flst_format = "(I3,A1)"
character(len=7), parameter :: ireg_space_format = "(7X,A1)"
integer :: nreal, nborn, i, u, mr
integer :: nleft, nright, nreg, nreg_diff
u = given_output_unit (unit); if (u < 0) return
mr = sregion%nregions; if (present (maxnregions)) mr = maxnregions
nreal = size (sregion%flst_real%flst)
nborn = size (sregion%flst_uborn%flst)
call write_vline (u)
write (u, '(A1)', advance = 'no') '['
do i = 1, nreal - 1
    write (u, flst_format, advance = 'no') sregion%flst_real%flst(i), ', '
end do
write (u, flst_format, advance = 'no') sregion%flst_real%flst(nreal), ']'
call write_vline (u)
write (u, '(I6)', advance = 'no') sregion%real_index
call write_vline (u)
write (u, '(I3)', advance = 'no') sregion%emitter
call write_vline (u)
write (u, '(I3)', advance = 'no') sregion%mult
call write_vline (u)
write (u, '(I4)', advance = 'no') sregion%nregions
call write_vline (u)
if (sregion%i_res > 0) then
    write (u, '(I3)', advance = 'no') sregion%i_res
    call write_vline (u)
end if
nreg = sregion%nregions
if (nreg == mr) then
    nleft = 0
    nright = 0
else
    nreg_diff = mr - nreg
    nleft = nreg_diff / 2
    if (mod(nreg_diff, 2) == 0) then
        nright = nleft
    else
        nright = nleft + 1
    end if
end if
if (nleft > 0) then
    do i = 1, nleft
        write(u, ireg_space_format, advance='no') ' '
    end do
end if
write (u, '(A)', advance = 'no') char (ftuple_string (sregion%ftuples, .false.))
call write_vline (u)
write (u, '(A1)', advance = 'no') '['
do i = 1, nborn - 1
    write(u, flst_format, advance = 'no') sregion%flst_uborn%flst(i), ', '
end do
write (u, flst_format, advance = 'no') sregion%flst_uborn%flst(nborn), ']'

```

```

call write_vline (u)
write (u, '(I7)', advance = 'no') sregion%uborn_index
call write_vline (u)
if (sregion%nlo_correction_type == "EW") then
  write (u, '(A3)', advance = 'no') 'ew'
else if (sregion%nlo_correction_type == "QCD") then
  write (u, '(A4)', advance = 'no') 'qcd'
else
  write (u, '(A5)', advance = 'no') 'none'
end if
write (u, '(A)')
end subroutine singular_region_write

```

<fks regions: singular region: TBP>+≡

```

procedure :: write_latex => singular_region_write_latex

```

<fks regions: procedures>+≡

```

subroutine singular_region_write_latex (region, unit)
  class(singular_region_t), intent(in) :: region
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(I2,A3,A,A3,I2,A3,I1,A3,I1,A3,A,A3,I2,A3,A,A3)" &
    region%alr, " & ", char (region%flst_real%to_string ()), &
    " & ", region%real_index, " & ", region%emitter, " & ", &
    region%mult, " & ", char (ftuple_string (region%ftuples, .true.)), &
    " & ", region%uborn_index, " & ", char (region%flst_uborn%to_string ()), &
    " \\")
end subroutine singular_region_write_latex

```

In case of a $g \rightarrow gg$ splitting, the factor

$$\frac{2E_{\text{em}}}{E_{\text{em}} + E_{\text{rad}}}$$

is multiplied to the real matrix element. This way, the symmetry of the splitting is used and only one singular region has to be taken into account. However, the factor ensures that there is only a soft singularity if the radiated parton becomes soft.

<fks regions: singular region: TBP>+≡

```

procedure :: set_splitting_info => singular_region_set_splitting_info

```

<fks regions: procedures>+≡

```

subroutine singular_region_set_splitting_info (region, n_in)
  class(singular_region_t), intent(inout) :: region
  integer, intent(in) :: n_in
  integer :: i1, i2
  integer :: reg
  region%double_fsr = .false.
  region%soft_divergence = .false.
  associate (ftuple => region%ftuples)
    do reg = 1, region%nregions
      call ftuple(reg)%get (i1, i2)
      if (i1 /= region%emitter .or. i2 /= region%flst_real%nlegs) then

```

```

        cycle
    else
        if (ftuple(reg)%splitting_type == V_TO_VV .or. &
            ftuple(reg)%splitting_type == F_TO_FV ) then
            region%soft_divergence = .true.
        end if

        if (i1 == 0) then
            region%coll_divergence = .not. all (region%flst_real%massive(1:n_in))
        else
            region%coll_divergence = .not. region%flst_real%massive(i1)
        end if

        if (ftuple(reg)%splitting_type == V_TO_VV) then
            if (all (ftuple(reg)%ireg > n_in)) &
                region%double_fsr = all (is_gluon (region%flst_real%flst(ftuple(reg)%ireg)))
            exit
        else if (ftuple(reg)%splitting_type == UNDEFINED_SPLITTING) then
            call msg_fatal ("All splittings should be defined!")
        end if
    end if
end do
if (.not. region%soft_divergence .and. .not. region%coll_divergence) &
    call msg_fatal ("Singular region defined without divergence!")
end associate
end subroutine singular_region_set_splitting_info

```

<fks regions: singular region: TBP>+≡
 procedure :: double_fsr_factor => singular_region_double_fsr_factor

<fks regions: procedures>+≡
 function singular_region_double_fsr_factor (region, p) result (val)
 class(singular_region_t), intent(in) :: region
 type(vector4_t), intent(in), dimension(:) :: p
 real(default) :: val
 real(default) :: E_rad, E_em
 if (region%double_fsr) then
 E_em = energy (p(region%emitter))
 E_rad = energy (p(region%flst_real%nlegs))
 val = two * E_em / (E_em + E_rad)
 else
 val = one
 end if
 end function singular_region_double_fsr_factor

<fks regions: singular region: TBP>+≡
 procedure :: has_soft_divergence => singular_region_has_soft_divergence

<fks regions: procedures>+≡
 function singular_region_has_soft_divergence (region) result (div)
 logical :: div
 class(singular_region_t), intent(in) :: region
 div = region%soft_divergence
 end function singular_region_has_soft_divergence

```

<fks regions: singular region: TBP>+≡
  procedure :: has_collinear_divergence => &
    singular_region_has_collinear_divergence

<fks regions: procedures>+≡
  function singular_region_has_collinear_divergence (region) result (div)
    logical :: div
    class(singular_region_t), intent(in) :: region
    div = region%coll_divergence
  end function singular_region_has_collinear_divergence

<fks regions: singular region: TBP>+≡
  procedure :: has_identical_ftuples => singular_region_has_identical_ftuples

<fks regions: procedures>+≡
  elemental function singular_region_has_identical_ftuples (sregion) result (value)
    logical :: value
    class(singular_region_t), intent(in) :: sregion
    integer :: alr
    value = .false.
    do alr = 1, sregion%nregions
      value = value .or. (count (sregion%ftuples(alr) == sregion%ftuples) > 1)
    end do
  end function singular_region_has_identical_ftuples

<fks regions: interfaces>+≡
  interface assignment(=)
    module procedure singular_region_assign
  end interface

<fks regions: procedures>+≡
  subroutine singular_region_assign (reg_out, reg_in)
    type(singular_region_t), intent(out) :: reg_out
    type(singular_region_t), intent(in) :: reg_in
    reg_out%alr = reg_in%alr
    reg_out%i_res = reg_in%i_res
    reg_out%flst_real = reg_in%flst_real
    reg_out%flst_uborn = reg_in%flst_uborn
    reg_out%mult = reg_in%mult
    reg_out%emitter = reg_in%emitter
    reg_out%nregions = reg_in%nregions
    reg_out%real_index = reg_in%real_index
    reg_out%uborn_index = reg_in%uborn_index
    reg_out%double_fsr = reg_in%double_fsr
    reg_out%soft_divergence = reg_in%soft_divergence
    reg_out%coll_divergence = reg_in%coll_divergence
    reg_out%nlo_correction_type = reg_in%nlo_correction_type
    if (allocated (reg_in%ftuples)) then
      allocate (reg_out%ftuples (size (reg_in%ftuples)))
      reg_out%ftuples = reg_in%ftuples
    else
      call msg_bug ("singular_region_assign: Trying to copy a singular region without allocated f
    end if
  end subroutine singular_region_assign

```


Two singular regions match if they would produce the same amplitude. For this we have to check that their real and underlying Born flavor structures are equivalent, as determined by the `prc_core`. However, since there are more aspects of a singular region that make it unique, we have to check other attributes as well.

```

<fks regions: interfaces>+≡
  interface operator(.match.)
    module procedure singular_region_match
  end interface

<fks regions: procedures>+≡
  function singular_region_match (reg1, reg2) result (match)
    type(singular_region_t), intent(in) :: reg1, reg2
    logical :: match
    match = all ([reg1%flst_real%eqv_index, reg2%flst_real%eqv_index] > 0)
    match = match .and. (reg1%flst_real%eqv_index == reg2%flst_real%eqv_index)
    match = match .and. (reg1%flst_uborn%eqv_index == reg2%flst_uborn%eqv_index)
    match = match .and. (reg1%mult == reg2%mult)
    match = match .and. (reg1%emitter == reg2%emitter)
    match = match .and. (reg1%nregions == reg2%nregions)
    match = match .and. (reg1%double_fsr .eqv. reg2%double_fsr)
    match = match .and. (reg1%soft_divergence .eqv. reg2%soft_divergence)
    match = match .and. (reg1%coll_divergence .eqv. reg2%coll_divergence)
    match = match .and. (char (reg1%nlo_correction_type) == char (reg2%nlo_correction_type))
    if (match) match = match .and. (all (reg1%ftuples == reg2%ftuples))
  end function singular_region_match

<fks regions: types>+≡
  type :: resonance_mapping_t
    type(resonance_history_t), dimension(:), allocatable :: res_histories
    integer, dimension(:), allocatable :: alr_to_i_res
    integer, dimension(:,:), allocatable :: i_res_to_alr
    type(vector4_t), dimension(:), allocatable :: p_res
  contains
    <fks regions: resonance mapping: TBP>
  end type resonance_mapping_t

```

Testing: Init resonance mapping for $\mu\mu b\bar{b}$ final state.

```

<fks regions: resonance mapping: TBP>≡
  procedure :: init => resonance_mapping_init

<fks regions: procedures>+≡
  subroutine resonance_mapping_init (res_map, res_hist)
    class(resonance_mapping_t), intent(inout) :: res_map
    type(resonance_history_t), intent(in), dimension(:) :: res_hist
    integer :: n_hist, i_hist1, i_hist2, n_contributors
    n_contributors = 0
    n_hist = size (res_hist)
    allocate (res_map%res_histories (n_hist))
    do i_hist1 = 1, n_hist
      if (i_hist1 + 1 <= n_hist) then
        do i_hist2 = i_hist1 + 1, n_hist
          if (.not. (res_hist(i_hist1) .contains. res_hist(i_hist2))) &

```

```

        n_contributors = n_contributors + res_hist(i_hist2)%n_resonances
    end do
    else
        n_contributors = n_contributors + res_hist(i_hist1)%n_resonances
    end if
end do
allocate (res_map%p_res (n_contributors))
res_map%res_histories = res_hist
res_map%p_res = vector4_null
end subroutine resonance_mapping_init

```

(fks regions: resonance mapping: TBP)+≡

```

procedure :: set_alr_to_i_res => resonance_mapping_set_alr_to_i_res

```

(fks regions: procedures)+≡

```

subroutine resonance_mapping_set_alr_to_i_res (res_map, regions, alr_new_to_old)
    class(resonance_mapping_t), intent(inout) :: res_map
    type(singular_region_t), intent(in), dimension(:) :: regions
    integer, intent(out), dimension(:), allocatable :: alr_new_to_old
    integer :: alr, i_res
    integer :: alr_new, n_alr_res
    integer :: k
    if (debug_on) call msg_debug (D_SUBTRACTION, "resonance_mapping_set_alr_to_i_res")
    n_alr_res = 0
    do alr = 1, size (regions)
        do i_res = 1, size (res_map%res_histories)
            if (res_map%res_histories(i_res)%contains_leg (regions(alr)%emitter)) &
                n_alr_res = n_alr_res + 1
        end do
    end do

    allocate (res_map%alr_to_i_res (n_alr_res))
    allocate (res_map%i_res_to_alr (size (res_map%res_histories), 10))
    res_map%i_res_to_alr = 0
    allocate (alr_new_to_old (n_alr_res))
    alr_new = 1
    do alr = 1, size (regions)
        do i_res = 1, size (res_map%res_histories)
            if (res_map%res_histories(i_res)%contains_leg (regions(alr)%emitter)) then
                res_map%alr_to_i_res (alr_new) = i_res
                alr_new_to_old (alr_new) = alr
                alr_new = alr_new + 1
            end if
        end do
    end do

    do i_res = 1, size (res_map%res_histories)
        k = 1
        do alr = 1, size (regions)
            if (res_map%res_histories(i_res)%contains_leg (regions(alr)%emitter)) then
                res_map%i_res_to_alr (i_res, k) = alr
                k = k + 1
            end if
        end do
    end do

```

```

        end do
        if (debug_active (D_SUBTRACTION)) then
            print *, 'i_res_to_alr:'
            do i_res = 1, size(res_map%i_res_to_alr, dim=1)
                print *, res_map%i_res_to_alr (i_res, :)
            end do
            print *, 'alr_new_to_old:', alr_new_to_old
        end if
    end subroutine resonance_mapping_set_alr_to_i_res

<fks regions: resonance mapping: TBP>+≡
    procedure :: get_resonance_history => resonance_mapping_get_resonance_history

<fks regions: procedures>+≡
    function resonance_mapping_get_resonance_history (res_map, alr) result (res_hist)
        type(resonance_history_t) :: res_hist
        class(resonance_mapping_t), intent(in) :: res_map
        integer, intent(in) :: alr
        res_hist = res_map%res_histories(res_map%alr_to_i_res (alr))
    end function resonance_mapping_get_resonance_history

<fks regions: resonance mapping: TBP>+≡
    procedure :: write => resonance_mapping_write

<fks regions: procedures>+≡
    subroutine resonance_mapping_write (res_map)
        class(resonance_mapping_t), intent(in) :: res_map
        integer :: i_res
        do i_res = 1, size (res_map%res_histories)
            call res_map%res_histories(i_res)%write ()
        end do
    end subroutine resonance_mapping_write

<fks regions: resonance mapping: TBP>+≡
    procedure :: get_resonance_value => resonance_mapping_get_resonance_value

<fks regions: procedures>+≡
    function resonance_mapping_get_resonance_value (res_map, i_res, p, i_gluon) result (p_map)
        real(default) :: p_map
        class(resonance_mapping_t), intent(in) :: res_map
        integer, intent(in) :: i_res
        type(vector4_t), intent(in), dimension(:) :: p
        integer, intent(in), optional :: i_gluon
        p_map = res_map%res_histories(i_res)%mapping (p, i_gluon)
    end function resonance_mapping_get_resonance_value

<fks regions: resonance mapping: TBP>+≡
    procedure :: get_resonance_all => resonance_mapping_get_resonance_all

<fks regions: procedures>+≡
    function resonance_mapping_get_resonance_all (res_map, alr, p, i_gluon) result (p_map)
        real(default) :: p_map
        class(resonance_mapping_t), intent(in) :: res_map
        integer, intent(in) :: alr

```

```

type(vector4_t), intent(in), dimension(:) :: p
integer, intent(in), optional :: i_gluon
integer :: i_res
p_map = zero
do i_res = 1, size (res_map%res_histories)
    associate (res => res_map%res_histories(i_res))
        if (any (res_map%i_res_to_alr (i_res, :) == alr)) &
            p_map = p_map + res%mapping (p, i_gluon)
        end associate
    end do
end function resonance_mapping_get_resonance_all

<fks regions: resonance mapping: TBP>+≡
procedure :: get_weight => resonance_mapping_get_weight

<fks regions: procedures>+≡
function resonance_mapping_get_weight (res_map, alr, p) result (pfr)
    real(default) :: pfr
    class(resonance_mapping_t), intent(in) :: res_map
    integer, intent(in) :: alr
    type(vector4_t), intent(in), dimension(:) :: p
    real(default) :: sumpfr
    integer :: i_res
    sumpfr = zero
    do i_res = 1, size (res_map%res_histories)
        sumpfr = sumpfr + res_map%get_resonance_value (i_res, p)
    end do
    pfr = res_map%get_resonance_value (res_map%alr_to_i_res (alr), p) / sumpfr
end function resonance_mapping_get_weight

<fks regions: resonance mapping: TBP>+≡
procedure :: get_resonance_alr => resonance_mapping_get_resonance_alr

<fks regions: procedures>+≡
function resonance_mapping_get_resonance_alr (res_map, alr, p, i_gluon) result (p_map)
    real(default) :: p_map
    class(resonance_mapping_t), intent(in) :: res_map
    integer, intent(in) :: alr
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in), optional :: i_gluon
    integer :: i_res
    i_res = res_map%alr_to_i_res (alr)
    p_map = res_map%res_histories(i_res)%mapping (p, i_gluon)
end function resonance_mapping_get_resonance_alr

<fks regions: interfaces>+≡
interface assignment(=)
    module procedure resonance_mapping_assign
end interface

<fks regions: procedures>+≡
subroutine resonance_mapping_assign (res_map_out, res_map_in)
    type(resonance_mapping_t), intent(out) :: res_map_out

```

```

type(resonance_mapping_t), intent(in) :: res_map_in
if (allocated (res_map_in%res_histories)) then
  allocate (res_map_out%res_histories (size (res_map_in%res_histories)))
  res_map_out%res_histories = res_map_in%res_histories
end if
if (allocated (res_map_in%alr_to_i_res)) then
  allocate (res_map_out%alr_to_i_res (size (res_map_in%alr_to_i_res)))
  res_map_out%alr_to_i_res = res_map_in%alr_to_i_res
end if
if (allocated (res_map_in%i_res_to_alr)) then
  allocate (res_map_out%i_res_to_alr &
    (size (res_map_in%i_res_to_alr, 1), size (res_map_in%i_res_to_alr, 2)))
  res_map_out%i_res_to_alr = res_map_in%i_res_to_alr
end if
if (allocated (res_map_in%p_res)) then
  allocate (res_map_out%p_res (size (res_map_in%p_res)))
  res_map_out%p_res = res_map_in%p_res
end if
end subroutine resonance_mapping_assign

```

Every FKS mapping should store the $\sum_{\alpha} d_{ij}^{-1}$ and $\sum_{\alpha} d_{ij,\text{soft}}^{-1}$. Also we keep the option open to use a normlization factor, which ensures $\sum_{\alpha} S_{\alpha} = 1$.

```

⟨fks regions: types⟩+≡
  type, abstract :: fks_mapping_t
    real(default) :: sumdijs
    real(default) :: sumdijs_soft
    logical :: pseudo_isr = .false.
    real(default) :: normalization_factor = one
  contains
  ⟨fks regions: fks mapping: TBP⟩
end type fks_mapping_t

⟨fks regions: public⟩+≡
  public :: fks_mapping_default_t

⟨fks regions: types⟩+≡
  type, extends (fks_mapping_t) :: fks_mapping_default_t
    real(default) :: exp_1, exp_2
    integer :: n_in
  contains
  ⟨fks regions: fks mapping default: TBP⟩
end type fks_mapping_default_t

⟨fks regions: public⟩+≡
  public :: fks_mapping_resonances_t

⟨fks regions: types⟩+≡
  type, extends (fks_mapping_t) :: fks_mapping_resonances_t
    real(default) :: exp_1, exp_2
    type(resonance_mapping_t) :: res_map
    integer :: i_con = 0
  contains
  ⟨fks regions: fks mapping resonances: TBP⟩

```

```

end type fks_mapping_resonances_t

<fks regions: public>+≡
public :: operator(.equiv.)
public :: operator(.equivtag.)

<fks regions: interfaces>+≡
interface operator(.equiv.)
  module procedure flv_structure_equivalent_no_tag
end interface

interface operator(.equivtag.)
  module procedure flv_structure_equivalent_with_tag
end interface

interface assignment(=)
  module procedure flv_structure_assign_flv
  module procedure flv_structure_assign_integer
end interface

<fks regions: public>+≡
public :: region_data_t

<fks regions: types>+≡
type :: region_data_t
  type(singular_region_t), dimension(:), allocatable :: regions
  type(flv_structure_t), dimension(:), allocatable :: flv_born
  type(flv_structure_t), dimension(:), allocatable :: flv_real
  integer, dimension(:), allocatable :: eqv_flv_index_born
  integer, dimension(:), allocatable :: eqv_flv_index_real
  integer, dimension(:), allocatable :: emitters
  integer :: n_regions = 0
  integer :: n_emitters = 0
  integer :: n_flv_born = 0
  integer :: n_flv_real = 0
  integer :: n_in = 0
  integer :: n_legs_born = 0
  integer :: n_legs_real = 0
  integer :: n_phs = 0
  integer :: alpha_power = 0
  integer :: alphas_power = 0
  type(string_t) :: nlo_correction_type
  class(fks_mapping_t), allocatable :: fks_mapping
  integer, dimension(:), allocatable :: resonances
  type(resonance_contributors_t), dimension(:), allocatable :: alr_contributors
  integer, dimension(:), allocatable :: alr_to_i_contributor
  integer, dimension(:), allocatable :: i_phs_to_i_con
contains
  <fks regions: reg data: TBP>
end type region_data_t

<fks regions: reg data: TBP>≡
procedure :: allocate_fks_mappings => region_data_allocate_fks_mappings

```

```

(fks regions: procedures)+≡
subroutine region_data_allocate_fks_mappings (reg_data, mapping_type)
  class(region_data_t), intent(inout) :: reg_data
  integer, intent(in) :: mapping_type

  select case (mapping_type)
  case (FKS_DEFAULT)
    allocate (fks_mapping_default_t :: reg_data%fks_mapping)
  case (FKS_RESONANCES)
    allocate (fks_mapping_resonances_t :: reg_data%fks_mapping)
  case default
    call msg_fatal ("Init region_data: FKS mapping not implemented!")
  end select
end subroutine region_data_allocate_fks_mappings

(fks regions: reg data: TBP)+≡
procedure :: init => region_data_init

(fks regions: procedures)+≡
subroutine region_data_init (reg_data, n_in, model, flavor_born, &
  flavor_real, nlo_correction_type, alpha_pow, alphas_pow)
  class(region_data_t), intent(out) :: reg_data
  integer, intent(in) :: n_in, alpha_pow, alphas_pow
  type(model_t), intent(in) :: model
  integer, intent(in), dimension(:,:) :: flavor_born, flavor_real
  integer, dimension(:,:), allocatable :: flv_real_tmp
  type(ftuple_list_t), dimension(:), allocatable :: ftuples
  integer, dimension(:), allocatable :: emitter
  type(flv_structure_t), dimension(:), allocatable :: flst_alr
  integer :: i, n_real
  integer :: n_flv_real_before_check
  type(string_t), intent(in) :: nlo_correction_type
  reg_data%n_in = n_in
  reg_data%alpha_power = alpha_pow
  reg_data%alphas_power = alphas_pow
  reg_data%n_flv_born = size (flavor_born, dim = 2)
  reg_data%n_legs_born = size (flavor_born, dim = 1)
  reg_data%n_legs_real = reg_data%n_legs_born + 1
  reg_data%nlo_correction_type = nlo_correction_type
  n_flv_real_before_check = size (flavor_real, dim = 2)
  allocate (reg_data%flv_born (reg_data%n_flv_born))
  allocate (flv_real_tmp (reg_data%n_legs_real, n_flv_real_before_check))
  do i = 1, reg_data%n_flv_born
    call reg_data%flv_born(i)%init (flavor_born (:, i), n_in)
  end do
  n_real = 0
  do i = 1, n_flv_real_before_check
    if (nlo_correction_type == "EW") then
      if (.not. (query_coupling_powers &
        (flavor_real (:, i), reg_data%alpha_power + 1, reg_data%alphas_power))) cycle
    end if
    n_real = n_real + 1
    flv_real_tmp (:, n_real) = flavor_real (:, i)
  end do

```

```

allocate (reg_data%flv_real (n_real))
do i = 1, n_real
    call reg_data%flv_real(i)%init (flv_real_tmp (:, i), n_in)
end do

call reg_data%find_regions (model, ftuples, emitter, flst_alr)
call reg_data%init_singular_regions (ftuples, emitter, flst_alr, nlo_correction_type)
reg_data%n_flv_real = maxval (reg_data%regions%real_index)
call reg_data%find_emitters ()
call reg_data%set_mass_color_and_charge (model)
call reg_data%set_splitting_info ()
end subroutine region_data_init

<fks regions: reg data: TBP>+≡
procedure :: init_resonance_information => region_data_init_resonance_information

<fks regions: procedures>+≡
subroutine region_data_init_resonance_information (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    call reg_data%enlarge_singular_regions_with_resonances ()
    call reg_data%find_resonances ()
end subroutine region_data_init_resonance_information

<fks regions: reg data: TBP>+≡
procedure :: set_resonance_mappings => region_data_set_resonance_mappings

<fks regions: procedures>+≡
subroutine region_data_set_resonance_mappings (reg_data, resonance_histories)
    class(region_data_t), intent(inout) :: reg_data
    type(resonance_history_t), intent(in), dimension(:) :: resonance_histories
    select type (map => reg_data%fks_mapping)
        type is (fks_mapping_resonances_t)
            call map%res_map%init (resonance_histories)
        end select
    end select
end subroutine region_data_set_resonance_mappings

<fks regions: reg data: TBP>+≡
procedure :: setup_fks_mappings => region_data_setup_fks_mappings

<fks regions: procedures>+≡
subroutine region_data_setup_fks_mappings (reg_data, template, n_in)
    class(region_data_t), intent(inout) :: reg_data
    type(fks_template_t), intent(in) :: template
    integer, intent(in) :: n_in
    call reg_data%allocate_fks_mappings (template%mapping_type)
    select type (map => reg_data%fks_mapping)
        type is (fks_mapping_default_t)
            call map%set_parameter (n_in, template%fks_dij_exp1, template%fks_dij_exp2)
        end select
    end select
end subroutine region_data_setup_fks_mappings

```


So far, we have only created singular regions for a non-resonant case. When resonance mappings are required, we have more singular regions, since they must now be identified by their emitter-resonance pair index, where the emitter must be compatible with the resonance.

```

(fks regions: reg data: TBP)+≡
  procedure :: enlarge_singular_regions_with_resonances &
    => region_data_enlarge_singular_regions_with_resonances

(fks regions: procedures)+≡
  subroutine region_data_enlarge_singular_regions_with_resonances (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    integer :: alr
    integer, dimension(:), allocatable :: alr_new_to_old
    integer :: n_alr_new
    type(singular_region_t), dimension(:), allocatable :: save_regions
    if (debug_on) call msg_debug (D_SUBTRACTION, "region_data_enlarge_singular_regions_with_resona
    call debug_input_values ()
    select type (fks_mapping => reg_data%fks_mapping)
    type is (fks_mapping_default_t)
      return
    type is (fks_mapping_resonances_t)
      allocate (save_regions (reg_data%n_regions))
      do alr = 1, reg_data%n_regions
        save_regions(alr) = reg_data%regions(alr)
      end do

      associate (res_map => fks_mapping%res_map)
        call res_map%set_alr_to_i_res (reg_data%regions, alr_new_to_old)
        deallocate (reg_data%regions)
        n_alr_new = size (alr_new_to_old)
        reg_data%n_regions = n_alr_new
        allocate (reg_data%regions (n_alr_new))
        do alr = 1, n_alr_new
          reg_data%regions(alr) = save_regions(alr_new_to_old (alr))
          reg_data%regions(alr)%i_res = res_map%alr_to_i_res (alr)
        end do
      end associate
    end select

contains

    subroutine debug_input_values ()
      if (debug2_active (D_SUBTRACTION)) then
        call reg_data%write ()
      end if
    end subroutine debug_input_values

  end subroutine region_data_enlarge_singular_regions_with_resonances

(fks regions: reg data: TBP)+≡
  procedure :: set_isr_pseudo_regions => region_data_set_isr_pseudo_regions

(fks regions: procedures)+≡
  subroutine region_data_set_isr_pseudo_regions (reg_data)

```

```

class(region_data_t), intent(inout) :: reg_data
integer :: alr
integer :: n_alr_new
!!! Subroutine called for threshold factorization ->
!!! Size of singular regions at this point is fixed
type(singular_region_t), dimension(2) :: save_regions
integer, dimension(4) :: alr_new_to_old
do alr = 1, reg_data%n_regions
    save_regions(alr) = reg_data%regions(alr)
end do
n_alr_new = reg_data%n_regions * 2
alr_new_to_old = [1, 1, 2, 2]
deallocate (reg_data%regions)
allocate (reg_data%regions (n_alr_new))
reg_data%n_regions = n_alr_new
do alr = 1, n_alr_new
    reg_data%regions(alr) = save_regions(alr_new_to_old (alr))
    call add_pseudo_emitters (reg_data%regions(alr))
    if (mod (alr, 2) == 0) reg_data%regions(alr)%pseudo_isr = .true.
end do
contains
subroutine add_pseudo_emitters (sregion)
    type(singular_region_t), intent(inout) :: sregion
    type(ftuple_t), dimension(2) :: ftuples_save
    integer :: alr
    do alr = 1, 2
        ftuples_save(alr) = sregion%ftuples(alr)
    end do
    deallocate (sregion%ftuples)
    sregion%nregions = sregion%nregions * 2
    allocate (sregion%ftuples (sregion%nregions))
    do alr = 1, sregion%nregions
        sregion%ftuples(alr) = ftuples_save (alr_new_to_old(alr))
        if (mod (alr, 2) == 0) sregion%ftuples(alr)%pseudo_isr = .true.
    end do
end subroutine add_pseudo_emitters
end subroutine region_data_set_isr_pseudo_regions

```

This subroutine splits up the ftuple-list of the singular regions into interference-free lists, i.e. lists which only contain the same emitter. This is relevant for factorized NLO calculations. In the current implementation, it is hand-tailored for the threshold computation, but should be generalized further in the future.

<fks regions: reg data: TBP>+≡

```

procedure :: split_up_interference_regions_for_threshold => &
    region_data_split_up_interference_regions_for_threshold

```

<fks regions: procedures>+≡

```

subroutine region_data_split_up_interference_regions_for_threshold (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    integer :: alr, i_ftuple
    integer :: current_emitter
    integer :: i1, i2
    integer :: n_new_reg
    type(ftuple_t), dimension(2) :: ftuples

```

```

do alr = 1, reg_data%n_regions
  associate (region => reg_data%regions(alr))
    current_emitter = region%emitter
    n_new_reg = 0
    do i_ftuple = 1, region%nregions
      call region%ftuples(i_ftuple)%get (i1, i2)
      if (i1 == current_emitter) then
        n_new_reg = n_new_reg + 1
        ftuples(n_new_reg) = region%ftuples(i_ftuple)
      end if
    end do
    deallocate (region%ftuples)
    allocate (region%ftuples(n_new_reg))
    region%ftuples = ftuples (1 : n_new_reg)
    region%nregions = n_new_reg
  end associate
end do
reg_data%fks_mapping%normalization_factor = 0.5_default
end subroutine region_data_split_up_interference_regions_for_threshold

```

<fks regions: reg data: TBP>+≡

```

procedure :: set_mass_color_and_charge => region_data_set_mass_color_and_charge

```

<fks regions: procedures>+≡

```

subroutine region_data_set_mass_color_and_charge (reg_data, model)
  class(region_data_t), intent(inout) :: reg_data
  type(model_t), intent(in) :: model
  integer :: i
  do i = 1, reg_data%n_regions
    associate (region => reg_data%regions(i))
      call region%flst_uborn%init_mass_color_and_charge (model)
      call region%flst_real%init_mass_color_and_charge (model)
    end associate
  end do
  do i = 1, reg_data%n_flv_born
    call reg_data%flv_born(i)%init_mass_color_and_charge (model)
  end do
  do i = 1, size (reg_data%flv_real)
    call reg_data%flv_real(i)%init_mass_color_and_charge (model)
  end do
end subroutine region_data_set_mass_color_and_charge

```

<fks regions: reg data: TBP>+≡

```

procedure :: uses_resonances => region_data_uses_resonances

```

<fks regions: procedures>+≡

```

function region_data_uses_resonances (reg_data) result (val)
  logical :: val
  class(region_data_t), intent(in) :: reg_data
  select type (fks_mapping => reg_data%fks_mapping)
    type is (fks_mapping_resonances_t)
      val = .true.
  class default
    val = .false.

```

```

end select
end function region_data_uses_resonances

```

Creates a list containing the emitter of each singular region.

```

(fks regions: reg data: TBP)+≡
  procedure :: get_emitter_list => region_data_get_emitter_list

(fks regions: procedures)+≡
  pure function region_data_get_emitter_list (reg_data) result (emitters)
    class(region_data_t), intent(in) :: reg_data
    integer, dimension(:), allocatable :: emitters
    integer :: i
    allocate (emitters (reg_data%n_regions))
    do i = 1, reg_data%n_regions
      emitters(i) = reg_data%regions(i)%emitter
    end do
  end function region_data_get_emitter_list

```

Returns the number of emitters not equal to 0 to avoid double counting between emitters 0, 1 and 2.

```

(fks regions: reg data: TBP)+≡
  procedure :: get_n_emitters_sc => region_data_get_n_emitters_sc

(fks regions: procedures)+≡
  function region_data_get_n_emitters_sc (reg_data) result (n_emitters_sc)
    class(region_data_t), intent(in) :: reg_data
    integer :: n_emitters_sc
    n_emitters_sc = count (reg_data%emitters /= 0)
  end function region_data_get_n_emitters_sc

```

```

(fks regions: reg data: TBP)+≡
  procedure :: get_associated_resonances => region_data_get_associated_resonances

(fks regions: procedures)+≡
  function region_data_get_associated_resonances (reg_data, emitter) result (res)
    integer, dimension(:), allocatable :: res
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: emitter
    integer :: alr, i
    integer :: n_res
    select type (fks_mapping => reg_data%fks_mapping)
    type is (fks_mapping_resonances_t)
      n_res = 0

      do alr = 1, reg_data%n_regions
        if (reg_data%regions(alr)%emitter == emitter) &
          n_res = n_res + 1
      end do

      if (n_res > 0) then
        allocate (res (n_res))
      else
        return
      end if
    end select
  end function region_data_get_associated_resonances

```

```

        i = 1

        do alr = 1, reg_data%n_regions
            if (reg_data%regions(alr)%emitter == emitter) then
                res (i) = fks_mapping%res_map%alr_to_i_res (alr)
                i = i + 1
            end if
        end do
    end select
end function region_data_get_associated_resonances

```

<fks regions: reg data: TBP>+≡

```

    procedure :: emitter_is_compatible_with_resonance => &
        region_data_emitter_is_compatible_with_resonance

```

<fks regions: procedures>+≡

```

    function region_data_emitter_is_compatible_with_resonance &
        (reg_data, i_res, emitter) result (compatible)
        logical :: compatible
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_res, emitter
        integer :: i_res_alr, alr
        compatible = .false.
        select type (fks_mapping => reg_data%fks_mapping)
        type is (fks_mapping_resonances_t)
            do alr = 1, reg_data%n_regions
                i_res_alr = fks_mapping%res_map%alr_to_i_res (alr)
                if (i_res_alr == i_res .and. reg_data%get_emitter(alr) == emitter) then
                    compatible = .true.
                    exit
                end if
            end do
        end select
    end function region_data_emitter_is_compatible_with_resonance

```

<fks regions: reg data: TBP>+≡

```

    procedure :: emitter_is_in_resonance => region_data_emitter_is_in_resonance

```

<fks regions: procedures>+≡

```

    function region_data_emitter_is_in_resonance (reg_data, i_res, emitter) result (exist)
        logical :: exist
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: i_res, emitter
        integer :: i
        exist = .false.
        select type (fks_mapping => reg_data%fks_mapping)
        type is (fks_mapping_resonances_t)
            associate (res_history => fks_mapping%res_map%res_histories(i_res))
                do i = 1, res_history%n_resonances
                    exist = exist .or. any (res_history%resonances(i)%contributors%c == emitter)
                end do
            end associate
        end select
    end function region_data_emitter_is_in_resonance

```

```

<fks regions: reg data: TBP>+≡
  procedure :: get_contributors => region_data_get_contributors

<fks regions: procedures>+≡
  subroutine region_data_get_contributors (reg_data, i_res, emitter, c, success)
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: i_res, emitter
    integer, intent(inout), dimension(:), allocatable :: c
    logical, intent(out) :: success
    integer :: i
    success = .false.
    select type (fks_mapping => reg_data%fks_mapping)
    type is (fks_mapping_resonances_t)
      associate (res_history => fks_mapping%res_map%res_histories (i_res))
        do i = 1, res_history%n_resonances
          if (any (res_history%resonances(i)%contributors%c == emitter)) then
            allocate (c (size (res_history%resonances(i)%contributors%c)))
            c = res_history%resonances(i)%contributors%c
            success = .true.
            exit
          end if
        end do
      end associate
    end select
  end subroutine region_data_get_contributors

<fks regions: reg data: TBP>+≡
  procedure :: get_emitter => region_data_get_emitter

<fks regions: procedures>+≡
  pure function region_data_get_emitter (reg_data, alr) result (emitter)
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: alr
    integer :: emitter
    emitter = reg_data%regions(alr)%emitter
  end function region_data_get_emitter

<fks regions: reg data: TBP>+≡
  procedure :: map_real_to_born_index => region_data_map_real_to_born_index

<fks regions: procedures>+≡
  function region_data_map_real_to_born_index (reg_data, real_index) result (uborn_index)
    integer :: uborn_index
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: real_index
    integer :: alr
    uborn_index = 0
    do alr = 1, size (reg_data%regions)
      if (reg_data%regions(alr)%real_index == real_index) then
        uborn_index = reg_data%regions(alr)%uborn_index
        exit
      end if
    end do
  end function region_data_map_real_to_born_index

```

```

(fks regions: reg data: TBP)+≡
generic :: get_flv_states_born => get_flv_states_born_single, get_flv_states_born_array
procedure :: get_flv_states_born_single => region_data_get_flv_states_born_single
procedure :: get_flv_states_born_array => region_data_get_flv_states_born_array

(fks regions: procedures)+≡
function region_data_get_flv_states_born_array (reg_data) result (flv_states)
    integer, dimension(:,:), allocatable :: flv_states
    class(region_data_t), intent(in) :: reg_data
    integer :: i_flv
    allocate (flv_states (reg_data%n_legs_born, reg_data%n_flv_born))
    do i_flv = 1, reg_data%n_flv_born
        flv_states (:, i_flv) = reg_data%flv_born(i_flv)%flst
    end do
end function region_data_get_flv_states_born_array

function region_data_get_flv_states_born_single (reg_data, i_flv) result (flv_states)
    integer, dimension(:), allocatable :: flv_states
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: i_flv
    allocate (flv_states (reg_data%n_legs_born))
    flv_states = reg_data%flv_born(i_flv)%flst
end function region_data_get_flv_states_born_single

(fks regions: reg data: TBP)+≡
generic :: get_flv_states_real => get_flv_states_real_single, get_flv_states_real_array
procedure :: get_flv_states_real_single => region_data_get_flv_states_real_single
procedure :: get_flv_states_real_array => region_data_get_flv_states_real_array

(fks regions: procedures)+≡
function region_data_get_flv_states_real_single (reg_data, i_flv) result (flv_states)
    integer, dimension(:), allocatable :: flv_states
    class(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: i_flv
    integer :: i_reg
    allocate (flv_states (reg_data%n_legs_real))
    do i_reg = 1, reg_data%n_regions
        if (i_flv == reg_data%regions(i_reg)%real_index) then
            flv_states = reg_data%regions(i_reg)%flst_real%flst
            exit
        end if
    end do
end function region_data_get_flv_states_real_single

function region_data_get_flv_states_real_array (reg_data) result (flv_states)
    integer, dimension(:,:), allocatable :: flv_states
    class(region_data_t), intent(in) :: reg_data
    integer :: i_flv
    allocate (flv_states (reg_data%n_legs_real, reg_data%n_flv_real))
    do i_flv = 1, reg_data%n_flv_real
        flv_states (:, i_flv) = reg_data%get_flv_states_real (i_flv)
    end do
end function region_data_get_flv_states_real_array

```

```

(fks regions: reg data: TBP)+≡
  procedure :: get_all_flv_states => region_data_get_all_flv_states

(fks regions: procedures)+≡
  subroutine region_data_get_all_flv_states (reg_data, flv_born, flv_real)
    class(region_data_t), intent(in) :: reg_data
    integer, dimension(:,:), allocatable, intent(out) :: flv_born, flv_real
    allocate (flv_born (reg_data%n_legs_born, reg_data%n_flv_born))
    flv_born = reg_data%get_flv_states_born ()
    allocate (flv_real (reg_data%n_legs_real, reg_data%n_flv_real))
    flv_real = reg_data%get_flv_states_real ()
  end subroutine region_data_get_all_flv_states

(fks regions: reg data: TBP)+≡
  procedure :: get_n_in => region_data_get_n_in

(fks regions: procedures)+≡
  function region_data_get_n_in (reg_data) result (n_in)
    integer :: n_in
    class(region_data_t), intent(in) :: reg_data
    n_in = reg_data%n_in
  end function region_data_get_n_in

(fks regions: reg data: TBP)+≡
  procedure :: get_n_legs_real => region_data_get_n_legs_real

(fks regions: procedures)+≡
  function region_data_get_n_legs_real (reg_data) result (n_legs)
    integer :: n_legs
    class(region_data_t), intent(in) :: reg_data
    n_legs = reg_data%n_legs_real
  end function region_data_get_n_legs_real

(fks regions: reg data: TBP)+≡
  procedure :: get_n_legs_born => region_data_get_n_legs_born

(fks regions: procedures)+≡
  function region_data_get_n_legs_born (reg_data) result (n_legs)
    integer :: n_legs
    class(region_data_t), intent(in) :: reg_data
    n_legs = reg_data%n_legs_born
  end function region_data_get_n_legs_born

(fks regions: reg data: TBP)+≡
  procedure :: get_n_flv_real => region_data_get_n_flv_real

(fks regions: procedures)+≡
  function region_data_get_n_flv_real (reg_data) result (n_flv)
    integer :: n_flv
    class(region_data_t), intent(in) :: reg_data
    n_flv = reg_data%n_flv_real
  end function region_data_get_n_flv_real

(fks regions: reg data: TBP)+≡
  procedure :: get_n_flv_born => region_data_get_n_flv_born

```



```

(fks regions: procedures)+≡
function region_data_get_n_flv_born (reg_data) result (n_flv)
  integer :: n_flv
  class(region_data_t), intent(in) :: reg_data
  n_flv = reg_data%n_flv_born
end function region_data_get_n_flv_born

```

Returns $S_i = \frac{1}{\mathcal{D}_{d_i}}$ or $S_{ij} = \frac{1}{\mathcal{D}_{d_{ij}}}$ for one particular singular region. At this point, the flavor array should be rearranged in such a way that the emitted particle is at the last position of the flavor structure list.

```

(fks regions: reg data: TBP)+≡
generic :: get_svalue => get_svalue_last_pos, get_svalue_ij
procedure :: get_svalue_last_pos => region_data_get_svalue_last_pos
procedure :: get_svalue_ij => region_data_get_svalue_ij

(fks regions: procedures)+≡
function region_data_get_svalue_ij (reg_data, p_real, alr, i, j, i_res) result (sval)
  class(region_data_t), intent(inout) :: reg_data
  type(vector4_t), intent(in), dimension(:) :: p_real
  integer, intent(in) :: alr, i, j
  integer, intent(in) :: i_res
  real(default) :: sval
  associate (map => reg_data%fks_mapping)
    call map%compute_sumdij (reg_data%regions(alr), p_real)
    select type (map)
      type is (fks_mapping_resonances_t)
        map%i_con = reg_data%alr_to_i_contributor (alr)
      end select
    map%pseudo_isr = reg_data%regions(alr)%pseudo_isr
    sval = map%svalue (p_real, i, j, i_res) * map%normalization_factor
  end associate
end function region_data_get_svalue_ij

function region_data_get_svalue_last_pos (reg_data, p, alr, emitter, i_res) result (sval)
  class(region_data_t), intent(inout) :: reg_data
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in) :: alr, emitter
  integer, intent(in) :: i_res
  real(default) :: sval
  sval = reg_data%get_svalue (p, alr, emitter, reg_data%n_legs_real, i_res)
end function region_data_get_svalue_last_pos

```

The same as above, but for the soft limit.

```

(fks regions: reg data: TBP)+≡
procedure :: get_svalue_soft => region_data_get_svalue_soft

(fks regions: procedures)+≡
function region_data_get_svalue_soft &
  (reg_data, p_born, p_soft, alr, emitter, i_res) result (sval)
  class(region_data_t), intent(inout) :: reg_data
  type(vector4_t), intent(in), dimension(:) :: p_born
  type(vector4_t), intent(in) :: p_soft
  integer, intent(in) :: alr, emitter, i_res

```

```

real(default) :: sval
associate (map => reg_data%fks_mapping)
  call map%compute_sumdij_soft (reg_data%regions(alr), p_born, p_soft)
  select type (map)
  type is (fks_mapping_resonances_t)
    map%i_con = reg_data%alr_to_i_contributor (alr)
  end select
  map%pseudo_isr = reg_data%regions(alr)%pseudo_isr
  sval = map%value_soft (p_born, p_soft, emitter, i_res) * map%normalization_factor
end associate
end function region_data_get_svalue_soft

```

This subroutine starts with a specification of N - and $N + 1$ -particle configurations, `flst_born` and `flst_real`, saved in `reg_data`. From these, it creates a list of fundamental tuples, a list of emitters and a list containing the $N + 1$ -particle configuration, rearranged in such a way that the emitter-radiation pair is last (`flst_alr`). For the $e^+ e^- \rightarrow u \bar{u} g$ - example, the generated objects are shown in table 27.2. Note that at this point, `flst_alr` is arranged in such a way that the emitter can only be equal to $n_{legs} - 1$ for final-state radiation or 0, 1, or 2 for initial-state radiation. Further, it occurs that regions can be equivalent. For example in table 27.2 the regions corresponding to `alr = 1` and `alr = 3` as well as `alr = 2` and `alr = 4` describe the same physics and are therefore equivalent.

```

<fks regions: reg_data: TBP>+≡
  procedure :: find_regions => region_data_find_regions

<fks regions: procedures>+≡
  subroutine region_data_find_regions &
    (reg_data, model, ftuples, emitters, flst_alr)
    class(region_data_t), intent(in) :: reg_data
    type(model_t), intent(in) :: model
    type(ftuple_list_t), intent(out), dimension(:), allocatable :: ftuples
    integer, intent(out), dimension(:), allocatable :: emitters
    type(flv_structure_t), intent(out), dimension(:), allocatable :: flst_alr
    type(ftuple_list_t), dimension(:,:), allocatable :: ftuples_tmp
    integer, dimension(:,:), allocatable :: ftuple_index
    integer :: n_born, n_real
    integer :: n_legreal
    integer :: i_born, i_real, i_ftuple
    integer :: last_registered_i_born, last_registered_i_real

    n_born = size (reg_data%flv_born)
    n_real = size (reg_data%flv_real)
    n_legreal = size (reg_data%flv_real(1)%flst)
    allocate (emitters (0))
    allocate (flst_alr (0))
    allocate (ftuples (0))
    i_ftuple = 0
    last_registered_i_born = 0; last_registered_i_real = 0

    do i_real = 1, n_real
      do i_born = 1, n_born
        call setup_flsts_emitters_and_ftuples_fsr &
          (i_real, i_born, i_ftuple, flst_alr, emitters, ftuples)

```

```

        call setup_flsts_emitters_and_ftuples_isr &
            (i_real, i_born, i_ftuple, flst_alr, emitters, ftuples)
    end do
end do

contains

function incr_i_ftuple_if_required (i_born, i_real, i_ftuple_in) result (i_ftuple)
    integer :: i_ftuple
    integer, intent(in) :: i_born, i_real, i_ftuple_in
    if (last_registered_i_born /= i_born .or. last_registered_i_real /= i_real) then
        last_registered_i_born = i_born
        last_registered_i_real = i_real
        i_ftuple = i_ftuple_in + 1
    else
        i_ftuple = i_ftuple_in
    end if
end function incr_i_ftuple_if_required

subroutine setup_flsts_emitters_and_ftuples_fsr &
    (i_real, i_born, i_ftuple, flst_alr, emitters, ftuples)
    integer, intent(in) :: i_real, i_born
    integer, intent(inout) :: i_ftuple
    type(flv_structure_t), intent(inout), dimension(:), allocatable :: flst_alr
    integer, intent(inout), dimension(:), allocatable :: emitters
    type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
    type(ftuple_list_t) :: ftuples_tmp
    type(flv_structure_t) :: flst_alr_tmp
    type(ftuple_t) :: current_ftuple
    integer :: leg1, leg2
    logical :: valid
    associate (flv_born => reg_data%flv_born(i_born), &
        flv_real => reg_data%flv_real(i_real))
    do leg1 = reg_data%n_in + 1, n_legreal
    do leg2 = leg1 + 1, n_legreal
        valid = flv_real%valid_pair(leg1, leg2, flv_born, model)
        if (valid) then
            if (is_vector(flv_real%flst(leg1)) .and. &
                is_fermion(flv_real%flst(leg2))) then
                flst_alr_tmp = create_alr (flv_real, &
                    reg_data%n_in, leg2, leg1)
            else
                flst_alr_tmp = create_alr (flv_real, &
                    reg_data%n_in, leg1, leg2)
            end if
            flst_alr = [flst_alr, flst_alr_tmp]
            emitters = [emitters, n_legreal - 1]
            call current_ftuple%set (leg1, leg2)
            call current_ftuple%determine_splitting_type_fsr &
                (flv_real, leg1, leg2)
            call current_ftuple%determine_sub_correction_type &
                (flv_born, flv_real, leg1, leg2)
            i_ftuple = incr_i_ftuple_if_required (i_born, i_real, i_ftuple)
            if (i_ftuple > size (ftuples)) then
                call ftuples_tmp%append (current_ftuple)
            end if
        end if
    end do
    end do
end subroutine setup_flsts_emitters_and_ftuples_fsr

```

```

        ftuples = [ftuples, ftuples_tmp]
    else
        call ftuples(i_ftuple)%append (current_ftuple)
    end if
end if
end do
end do
end associate
end subroutine setup_flsts_emitters_and_ftuples_fsr

subroutine setup_flsts_emitters_and_ftuples_isr &
    (i_real, i_born, i_ftuple, flst_alr, emitters, ftuples)
integer, intent(in) :: i_real, i_born
integer, intent(inout) :: i_ftuple
type(flv_structure_t), intent(inout), dimension(:), allocatable :: flst_alr
integer, intent(inout), dimension(:), allocatable :: emitters
type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
type(ftuple_list_t) :: ftuples_tmp
type(flv_structure_t) :: flst_alr_tmp
type(ftuple_t) :: current_ftuple
integer :: leg, emitter
logical :: valid1, valid2
associate (flv_born => reg_data%flv_born(i_born), &
    flv_real => reg_data%flv_real(i_real))
do leg = reg_data%n_in + 1, n_legreal
    valid1 = flv_real%valid_pair(1, leg, flv_born, model)
    if (reg_data%n_in > 1) then
        valid2 = flv_real%valid_pair(2, leg, flv_born, model)
    else
        valid2 = .false.
    end if
    if (valid1 .and. valid2) then
        emitter = 0
    else if (valid1 .and. .not. valid2) then
        emitter = 1
    else if (.not. valid1 .and. valid2) then
        emitter = 2
    else
        emitter = -1
    end if
    if (valid1.or. valid2) then
        flst_alr_tmp = create_alr (flv_real, reg_data%n_in, emitter, leg)
        flst_alr = [flst_alr, flst_alr_tmp]
        emitters = [emitters, emitter]
        call current_ftuple%set(emitter, leg)
        call current_ftuple%determine_splitting_type_isr &
            (flv_real, emitter, leg)
        call current_ftuple%determine_sub_correction_type &
            (flv_born, flv_real, emitter, leg)
        i_ftuple = incr_i_ftuple_if_required (i_born, i_real, i_ftuple)
        if (i_ftuple > size (ftuples)) then
            call ftuples_tmp%append (current_ftuple)
            ftuples = [ftuples, ftuples_tmp]
        else

```

```

        call ftuples(i_ftuple)%append (current_ftuple)
    end if
end if
end do
end associate
end subroutine setup_flsts_emitters_and_ftuples_isr

end subroutine region_data_find_regions

```

We transfer the mapping of flavor structures that lead to the same amplitude (with structure functions already accounted for!) to the Born and real `flv_structure` of each `singular_region`. We then use this information, besides other data of each `singular_region`, to determine which produce the same amplitude for the non-subtracted real and real subtraction terms and set up the equivalence index mapping for each region.

```

<fks regions: reg data: TBP>+≡
    procedure :: find_eqv_regions => region_data_find_eqv_regions

<fks regions: procedures>+≡
    subroutine region_data_find_eqv_regions (reg_data, optimize)
        class(region_data_t), intent(inout) :: reg_data
        logical, intent(in) :: optimize
        integer :: n_reg, alr1, alr2
        n_reg = reg_data%n_regions
        if (optimize) then
            do alr1 = 1, n_reg
                reg_data%regions(alr1)%flst_uborn%eqv_index = &
                    reg_data%eqv_flv_index_born(reg_data%regions(alr1)%uborn_index)
                reg_data%regions(alr1)%flst_real%eqv_index = &
                    reg_data%eqv_flv_index_real(reg_data%regions(alr1)%real_index)
            end do
            do alr1 = 1, n_reg
                do alr2 = 1, alr1
                    if (reg_data%regions(alr2) .match. reg_data%regions(alr1)) then
                        reg_data%regions(alr1)%eqv_index = alr2
                        exit
                    end if
                end do
            end do
        else
            do alr1 = 1, n_reg
                reg_data%regions(alr1)%eqv_index = alr1
            end do
        end if
    end subroutine region_data_find_eqv_regions

```

Creates singular regions according to table 27.1. It scans all regions in table 27.2 and records the real flavor structures. If they are equivalent, the flavor structure is not recorded, but the multiplicity of the present one is increased.

```

<fks regions: reg data: TBP>+≡
    procedure :: init_singular_regions => region_data_init_singular_regions

```

(fks regions: procedures)+≡

```

subroutine region_data_init_singular_regions &
    (reg_data, ftuples, emitter, flv_alr, nlo_correction_type)
    class(region_data_t), intent(inout) :: reg_data
    type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
    type(string_t), intent(in) :: nlo_correction_type
    type(string_t), dimension(:), allocatable :: nlo_correction_type_dyn
    integer :: n_independent_flv
    integer, intent(in), dimension(:) :: emitter
    type(flv_structure_t), intent(in), dimension(:) :: flv_alr
    type(flv_structure_t), dimension(:), allocatable :: flv_uborn, flv_alr_registered
    integer, dimension(:), allocatable :: mult
    integer, dimension(:), allocatable :: flst_emitter
    integer :: n_regions, maxregions
    integer, dimension(:), allocatable :: index
    integer :: i, i_flv, n_legs
    logical :: equiv, valid_fs_splitting, pure_corr_type, corr_type_valid, non_singular_reg
    integer :: i_first, i_reg, i_reg_prev
    integer, dimension(:), allocatable :: region_to_ftuple, alr_limits
    integer, dimension(:), allocatable :: equiv_index

    maxregions = size (emitter)
    n_legs = flv_alr(1)%nlegs

    allocate (flv_uborn (maxregions))
    allocate (flv_alr_registered (maxregions))
    allocate (mult (maxregions))
    mult = 0
    allocate (flst_emitter (maxregions))
    allocate (index (0))
    allocate (region_to_ftuple (maxregions))
    allocate (equiv_index (maxregions))
    allocate (nlo_correction_type_dyn (maxregions))

    call setup_region_mappings (n_independent_flv, alr_limits, region_to_ftuple)
    nlo_correction_type_dyn = nlo_correction_type
    i_first = 1
    i_reg = 1
    SCAN_FLAVORS: do i_flv = 1, n_independent_flv
        SCAN_FTUPLES: do i = i_first, i_first + alr_limits (i_flv) - 1
            equiv = .false.
            corr_type_valid = .true.
            non_singular_reg = .false.
            if (i == i_first) then
                flv_alr_registered(i_reg) = flv_alr(i)
                if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
                    nlo_correction_type_dyn (i_reg) = set_dynamic_correction_type (i)
                end if
                flv_uborn(i_reg) = flv_alr(i)%create_uborn (emitter(i), &
                    nlo_correction_type_dyn (i_reg))
                flst_emitter(i_reg) = emitter(i)
                equiv_index(i_reg) = region_to_ftuple(i)
                if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
                    corr_type_valid = (nlo_correction_type_dyn (i_reg) == "EW" .and. &

```

```

        query_coupling_powers (flv_uborn(i_reg)%flst, &
        reg_data%alpha_power, reg_data%alphas_power)) &
        .or. (nlo_correction_type_dyn (i_reg) == "QCD" .and. &
        query_coupling_powers (flv_uborn(i_reg)%flst, &
        reg_data%alpha_power + 1, reg_data%alphas_power - 1))
non_singular_reg = .not. corr_type_valid .and. &
        qcd_ew_interferences (flv_alr_registered(i_reg)%flst) &
        .and. .not. qcd_ew_interferences (flv_uborn(i_reg)%flst) &
        .and. nlo_correction_type_dyn (i_reg) == "QCD"
    if (non_singular_reg) nlo_correction_type_dyn (i_reg) = "none"
end if
if (corr_type_valid .or. non_singular_reg) then
    mult(i_reg) = mult(i_reg) + 1
    index = [index, region_to_real_index(ftuples, i)]
    i_reg = i_reg + 1
end if
else
    !!! Check for equivalent flavor structures
    do i_reg_prev = 1, i_reg - 1
        if (emitter(i) == flst_emitter(i_reg_prev) .and. emitter(i) > reg_data%n_in) then
            valid_fs_splitting = check_fs_splitting (flv_alr(i)%get_last_two(n_legs), &
            flv_alr_registered(i_reg_prev)%get_last_two(n_legs), &
            flv_alr(i)%tag(n_legs - 1), flv_alr_registered(i_reg_prev)%tag(n_legs -
            if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
                nlo_correction_type_dyn (i_reg) = set_dynamic_correction_type (i)
            end if
            pure_corr_type = nlo_correction_type_dyn (i_reg) &
                == nlo_correction_type_dyn (i_reg_prev)
            if ((flv_alr(i) .equiv. flv_alr_registered(i_reg_prev)) &
                .and. valid_fs_splitting .and. pure_corr_type) then
                mult(i_reg_prev) = mult(i_reg_prev) + 1
                equiv = .true.
                call ftuples(region_to_real_index(ftuples, i))%set_equiv &
                    (equiv_index(i_reg_prev), region_to_ftuple(i))
                exit
            end if
        else if (emitter(i) == flst_emitter(i_reg_prev) .and. emitter(i) <= reg_data%n_in)
            if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
                nlo_correction_type_dyn (i_reg) = set_dynamic_correction_type (i)
            end if
            pure_corr_type = nlo_correction_type_dyn (i_reg) &
                == nlo_correction_type_dyn (i_reg_prev)
            if ((flv_alr(i) .equiv. flv_alr_registered(i_reg_prev)) &
                .and. pure_corr_type) then
                mult(i_reg_prev) = mult(i_reg_prev) + 1
                equiv = .true.
                call ftuples(region_to_real_index(ftuples, i))%set_equiv &
                    (equiv_index(i_reg_prev), region_to_ftuple(i))
                exit
            end if
        end if
    end do
    if (.not. equiv) then
        flv_alr_registered(i_reg) = flv_alr(i)
    end if
end if

```

```

        if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
            nlo_correction_type_dyn (i_reg) = set_dynamic_correction_type (i)
        end if
        flv_uborn(i_reg) = flv_alr(i)%create_uborn (emitter(i), &
            nlo_correction_type_dyn (i_reg))
        flst_emitter(i_reg) = emitter(i)
        equiv_index (i_reg) = region_to_ftuple(i)
        if (nlo_correction_type == "EW" .and. reg_data%alphas_power > 0) then
            corr_type_valid = (nlo_correction_type_dyn (i_reg) == "EW" .and. &
                query_coupling_powers (flv_uborn(i_reg)%flst, &
                    reg_data%alpha_power, reg_data%alphas_power)) &
                .or. (nlo_correction_type_dyn (i_reg) == "QCD" .and. &
                    query_coupling_powers (flv_uborn(i_reg)%flst, &
                        reg_data%alpha_power + 1, reg_data%alphas_power - 1))
            non_singular_reg = .not. corr_type_valid .and. &
                qcd_ew_interferences (flv_alr_registered(i_reg)%flst) &
                .and. .not. qcd_ew_interferences (flv_uborn(i_reg)%flst) &
                .and. nlo_correction_type_dyn (i_reg) == "QCD"
            if (non_singular_reg) nlo_correction_type_dyn (i_reg) = "none"
        end if
        if (corr_type_valid .or. non_singular_reg) then
            mult(i_reg) = mult(i_reg) + 1
            index = [index, region_to_real_index(ftuples, i)]
            i_reg = i_reg + 1
        end if
    end if
end if
end do SCAN_FTUPLES
i_first = i_first + alr_limits(i_flv)
end do SCAN_FLAVORS
n_regions = i_reg - 1

allocate (reg_data%regions (n_regions))
reg_data%n_regions = n_regions
call account_for_regions_from_other_uborns (ftuples)
call init_regions_with_permuted_flavors ()
call assign_real_indices ()

deallocate (flv_uborn)
deallocate (flv_alr_registered)
deallocate (mult)
deallocate (flst_emitter)
deallocate (index)
deallocate (region_to_ftuple)
deallocate (equiv_index)

contains

subroutine account_for_regions_from_other_uborns (ftuples)
    type(ftuple_list_t), intent(inout), dimension(:), allocatable :: ftuples
    integer :: alr1, alr2, i
    type(ftuple_t), dimension(:), allocatable :: ftuples_alr1, ftuples_alr2
    type(flavor_permutation_t) :: perm_list
    logical, dimension(:,:), allocatable :: equivalences

```



```

do alr1 = 1, n_regions
  do alr2 = 1, n_regions
    if (index(alr1) == index(alr2)) cycle
    if (flv_alr_registered(alr1) .equiv. flv_alr_registered(alr2)) then
      call ftuples(index(alr1))%to_array (ftuples_alr1, equivalences, .false.)
      call ftuples(index(alr2))%to_array (ftuples_alr2, equivalences, .false.)
      do i = 1, size (ftuples_alr2)
        if (.not. any (ftuple_equal_ireg (ftuples_alr1, ftuples_alr2(i)))) then
          call ftuples(index(alr1))%append (ftuples_alr2(i))
        end if
      end do
    end if
  end do
end do
end subroutine account_for_regions_from_other_uborns

subroutine setup_region_mappings (n_independent_flv, &
  alr_limits, region_to_ftuple)
  integer, intent(inout) :: n_independent_flv
  integer, intent(inout), dimension(:), allocatable :: alr_limits
  integer, intent(inout), dimension(:), allocatable :: region_to_ftuple
  integer :: i, j, i_flv
  if (any (ftuples%get_n_tuples() == 0)) &
    call msg_fatal ("Inconsistent collection of FKS pairs!")
  n_independent_flv = size (ftuples)
  alr_limits = ftuples%get_n_tuples()
  if (.not. (sum (alr_limits) == maxregions)) &
    call msg_fatal ("Too many regions!")
  j = 1
  do i_flv = 1, n_independent_flv
    do i = 1, alr_limits(i_flv)
      region_to_ftuple(j) = i
      j = j + 1
    end do
  end do
end subroutine setup_region_mappings

subroutine check_permutation (perm, flv_perm, flv_orig, i_reg)
  type(flavor_permutation_t), intent(in) :: perm
  type(flv_structure_t), intent(in) :: flv_perm, flv_orig
  integer, intent(in) :: i_reg
  type(flv_structure_t) :: flv_test
  flv_test = perm%apply (flv_orig, invert = .true.)
  if (.not. all (flv_test%flst == flv_perm%flst)) then
    print *, 'Fail at: ', i_reg
    print *, 'Original flavor structure: ', flv_orig%flst
    call perm%write ()
    print *, 'Permuted flavor: ', flv_perm%flst
    print *, 'Should be: ', flv_test%flst
    call msg_fatal ("Permutation does not reproduce original flavor!")
  end if
end subroutine check_permutation

subroutine init_regions_with_permuted_flavors ()

```

```

type(flavor_permutation_t) :: perm_list
type(ftuple_t), dimension(:), allocatable :: ftuple_array
logical, dimension(:,:), allocatable :: equivalences
integer :: i, j
do j = 1, n_regions
  do i = 1, reg_data%n_flv_born
    if (reg_data%flv_born(i) .equiv. flv_uborn(j)) then
      call perm_list%reset()
      call perm_list%init(reg_data%flv_born(i), flv_uborn(j), &
        reg_data%n_in, reg_data%n_legs_born, .true.)
      flv_uborn(j) = perm_list%apply(flv_uborn(j))
      flv_alr_registered(j) = perm_list%apply(flv_alr_registered(j))
      flst_emitter(j) = perm_list%apply(flst_emitter(j))
    end if
  end do
  call ftuples(index(j))%to_array(ftuple_array, equivalences, .false.)
  do i = 1, size(reg_data%flv_real)
    if (reg_data%flv_real(i) .equiv. flv_alr_registered(j)) then
      call perm_list%reset()
      call perm_list%init(flv_alr_registered(j), reg_data%flv_real(i), &
        reg_data%n_in, reg_data%n_legs_real, .false.)
      if (debug_active(D_SUBTRACTION)) call check_permutation &
        (perm_list, reg_data%flv_real(i), flv_alr_registered(j), j)
      ftuple_array = perm_list%apply(ftuple_array)
      call ftuple_sort_array(ftuple_array, equivalences)
    end if
  end do
  call reg_data%regions(j)%init(j, mult(j), 0, flv_alr_registered(j), &
    flv_uborn(j), reg_data%flv_born, flst_emitter(j), ftuple_array, &
    equivalences, nlo_correction_type_dyn(j))
  if (allocated(ftuple_array)) deallocate(ftuple_array)
  if (allocated(equivalences)) deallocate(equivalences)
end do
end subroutine init_regions_with_permuted_flavors

subroutine assign_real_indices()
  type(flv_structure_t) :: current_flv_real
  type(flv_structure_t), dimension(:), allocatable :: these_flv
  integer :: i_real, current_uborn_index
  integer :: i, j, this_i_real
  allocate(these_flv(size(flv_alr_registered)))
  i_real = 1
  associate(regions => reg_data%regions)
  do i = 1, reg_data%n_regions
    do j = 1, size(these_flv)
      if (.not. allocated(these_flv(j)%flst)) then
        this_i_real = i_real
        call these_flv(i_real)%init(flv_alr_registered(i)%flst, reg_data%n_in)
        i_real = i_real + 1
        exit
      else if (all(these_flv(j)%flst == flv_alr_registered(i)%flst)) then
        this_i_real = j
        exit
      end if
    end do
  end do
end subroutine assign_real_indices

```

```

        end do
        regions(i)%real_index = this_i_real
    end do
end associate
deallocate (these_flv)
end subroutine assign_real_indices

subroutine write_perm_list (perm_list)
    integer, intent(in), dimension(:,:) :: perm_list
    integer :: i
    do i = 1, size (perm_list(:,1))
        write (*,'(I1,1x,I1,A)', advance = "no" ) perm_list(i,1), perm_list(i,2), '/'
    end do
    print *, ''
end subroutine write_perm_list

function check_fs_splitting (flv1, flv2, tag1, tag2) result (valid)
    logical :: valid
    integer, intent(in), dimension(2) :: flv1, flv2
    integer, intent(in) :: tag1, tag2
    if (flv1(1) + flv1(2) == 0) then
        valid = abs(flv1(1)) == abs(flv2(1)) .and. abs(flv1(2)) == abs(flv2(2))
    else
        valid = flv1(1) == flv2(1) .and. flv1(2) == flv2(2) .and. tag1 == tag2
    end if
end function check_fs_splitting

function set_dynamic_correction_type (i_flv_alr) result (nlo_corr_type_dyn)
    type(string_t) :: nlo_corr_type_dyn
    type(ftuple_t) :: ftuple_tmp
    integer, intent(in) :: i_flv_alr
    ftuple_tmp = ftuples (region_to_real_index(ftuples, i_flv_alr))%get_ftuple &
        (region_to_ftuple(i_flv_alr))
    if (ftuple_tmp%qcd_split) then
        nlo_corr_type_dyn = var_str ("QCD")
    else
        nlo_corr_type_dyn = var_str ("EW")
    end if
end function set_dynamic_correction_type
end subroutine region_data_init_singular_regions

```

Create an array containing all emitters and resonances of `region_data`.

```

⟨fks regions: reg data: TBP⟩+≡
    procedure :: find_emitters => region_data_find_emitters

⟨fks regions: procedures⟩+≡
    subroutine region_data_find_emitters (reg_data)
        class(region_data_t), intent(inout) :: reg_data
        integer :: alr, j, n_em, em
        integer, dimension(:), allocatable :: em_count
        allocate (em_count(reg_data%n_regions))
        em_count = -1
        n_em = 0
    end subroutine region_data_find_emitters

```

```

!!!Count the number of different emitters
do alr = 1, reg_data%n_regions
  em = reg_data%regions(alr)%emitter
  if (.not. any (em_count == em)) then
    n_em = n_em + 1
    em_count(alr) = em
  end if
end do

if (n_em < 1) call msg_fatal ("region_data_find_emitters: No emitters found!")
reg_data%n_emitters = n_em
allocate (reg_data%emitters (reg_data%n_emitters))
reg_data%emitters = -1

j = 1
do alr = 1, size (reg_data%regions)
  em = reg_data%regions(alr)%emitter
  if (.not. any (reg_data%emitters == em)) then
    reg_data%emitters(j) = em
    j = j + 1
  end if
end do
end subroutine region_data_find_emitters

```

<fks regions: reg data: TBP>+≡

```

procedure :: find_resonances => region_data_find_resonances

```

<fks regions: procedures>+≡

```

subroutine region_data_find_resonances (reg_data)
  class(region_data_t), intent(inout) :: reg_data
  integer :: alr, j, k, n_res, n_contr
  integer :: res
  integer, dimension(10) :: res_count
  type(resonance_contributors_t), dimension(10) :: contributors_count
  type(resonance_contributors_t) :: contributors
  integer :: i_res, emitter
  logical :: share_emitter
  res_count = -1
  n_res = 0; n_contr = 0

  !!! Count the number of different resonances
  do alr = 1, reg_data%n_regions
    select type (fks_mapping => reg_data%fks_mapping)
      type is (fks_mapping_resonances_t)
        res = fks_mapping%res_map%alr_to_i_res (alr)
        if (.not. any (res_count == res)) then
          n_res = n_res + 1
          res_count(alr) = res
        end if
      end select
    end do

    if (n_res > 0) allocate (reg_data%resonances (n_res))
  end do

```

```

j = 1
select type (fks_mapping => reg_data%fks_mapping)
type is (fks_mapping_resonances_t)
do alr = 1, size (reg_data%regions)
  res = fks_mapping%res_map%alr_to_i_res (alr)
  if (.not. any (reg_data%resonances == res)) then
    reg_data%resonances(j) = res
    j = j + 1
  end if
end do

allocate (reg_data%alr_to_i_contributor (size (reg_data%regions)))
do alr = 1, size (reg_data%regions)
  i_res = fks_mapping%res_map%alr_to_i_res (alr)
  emitter = reg_data%regions(alr)%emitter
  call reg_data%get_contributors (i_res, emitter, contributors%c, share_emitter)
  if (.not. share_emitter) cycle
  if (.not. any (contributors_count == contributors)) then
    n_contr = n_contr + 1
    contributors_count(alr) = contributors
  end if
  if (allocated (contributors%c)) deallocate (contributors%c)
end do
allocate (reg_data%alr_contributors (n_contr))
j = 1
do alr = 1, size (reg_data%regions)
  i_res = fks_mapping%res_map%alr_to_i_res (alr)
  emitter = reg_data%regions(alr)%emitter
  call reg_data%get_contributors (i_res, emitter, contributors%c, share_emitter)
  if (.not. share_emitter) cycle
  if (.not. any (reg_data%alr_contributors == contributors)) then
    reg_data%alr_contributors(j) = contributors
    reg_data%alr_to_i_contributor (alr) = j
    j = j + 1
  else
    do k = 1, size (reg_data%alr_contributors)
      if (reg_data%alr_contributors(k) == contributors) exit
    end do
    reg_data%alr_to_i_contributor (alr) = k
  end if
  if (allocated (contributors%c)) deallocate (contributors%c)
end do
end select
call reg_data%extend_ftuples (n_res)
call reg_data%set_contributors ()

end subroutine region_data_find_resonances

```

```

<fks regions: reg data: TBP>+≡
  procedure :: set_i_phs_to_i_con => region_data_set_i_phs_to_i_con

<fks regions: procedures>+≡
  subroutine region_data_set_i_phs_to_i_con (reg_data)
    class(region_data_t), intent(inout) :: reg_data

```

```

integer :: alr
integer :: i_res, emitter, i_con, i_phs, i_em
type(phs_identifiers_t), dimension(:), allocatable :: phs_id_tmp
logical :: share_emitter, phs_exist
type(resonance_contributors_t) :: contributors
allocate (phs_id_tmp (reg_data%n_phs))
if (allocated (reg_data%resonances)) then
  allocate (reg_data%i_phs_to_i_con (reg_data%n_phs))
  do i_em = 1, size (reg_data%emitters)
    emitter = reg_data%emitters(i_em)
    do i_res = 1, size (reg_data%resonances)
      if (reg_data%emitter_is_compatible_with_resonance (i_res, emitter)) then
        alr = find_alr (emitter, i_res)
        if (alr == 0) call msg_fatal ("Could not find requested alpha region!")
        i_con = reg_data%alr_to_i_contributor (alr)
        call reg_data%get_contributors (i_res, emitter, contributors%c, share_emitter)
        if (.not. share_emitter) cycle
        call check_for_phs_identifier &
          (phs_id_tmp, reg_data%n_in, emitter, contributors%c, phs_exist, i_phs)
        if (phs_id_tmp(i_phs)%emitter < 0) then
          phs_id_tmp(i_phs)%emitter = emitter
          allocate (phs_id_tmp(i_phs)%contributors (size (contributors%c)))
          phs_id_tmp(i_phs)%contributors = contributors%c
        end if
        reg_data%i_phs_to_i_con (i_phs) = i_con
      end if
    end do
    if (allocated (contributors%c)) deallocate (contributors%c)
  end do
end do
end if
contains
function find_alr (emitter, i_res) result (alr)
integer :: alr
integer, intent(in) :: emitter, i_res
integer :: i
do i = 1, reg_data%n_regions
  if (reg_data%regions(i)%emitter == emitter .and. &
    reg_data%regions(i)%i_res == i_res) then
    alr = i
    return
  end if
end do
alr = 0
end function find_alr
end subroutine region_data_set_i_phs_to_i_con

```

<fks regions: reg data: TBP>+≡

```
procedure :: set_alr_to_i_phs => region_data_set_alr_to_i_phs
```

<fks regions: procedures>+≡

```

subroutine region_data_set_alr_to_i_phs (reg_data, phs_identifiers, alr_to_i_phs)
class(region_data_t), intent(inout) :: reg_data
type(phs_identifiers_t), intent(in), dimension(:) :: phs_identifiers
integer, intent(out), dimension(:) :: alr_to_i_phs

```

```

integer :: alr, i_phs
integer :: emitter, i_res
type(resonance_contributors_t) :: contributors
logical :: share_emitter, phs_exist
do alr = 1, reg_data%n_regions
  associate (region => reg_data%regions(alr))
    emitter = region%emitter
    i_res = region%i_res
    if (i_res /= 0) then
      call reg_data%get_contributors (i_res, emitter, &
        contributors%c, share_emitter)
      if (.not. share_emitter) cycle
    end if
    if (allocated (contributors%c)) then
      call check_for_phs_identifier (phs_identifiers, reg_data%n_in, &
        emitter, contributors%c, phs_exist = phs_exist, i_phs = i_phs)
    else
      call check_for_phs_identifier (phs_identifiers, reg_data%n_in, &
        emitter, phs_exist = phs_exist, i_phs = i_phs)
    end if
    if (.not. phs_exist) &
      call msg_fatal ("phs identifiers are not set up correctly!")
    alr_to_i_phs(alr) = i_phs
  end associate
  if (allocated (contributors%c)) deallocate (contributors%c)
end do
end subroutine region_data_set_alr_to_i_phs

```

<fks regions: reg data: TBP>+≡

```

procedure :: set_contributors => region_data_set_contributors

```

<fks regions: procedures>+≡

```

subroutine region_data_set_contributors (reg_data)
  class(region_data_t), intent(inout) :: reg_data
  integer :: alr, i_res, i_reg, i_con
  integer :: i1, i2, i_em
  integer, dimension(:), allocatable :: contributors
  logical :: share_emitter
  do alr = 1, size (reg_data%regions)
    associate (sregion => reg_data%regions(alr))
      allocate (sregion%i_reg_to_i_con (sregion%nregions))
      do i_reg = 1, sregion%nregions
        call sregion%ftuples(i_reg)%get (i1, i2)
        i_em = get_emitter_index (i1, i2, reg_data%n_legs_real)
        i_res = sregion%ftuples(i_reg)%i_res
        call reg_data%get_contributors (i_res, i_em, contributors, share_emitter)
        !!! Lookup contributor index
        do i_con = 1, size (reg_data%alr_contributors)
          if (all (reg_data%alr_contributors(i_con)%c == contributors)) then
            sregion%i_reg_to_i_con (i_reg) = i_con
            exit
          end if
        end do
      end do
    end associate
    deallocate (contributors)
  end do

```

```

        end do
    end associate
end do
contains
    function get_emitter_index (i1, i2, n) result (i_em)
        integer :: i_em
        integer, intent(in) :: i1, i2, n
        if (i1 == n) then
            i_em = i2
        else
            i_em = i1
        end if
    end function get_emitter_index
end subroutine region_data_set_contributors

```

This extension of the ftuples is still too naive as it assumes that the same resonances are possible for all ftuples

(fks regions: reg data: TBP)+≡

```

    procedure :: extend_ftuples => region_data_extend_ftuples

```

(fks regions: procedures)+≡

```

subroutine region_data_extend_ftuples (reg_data, n_res)
    class(region_data_t), intent(inout) :: reg_data
    integer, intent(in) :: n_res
    integer :: alr, n_reg_save
    integer :: i_reg, i_res, i_em, k
    type(ftuple_t), dimension(:), allocatable :: ftuple_save
    integer :: n_new
    do alr = 1, size (reg_data%regions)
        associate (sregion => reg_data%regions(alr))
            n_reg_save = sregion%nregions
            allocate (ftuple_save (n_reg_save))
            ftuple_save = sregion%ftuples
            n_new = count_n_new_ftuples (sregion, n_res)
            deallocate (sregion%ftuples)
            sregion%nregions = n_new
            allocate (sregion%ftuples (n_new))
            k = 1
            do i_res = 1, n_res
                do i_reg = 1, n_reg_save
                    associate (ftuple_new => sregion%ftuples(k))
                        i_em = ftuple_save(i_reg)%ireg(1)
                        if (reg_data%emitter_is_in_resonance (i_res, i_em)) then
                            call ftuple_new%set (i_em, ftuple_save(i_reg)%ireg(2))
                            ftuple_new%i_res = i_res
                            ftuple_new%splitting_type = ftuple_save(i_reg)%splitting_type
                            k = k + 1
                        end if
                    end associate
                end do
            end do
            deallocate (ftuple_save)
        end do
    end do
end subroutine region_data_extend_ftuples

```



```

contains
  function count_n_new_ftuples (sregion, n_res) result (n_new)
    integer :: n_new
    type(singular_region_t), intent(in) :: sregion
    integer, intent(in) :: n_res
    integer :: i_reg, i_res, i_em
    n_new = 0
    do i_reg = 1, sregion%nregions
      do i_res = 1, n_res
        i_em = sregion%ftuples(i_reg)%ireg(1)
        if (reg_data%emitter_is_in_resonance (i_res, i_em)) &
          n_new = n_new + 1
      end do
    end do
  end function count_n_new_ftuples
end subroutine region_data_extend_ftuples

```

<fks regions: reg data: TBP>+≡
 procedure :: get_flavor_indices => region_data_get_flavor_indices

<fks regions: procedures>+≡
 function region_data_get_flavor_indices (reg_data, born) result (i_flv)
 integer, dimension(:), allocatable :: i_flv
 class(region_data_t), intent(in) :: reg_data
 logical, intent(in) :: born
 allocate (i_flv (reg_data%n_regions))
 if (born) then
 i_flv = reg_data%regions%uborn_index
 else
 i_flv = reg_data%regions%real_index
 end if
 end function region_data_get_flavor_indices

<fks regions: reg data: TBP>+≡
 procedure :: get_matrix_element_index => region_data_get_matrix_element_index

<fks regions: procedures>+≡
 function region_data_get_matrix_element_index (reg_data, i_reg) result (i_me)
 integer :: i_me
 class(region_data_t), intent(in) :: reg_data
 integer, intent(in) :: i_reg
 i_me = reg_data%regions(i_reg)%real_index
 end function region_data_get_matrix_element_index

<fks regions: reg data: TBP>+≡
 procedure :: compute_number_of_phase_spaces &
 => region_data_compute_number_of_phase_spaces

<fks regions: procedures>+≡
 subroutine region_data_compute_number_of_phase_spaces (reg_data)
 class(region_data_t), intent(inout) :: reg_data
 integer :: i_em, i_res, i_phs
 integer :: emitter
 type(resonance_contributors_t) :: contributors

```

integer, parameter :: n_max_phs = 10
type(phs_identifer_t), dimension(n_max_phs) :: phs_id_tmp
logical :: share_emitter, phs_exist
if (allocated (reg_data%resonances)) then
    reg_data%n_phs = 0
    do i_em = 1, size (reg_data%emitters)
        emitter = reg_data%emitters(i_em)
        do i_res = 1, size (reg_data%resonances)
            if (reg_data%emitter_is_compatible_with_resonance (i_res, emitter)) then
                call reg_data%get_contributors (i_res, emitter, contributors%c, share_emitter)
                if (.not. share_emitter) cycle
                call check_for_phs_identifer &
                    (phs_id_tmp, reg_data%n_in, emitter, contributors%c, phs_exist, i_phs)
                if (.not. phs_exist) then
                    reg_data%n_phs = reg_data%n_phs + 1
                    if (reg_data%n_phs > n_max_phs) call msg_fatal &
                        ("Buffer of phase space identifierees: Too much phase spaces!")
                    call phs_id_tmp(i_phs)%init (emitter, contributors%c)
                end if
            end if
        end do
        if (allocated (contributors%c)) deallocate (contributors%c)
    end do
else
    reg_data%n_phs = size (remove_duplicates_from_int_array (reg_data%emitters))
end if
end subroutine region_data_compute_number_of_phase_spaces

```

<fks regions: reg data: TBP>+≡

```

procedure :: get_n_phs => region_data_get_n_phs

```

<fks regions: procedures>+≡

```

function region_data_get_n_phs (reg_data) result (n_phs)
    integer :: n_phs
    class(region_data_t), intent(in) :: reg_data
    n_phs = reg_data%n_phs
end function region_data_get_n_phs

```

<fks regions: reg data: TBP>+≡

```

procedure :: set_splitting_info => region_data_set_splitting_info

```

<fks regions: procedures>+≡

```

subroutine region_data_set_splitting_info (reg_data)
    class(region_data_t), intent(inout) :: reg_data
    integer :: alr
    do alr = 1, reg_data%n_regions
        call reg_data%regions(alr)%set_splitting_info (reg_data%n_in)
    end do
end subroutine region_data_set_splitting_info

```

<fks regions: reg data: TBP>+≡

```

procedure :: init_phs_identifiers => region_data_init_phs_identifiers

```

(fks regions: procedures)+≡

```

subroutine region_data_init_phs_identifiers (reg_data, phs_id)
  class(region_data_t), intent(in) :: reg_data
  type(phs_identifier_t), intent(out), dimension(:), allocatable :: phs_id
  integer :: i_em, i_res, i_phs
  integer :: emitter
  type(resonance_contributors_t) :: contributors
  logical :: share_emitter, phs_exist
  allocate (phs_id (reg_data%n_phs))
  do i_em = 1, size (reg_data%emitters)
    emitter = reg_data%emitters(i_em)
    if (allocated (reg_data%resonances)) then
      do i_res = 1, size (reg_data%resonances)
        call reg_data%get_contributors (i_res, emitter, contributors%c, share_emitter)
        if (.not. share_emitter) cycle
        call check_for_phs_identifier &
          (phs_id, reg_data%n_in, emitter, contributors%c, phs_exist, i_phs)
        if (.not. phs_exist) &
          call phs_id(i_phs)%init (emitter, contributors%c)
        if (allocated (contributors%c)) deallocate (contributors%c)
      end do
    else
      call check_for_phs_identifier (phs_id, reg_data%n_in, emitter, &
        phs_exist = phs_exist, i_phs = i_phs)
      if (.not. phs_exist) call phs_id(i_phs)%init (emitter)
    end if
  end do
end subroutine region_data_init_phs_identifiers

```

Gathers all ftuples from all ALRs. There are at most $n \cdot (n - 1)$ ftuples with i and j in the final state and up to $3n$ ftuples with i in the initial state.

(fks regions: reg data: TBP)+≡

```

procedure :: get_all_ftuples => region_data_get_all_ftuples

```

(fks regions: procedures)+≡

```

subroutine region_data_get_all_ftuples (reg_data, ftuples)
  class(region_data_t), intent(in) :: reg_data
  type(ftuple_t), intent(inout), dimension(:), allocatable :: ftuples
  type(ftuple_t), dimension(:), allocatable :: ftuple_tmp
  integer :: i, j, alr, n_fs
  j = 0
  n_fs = reg_data%n_legs_real - reg_data%n_in
  allocate (ftuple_tmp (n_fs * (n_fs - 1) + 3 * n_fs))
  do i = 1, reg_data%n_regions
    associate (region => reg_data%regions(i))
      do alr = 1, region%nregions
        if (.not. any (ftuple_equal_ireg (region%ftuples(alr), ftuple_tmp))) then
          j = j + 1
          ftuple_tmp(j) = region%ftuples(alr)
        end if
      end do
    end associate
  end do
  allocate (ftuples (j))

```

```

ftuples = ftuple_tmp(1:j)
deallocate (ftuple_tmp)
end subroutine region_data_get_all_ftuples

```

<fks regions: reg data: TBP>+≡

```

procedure :: write_to_file => region_data_write_to_file

```

<fks regions: procedures>+≡

```

subroutine region_data_write_to_file (reg_data, proc_id, latex, os_data)
  class(region_data_t), intent(inout) :: reg_data
  type(string_t), intent(in) :: proc_id
  logical, intent(in) :: latex
  type(os_data_t), intent(in) :: os_data
  type(string_t) :: filename
  integer :: u
  integer :: status

  if (latex) then
    filename = proc_id // "_fks_regions.tex"
  else
    filename = proc_id // "_fks_regions.out"
  end if
  u = free_unit ()
  open (u, file=char(filename), action = "write", status="replace")
  if (latex) then
    call reg_data%write_latex (u)
    close (u)
    call os_data%build_latex_file &
      (proc_id // "_fks_regions", stat_out = status)
    if (status /= 0) &
      call msg_error (char ("Failed to compile " // filename))
  else
    call reg_data%write (u)
    close (u)
  end if
end subroutine region_data_write_to_file

```

<fks regions: reg data: TBP>+≡

```

procedure :: write_latex => region_data_write_latex

```

<fks regions: procedures>+≡

```

subroutine region_data_write_latex (reg_data, unit)
  class(region_data_t), intent(in) :: reg_data
  integer, intent(in), optional :: unit
  integer :: i, u
  u = given_output_unit (); if (present (unit)) u = unit
  write (u, "(A)") "\documentclass{article}"
  write (u, "(A)") "\begin{document}"
  write (u, "(A)") "%FKS region data, automatically created by WHIZARD"
  write (u, "(A)") "\begin{table}"
  write (u, "(A)") "\begin{center}"
  write (u, "(A)") "\begin{tabular} {|c|c|c|c|c|c|c|c|}"
  write (u, "(A)") "\hline"
  write (u, "(A)") "$\alpha_r$ & $f_r$ & $i_r$ & $\varepsilon$ & $\sigma$ & $\mathcal{P}_{\rm r}$"

```

```

write (u, "(A)") "\hline"
do i = 1, reg_data%n_regions
    call reg_data%regions(i)%write_latex (u)
end do
write (u, "(A)") "\hline"
write (u, "(A)") "\end{tabular}"
write (u, "(A)") "\caption[List of singular regions]"
write (u, "(A)") "\begin{description}"
write (u, "(A)") "\item[$\alpha_r$] Index of the singular region"
write (u, "(A)") "\item[$f_r$] Real flavor structure"
write (u, "(A)") "\item[$i_r$] Index of the associated real flavor structure"
write (u, "(A)") "\item[$\varepsilon$] Emitter"
write (u, "(A)") "\item[$\varsigma$] Multiplicity" !!! The symbol used by 0908.4272 for multiplicity
write (u, "(A)") "\item[$\mathcal{P}_{\rm FKS}$] The set of singular FKS-pairs"
write (u, "(A)") "\item[$i_b$] Underlying Born index"
write (u, "(A)") "\item[$f_b$] Underlying Born flavor structure"
write (u, "(A)") "\end{description}"
write (u, "(A)") "\end{center}"
write (u, "(A)") "\end{table}"
write (u, "(A)") "\end{document}"
end subroutine region_data_write_latex

```

Creates a table with information about all singular regions and writes it to a file.

```

<fks regions: reg data: TBP>+≡
    procedure :: write => region_data_write

<fks regions: procedures>+≡
    subroutine region_data_write (reg_data, unit)
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in), optional :: unit
        integer :: j
        integer :: maxnregions, i_reg_max
        type(string_t) :: flst_title, ftuple_title
        integer :: n_res, u
        u = given_output_unit (unit); if (u < 0) return
        maxnregions = 1; i_reg_max = 1
        do j = 1, reg_data%n_regions
            if (size (reg_data%regions(j)%ftuples) > maxnregions) then
                maxnregions = reg_data%regions(j)%nregions
                i_reg_max = j
            end if
        end do
        flst_title = '(A' // flst_title_format(reg_data%n_legs_real) // ')'
        ftuple_title = '(A' // ftuple_title_format() // ')'
        write (u, '(A,1X,I4)') 'Total number of regions: ', size(reg_data%regions)
        write (u, '(A4)', advance = 'no') ' alr'
        call write_vline (u)
        write (u, char (flst_title), advance = 'no') 'flst_real'
        call write_vline (u)
        write (u, '(A6)', advance = 'no') 'i_real'
        call write_vline (u)
        write (u, '(A3)', advance = 'no') 'em'
        call write_vline (u)
    end subroutine

```

```

write (u, '(A3)', advance = 'no') 'mult'
call write_vline (u)
write (u, '(A4)', advance = 'no') 'nreg'
call write_vline (u)
if (allocated (reg_data%fks_mapping)) then
  select type (fks_mapping => reg_data%fks_mapping)
  type is (fks_mapping_resonances_t)
    write (u, '(A3)', advance = 'no') 'res'
    call write_vline (u)
  end select
end if
write (u, char (ftuple_title), advance = 'no') 'ftuples'
call write_vline (u)
flst_title = '(A' // flst_title_format(reg_data%n_legs_born) // ')'
write (u, char (flst_title), advance = 'no') 'flst_born'
call write_vline (u)
write (u, '(A7)', advance = 'no') 'i_born'
call write_vline (u)
write (u, '(A4)') 'corr'
do j = 1, reg_data%n_regions
  write (u, '(I4)', advance = 'no') j
  call reg_data%regions(j)%write (u, maxnregions)
end do
call write_separator (u)
if (allocated (reg_data%fks_mapping)) then
  select type (fks_mapping => reg_data%fks_mapping)
  type is (fks_mapping_resonances_t)
    write (u, '(A)')
    write (u, '(A)') "The FKS regions are combined with resonance information: "
    n_res = size (fks_mapping%res_map%res_histories)
    write (u, '(A,1X,I1)') "Number of QCD resonance histories: ", n_res
    do j = 1, n_res
      write (u, '(A,1X,I1)') "i_res = ", j
      call fks_mapping%res_map%res_histories(j)%write (u)
      call write_separator (u)
    end do
  end select
end if
contains

function flst_title_format (n) result (frmt)
  integer, intent(in) :: n
  type(string_t) :: frmt
  character(len=2) :: frmt_char
  write (frmt_char, '(I2)') 4 * n + 1
  frmt = var_str (frmt_char)
end function flst_title_format

function ftuple_title_format () result (frmt)
  type(string_t) :: frmt
  integer :: n_ftuple_char
  !!! An ftuple (x,x) consists of five characters. In the string, they
  !!! are separated by maxregions - 1 commas. In total these are

```

```

!!! 5 * maxnregions + maxnregions - 1 = 6 * maxnregions - 1 characters.
!!! The {} brackets at add two additional characters.
n_ftuple_char = 6 * maxnregions + 1
!!! If there are resonances, each ftuple with a resonance adds a ";x"
!!! to the ftuple
n_ftuple_char = n_ftuple_char + 2 * count (reg_data%regions(i_reg_max)%ftuples%i_res > 0)
!!! Pseudo-ISR regions are denoted with a * at the end
n_ftuple_char = n_ftuple_char + count (reg_data%regions(i_reg_max)%ftuples%pseudo_isr)
frmt = str (n_ftuple_char)
end function ftuple_title_format

end subroutine region_data_write

<fks regions: procedures>+≡
subroutine write_vline (u)
  integer, intent(in) :: u
  character(len=10), parameter :: sep_format = "(1X,A2,1X)"
  write (u, sep_format, advance = 'no') '||'
end subroutine write_vline

<fks regions: public>+≡
public :: assignment(=)

<fks regions: interfaces>+≡
interface assignment(=)
  module procedure region_data_assign
end interface

<fks regions: procedures>+≡
subroutine region_data_assign (reg_data_out, reg_data_in)
  type(region_data_t), intent(out) :: reg_data_out
  type(region_data_t), intent(in) :: reg_data_in
  integer :: i
  if (allocated (reg_data_in%regions)) then
    allocate (reg_data_out%regions (size (reg_data_in%regions)))
    do i = 1, size (reg_data_in%regions)
      reg_data_out%regions(i) = reg_data_in%regions(i)
    end do
  else
    call msg_warning ("Copying region data without allocated singular regions!")
  end if
  if (allocated (reg_data_in%flv_born)) then
    allocate (reg_data_out%flv_born (size (reg_data_in%flv_born)))
    do i = 1, size (reg_data_in%flv_born)
      reg_data_out%flv_born(i) = reg_data_in%flv_born(i)
    end do
  else
    call msg_warning ("Copying region data without allocated born flavor structure!")
  end if
  if (allocated (reg_data_in%flv_real)) then
    allocate (reg_data_out%flv_real (size (reg_data_in%flv_real)))
    do i = 1, size (reg_data_in%flv_real)
      reg_data_out%flv_real(i) = reg_data_in%flv_real(i)
    end do
  end if
end subroutine region_data_assign

```

```

        end do
    else
        call msg_warning ("Copying region data without allocated real flavor structure!")
    end if
    if (allocated (reg_data_in%emitters)) then
        allocate (reg_data_out%emitters (size (reg_data_in%emitters)))
        do i = 1, size (reg_data_in%emitters)
            reg_data_out%emitters(i) = reg_data_in%emitters(i)
        end do
    else
        call msg_warning ("Copying region data without allocated emitters!")
    end if
    reg_data_out%n_regions = reg_data_in%n_regions
    reg_data_out%n_emitters = reg_data_in%n_emitters
    reg_data_out%n_flv_born = reg_data_in%n_flv_born
    reg_data_out%n_flv_real = reg_data_in%n_flv_real
    reg_data_out%n_in = reg_data_in%n_in
    reg_data_out%n_legs_born = reg_data_in%n_legs_born
    reg_data_out%n_legs_real = reg_data_in%n_legs_real
    if (allocated (reg_data_in%fks_mapping)) then
        select type (fks_mapping_in => reg_data_in%fks_mapping)
            type is (fks_mapping_default_t)
                allocate (fks_mapping_default_t :: reg_data_out%fks_mapping)
                select type (fks_mapping_out => reg_data_out%fks_mapping)
                    type is (fks_mapping_default_t)
                        fks_mapping_out = fks_mapping_in
                    end select
            type is (fks_mapping_resonances_t)
                allocate (fks_mapping_resonances_t :: reg_data_out%fks_mapping)
                select type (fks_mapping_out => reg_data_out%fks_mapping)
                    type is (fks_mapping_resonances_t)
                        fks_mapping_out = fks_mapping_in
                    end select
            end select
    else
        call msg_warning ("Copying region data without allocated FKS regions!")
    end if
    if (allocated (reg_data_in%resonances)) then
        allocate (reg_data_out%resonances (size (reg_data_in%resonances)))
        reg_data_out%resonances = reg_data_in%resonances
    end if
    reg_data_out%n_phs = reg_data_in%n_phs
    if (allocated (reg_data_in%alr_contributors)) then
        allocate (reg_data_out%alr_contributors (size (reg_data_in%alr_contributors)))
        reg_data_out%alr_contributors = reg_data_in%alr_contributors
    end if
    if (allocated (reg_data_in%alr_to_i_contributor)) then
        allocate (reg_data_out%alr_to_i_contributor &
            (size (reg_data_in%alr_to_i_contributor)))
        reg_data_out%alr_to_i_contributor = reg_data_in%alr_to_i_contributor
    end if
end subroutine region_data_assign

```

Returns the index of the real flavor structure an ftuple belongs to.


```

(fks regions: procedures)+≡
function region_to_real_index (list, i) result(index)
  type(ftuple_list_t), intent(in), dimension(:), allocatable :: list
  integer, intent(in) :: i
  integer, dimension(:), allocatable :: nreg
  integer :: index, j
  allocate (nreg (0))
  index = 0
  do j = 1, size (list)
    nreg = [nreg, sum (list(:j)%get_n_tuples ())]
    if (j == 1) then
      if (i <= nreg(j)) then
        index = j
        exit
      end if
    else
      if (i > nreg(j - 1) .and. i <= nreg(j)) then
        index = j
        exit
      end if
    end if
  end do
end function region_to_real_index

```

Final state emission: Rearrange the flavor array in such a way that the emitted particle is last and the emitter is second last. *i1* is the index of the emitter, *i2* is the index of the emitted particle.

Initial state emission: Just put the emitted particle to the last position.

```

(fks regions: procedures)+≡
function create_alr (flv1, n_in, i_em, i_rad) result(flv2)
  type(flv_structure_t), intent(in) :: flv1
  integer, intent(in) :: n_in
  integer, intent(in) :: i_em, i_rad
  type(flv_structure_t) :: flv2
  integer :: n
  n = size (flv1%flst)
  allocate (flv2%flst (n), flv2%tag (n))
  flv2%nlegs = n
  flv2%n_in = n_in
  if (i_em > n_in) then
    flv2%flst(1 : n_in) = flv1%flst(1 : n_in)
    flv2%flst(n - 1) = flv1%flst(i_em)
    flv2%flst(n) = flv1%flst(i_rad)
    flv2%tag(1 : n_in) = flv1%tag(1 : n_in)
    flv2%tag(n - 1) = flv1%tag(i_em)
    flv2%tag(n) = flv1%tag(i_rad)
    call fill_remaining_flavors (n_in, .true.)
  else
    flv2%flst(1 : n_in) = flv1%flst(1 : n_in)
    flv2%flst(n) = flv1%flst(i_rad)
    flv2%tag(1 : n_in) = flv1%tag(1 : n_in)
    flv2%tag(n) = flv1%tag(i_rad)
    call fill_remaining_flavors (n_in, .false.)
  end if
end function create_alr

```

```

end if
call flv2%compute_prt_symm_fs (flv2%n_in)
contains

```

Order remaining particles according to their original position

```

<fks regions: procedures>+=
subroutine fill_remaining_flavors (n_in, final_final)
integer, intent(in) :: n_in
logical, intent(in) :: final_final
integer :: i, j
logical :: check
j = n_in + 1
do i = n_in + 1, n
if (final_final) then
check = (i /= i_em .and. i /= i_rad)
else
check = (i /= i_rad)
end if
if (check) then
flv2%flst(j) = flv1%flst(i)
flv2%tag(j) = flv1%tag(i)
j = j + 1
end if
end do
end subroutine fill_remaining_flavors
end function create_alr

```

```

<fks regions: reg data: TBP>+=
procedure :: has_pseudo_isr => region_data_has_pseudo_isr

```

```

<fks regions: procedures>+=
function region_data_has_pseudo_isr (reg_data) result (val)
logical :: val
class(region_data_t), intent(in) :: reg_data
val = any (reg_data%regions%pseudo_isr)
end function region_data_has_pseudo_isr

```

Performs consistency checks on `region_data`. Up to now only checks that no `ftuple` appears more than once.

```

<fks regions: reg data: TBP>+=
procedure :: check_consistency => region_data_check_consistency

<fks regions: procedures>+=
subroutine region_data_check_consistency (reg_data, fail_fatal, unit)
class(region_data_t), intent(in) :: reg_data
logical, intent(in) :: fail_fatal
integer, intent(in), optional :: unit
integer :: u
integer :: i_reg, alr
integer :: i1, f1, f2
logical :: undefined_ftuples, same_ftuple_indices, valid_splitting
logical, dimension(4) :: no_fail
u = given_output_unit(unit); if (u < 0) return
no_fail = .true.

```

```

call msg_message ("Check that no negative ftuple indices occur", unit = u)
do i_reg = 1, reg_data%n_regions
  if (any (reg_data%regions(i_reg)%ftuples%has_negative_elements ())) then
    !!! This error is so severe that we stop immediately
    call msg_fatal ("Negative ftuple indices!")
  end if
end do
call msg_message ("Success!", unit = u)
call msg_message ("Check that there is no ftuple with identical elements", unit = u)
do i_reg = 1, reg_data%n_regions
  if (any (reg_data%regions(i_reg)%ftuples%has_identical_elements ())) then
    !!! This error is so severe that we stop immediately
    call msg_fatal ("Identical ftuple indices!")
  end if
end do
call msg_message ("Success!", unit = u)
call msg_message ("Check that there are no duplicate ftuples in a region", unit = u)
do i_reg = 1, reg_data%n_regions
  if (reg_data%regions(i_reg)%has_identical_ftuples ()) then
    if (no_fail(1)) then
      call msg_error ("FAIL: ", unit = u)
      no_fail(1) = .false.
    end if
    write (u, '(A,1x,I3)') 'i_reg:', i_reg
  end if
end do
if (no_fail(1)) call msg_message ("Success!", unit = u)
call msg_message ("Check that ftuples add up to a valid splitting", unit = u)
do i_reg = 1, reg_data%n_regions
  do alr = 1, reg_data%regions(i_reg)%nregions
    associate (region => reg_data%regions(i_reg))
      i1 = region%ftuples(alr)%ireg(1)
      if (i1 == 0) i1 = 1 !!! Gluon emission from both initial-state particles
      f1 = region%flst_real%flst(i1)
      f2 = region%flst_real%flst(region%ftuples(alr)%ireg(2))
      ! Flip PDG sign of IS fermions to allow a q -> g q splitting
      ! in which the ftuple has the flavors (q,q).
      if (i1 <= reg_data%n_in .and. is_fermion(f1)) then
        f1 = -f1
      end if
      valid_splitting = f1 + f2 == 0 &
        .or. (is_gluon(f1) .and. is_gluon(f2)) &
        .or. (is_massive_vector(f1) .and. is_photon(f2)) &
        .or. is_fermion_vector_splitting (f1, f2)
      if (.not. valid_splitting) then
        if (no_fail(2)) then
          call msg_error ("FAIL: ", unit = u)
          no_fail(2) = .false.
        end if
        write (u, '(A,1x,I3)') 'i_reg:', i_reg
        exit
      end if
    end associate
  end do
end do

```

```

end do
if (no_fail(2)) call msg_message ("Success!", unit = u)
call msg_message ("Check that at least one ftuple contains the emitter", unit = u)
do i_reg = 1, reg_data%n_regions
  associate (region => reg_data%regions(i_reg))
    if (.not. any (region%emitter == region%ftuples%ireg(1))) then
      if (no_fail(3)) then
        call msg_error ("FAIL: ", unit = u)
        no_fail(3) = .false.
      end if
      write (u, '(A,1x,I3)') 'i_reg:', i_reg
    end if
  end associate
end do
if (no_fail(3)) call msg_message ("Success!", unit = u)
call msg_message ("Check that each region has at least one ftuple &
  &with index n + 1", unit = u)
do i_reg = 1, reg_data%n_regions
  if (.not. any (reg_data%regions(i_reg)%ftuples%ireg(2) == reg_data%n_legs_real)) then
    if (no_fail(4)) then
      call msg_error ("FAIL: ", unit = u)
      no_fail(4) = .false.
    end if
    write (u, '(A,1x,I3)') 'i_reg:', i_reg
  end if
end do
if (no_fail(4)) call msg_message ("Success!", unit = u)
if (.not. all (no_fail)) &
  call abort_with_message ("Stop due to inconsistent region data!")

contains
subroutine abort_with_message (msg)
  character(len=*), intent(in) :: msg
  if (fail_fatal) then
    call msg_fatal (msg)
  else
    call msg_error (msg, unit = u)
  end if
end subroutine abort_with_message

function is_fermion_vector_splitting (pdg_1, pdg_2) result (value)
  logical :: value
  integer, intent(in) :: pdg_1, pdg_2
  value = (is_fermion (pdg_1) .and. is_massless_vector (pdg_2)) .or. &
    (is_fermion (pdg_2) .and. is_massless_vector (pdg_1))
end function
end subroutine region_data_check_consistency

<fks regions: reg data: TBP>+≡
  procedure :: requires_spin_correlations => region_data_requires_spin_correlations

<fks regions: procedures>+≡
  function region_data_requires_spin_correlations (reg_data) result (val)
    class(region_data_t), intent(in) :: reg_data

```

```

logical :: val
integer :: alr
val = .false.
do alr = 1, reg_data%n_regions
    val = reg_data%regions(alr)%sc_required
    if (val) return
end do
end function region_data_requires_spin_correlations

```

We have to apply the symmetry factor for identical particles of the real flavor structure to the born squared matrix element. The corresponding factor from the born flavor structure has to be cancelled.

```

⟨fks regions: reg data: TBP⟩+≡
    procedure :: born_to_real_symm_factor_fs => region_data_born_to_real_symm_factor_fs

⟨fks regions: procedures⟩+≡
    function region_data_born_to_real_symm_factor_fs (reg_data, alr) result (factor)
        class(region_data_t), intent(in) :: reg_data
        integer, intent(in) :: alr
        real(default) :: factor
        associate (flv_real => reg_data%regions(alr)%flst_real, &
            flv_uborn => reg_data%regions(alr)%flst_uborn)
            factor = flv_real%prt_symm_fs / flv_uborn%prt_symm_fs
        end associate
    end function region_data_born_to_real_symm_factor_fs

⟨fks regions: reg data: TBP⟩+≡
    procedure :: final => region_data_final

⟨fks regions: procedures⟩+≡
    subroutine region_data_final (reg_data)
        class(region_data_t), intent(inout) :: reg_data
        if (allocated (reg_data%regions)) deallocate (reg_data%regions)
        if (allocated (reg_data%flv_born)) deallocate (reg_data%flv_born)
        if (allocated (reg_data%flv_real)) deallocate (reg_data%flv_real)
        if (allocated (reg_data%emitters)) deallocate (reg_data%emitters)
        if (allocated (reg_data%fks_mapping)) deallocate (reg_data%fks_mapping)
        if (allocated (reg_data%resonances)) deallocate (reg_data%resonances)
        if (allocated (reg_data%alr_contributors)) deallocate (reg_data%alr_contributors)
        if (allocated (reg_data%alr_to_i_contributor)) deallocate (reg_data%alr_to_i_contributor)
    end subroutine region_data_final

⟨fks regions: fks mapping: TBP⟩≡
    procedure (fks_mapping_dij), deferred :: dij

⟨fks regions: interfaces⟩+≡
    abstract interface
        function fks_mapping_dij (map, p, i, j, i_con) result (d)
            import
            real(default) :: d
            class(fks_mapping_t), intent(in) :: map
            type(vector4_t), intent(in), dimension(:) :: p
            integer, intent(in) :: i, j
            integer, intent(in), optional :: i_con

```

```

        end function fks_mapping_dij
    end interface

    <fks regions: fks mapping: TBP>+≡
        procedure (fks_mapping_compute_sumdij), deferred :: compute_sumdij

    <fks regions: interfaces>+≡
        abstract interface
            subroutine fks_mapping_compute_sumdij (map, sregion, p_real)
                import
                class(fks_mapping_t), intent(inout) :: map
                type(singular_region_t), intent(in) :: sregion
                type(vector4_t), intent(in), dimension(:) :: p_real
            end subroutine fks_mapping_compute_sumdij
        end interface

    <fks regions: fks mapping: TBP>+≡
        procedure (fks_mapping_svalue), deferred :: svalue

    <fks regions: interfaces>+≡
        abstract interface
            function fks_mapping_svalue (map, p, i, j, i_res) result (value)
                import
                real(default) :: value
                class(fks_mapping_t), intent(in) :: map
                type(vector4_t), intent(in), dimension(:) :: p
                integer, intent(in) :: i, j
                integer, intent(in), optional :: i_res
            end function fks_mapping_svalue
        end interface

    <fks regions: fks mapping: TBP>+≡
        procedure (fks_mapping_dij_soft), deferred :: dij_soft

    <fks regions: interfaces>+≡
        abstract interface
            function fks_mapping_dij_soft (map, p_born, p_soft, em, i_con) result (d)
                import
                real(default) :: d
                class(fks_mapping_t), intent(in) :: map
                type(vector4_t), intent(in), dimension(:) :: p_born
                type(vector4_t), intent(in) :: p_soft
                integer, intent(in) :: em
                integer, intent(in), optional :: i_con
            end function fks_mapping_dij_soft
        end interface

    <fks regions: fks mapping: TBP>+≡
        procedure (fks_mapping_compute_sumdij_soft), deferred :: compute_sumdij_soft

    <fks regions: interfaces>+≡
        abstract interface
            subroutine fks_mapping_compute_sumdij_soft (map, sregion, p_born, p_soft)
                import

```

```

        class(fks_mapping_t), intent(inout) :: map
        type(singular_region_t), intent(in) :: sregion
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(in) :: p_soft
    end subroutine fks_mapping_compute_sumdij_soft
end interface

<fks regions: fks mapping: TBP>+≡
    procedure (fks_mapping_svalue_soft), deferred :: svalue_soft

<fks regions: interfaces>+≡
    abstract interface
        function fks_mapping_svalue_soft (map, p_born, p_soft, em, i_res) result (value)
            import
            real(default) :: value
            class(fks_mapping_t), intent(in) :: map
            type(vector4_t), intent(in), dimension(:) :: p_born
            type(vector4_t), intent(in) :: p_soft
            integer, intent(in) :: em
            integer, intent(in), optional :: i_res
        end function fks_mapping_svalue_soft
    end interface

<fks regions: fks mapping default: TBP>≡
    procedure :: set_parameter => fks_mapping_default_set_parameter

<fks regions: procedures>+≡
    subroutine fks_mapping_default_set_parameter (map, n_in, dij_exp1, dij_exp2)
        class(fks_mapping_default_t), intent(inout) :: map
        integer, intent(in) :: n_in
        real(default), intent(in) :: dij_exp1, dij_exp2
        map%n_in = n_in
        map%exp_1 = dij_exp1
        map%exp_2 = dij_exp2
    end subroutine fks_mapping_default_set_parameter

```

Computes the d_{ij} -quantities defined als follows:

$$\begin{aligned}
 d_{0i} &= [E_i^2 (1 - y_i)]^{p_2} \\
 , d_{1i} &= [2E_i^2 (1 - y_i)]^{p_2} \\
 , d_{2i} &= [2E_i^2 (1 + y_i)]^{p_2} \\
 ,
 \end{aligned}$$

for initial state regions and

$$d_{ij} = \left[2(k_i \cdot k_j) \frac{E_i E_j}{(E_i + E_j)^2} \right]^{p_1}$$

for final state regions, c.f. [1002.2581, Eq. 4.23f]. The exponents p_1 and p_2 can be used for tuning the efficiency of the mapping and are set to 1 per default.

```

<fks regions: fks mapping default: TBP>+≡
    procedure :: dij => fks_mapping_default_dij

```

```

(fks regions: procedures)+≡
function fks_mapping_default_dij (map, p, i, j, i_con) result (d)
  real(default) :: d
  class(fks_mapping_default_t), intent(in) :: map
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in) :: i, j
  integer, intent(in), optional :: i_con
  d = zero
  if (map%pseudo_isr) then
    d = dij_threshold_gluon_from_top (i, j, p, map%exp_1)
  else if (i > map%n_in .and. j > map%n_in) then
    d = dij_fsr (p(i), p(j), map%exp_1)
  else
    d = dij_isr (map%n_in, i, j, p, map%exp_2)
  end if
contains

function dij_fsr (p1, p2, expo) result (d_ij)
  real(default) :: d_ij
  type(vector4_t), intent(in) :: p1, p2
  real(default), intent(in) :: expo
  real(default) :: E1, E2
  E1 = p1%p(0); E2 = p2%p(0)
  d_ij = (two * p1 * p2 * E1 * E2 / (E1 + E2)**2)**expo
end function dij_fsr

function dij_threshold_gluon_from_top (i, j, p, expo) result (d_ij)
  real(default) :: d_ij
  integer, intent(in) :: i, j
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(in) :: expo
  type(vector4_t) :: p_top
  if (i == THR_POS_B) then
    p_top = p(THR_POS_WP) + p(THR_POS_B)
  else
    p_top = p(THR_POS_WM) + p(THR_POS_BBAR)
  end if
  d_ij = dij_fsr (p_top, p(j), expo)
end function dij_threshold_gluon_from_top

function dij_isr (n_in, i, j, p, expo) result (d_ij)
  real(default) :: d_ij
  integer, intent(in) :: n_in, i, j
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(in) :: expo
  real(default) :: E, y
  select case (n_in)
  case (1)
    call get_emitter_variables (1, i, j, p, E, y)
    d_ij = (E**2 * (one - y**2))**expo
  case (2)
    if ((i == 0 .and. j > 2) .or. (j == 0 .and. i > 2)) then
      call get_emitter_variables (0, i, j, p, E, y)
      d_ij = (E**2 * (one - y**2))**expo
    end if
  end select
end function dij_isr

```



```

        else if ((i == 1 .and. j > 2) .or. (j == 1 .and. i > 2)) then
            call get_emitter_variables (1, i, j, p, E, y)
            d_ij = (two * E**2 * (one - y))**expo
        else if ((i == 2 .and. j > 2) .or. (j == 2 .and. i > 2)) then
            call get_emitter_variables (2, i, j, p, E, y)
            d_ij = (two * E**2 * (one + y))**expo
        end if
    end select
end function dij_isr

subroutine get_emitter_variables (i_check, i, j, p, E, y)
    integer, intent(in) :: i_check, i, j
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(out) :: E, y
    if (j == i_check) then
        E = energy (p(i))
        y = polar_angle_ct (p(i))
    else
        E = energy (p(j))
        y = polar_angle_ct(p(j))
    end if
end subroutine get_emitter_variables

end function fks_mapping_default_dij

```

Computes the quantity

$$\mathcal{D} = \sum_k \frac{1}{d_{0k}} + \sum_{kl} \frac{1}{d_{kl}}.$$

where the sum goes over all ftuples of a single singular region.

```

<fks regions: fks mapping default: TBP>+≡
    procedure :: compute_sumdij => fks_mapping_default_compute_sumdij

<fks regions: procedures>+≡
    subroutine fks_mapping_default_compute_sumdij (map, sregion, p_real)
        class(fks_mapping_default_t), intent(inout) :: map
        type(singular_region_t), intent(in) :: sregion
        type(vector4_t), intent(in), dimension(:) :: p_real
        real(default) :: d
        integer :: i_ftuple, i, j

        associate (ftuples => sregion%ftuples)
            d = zero
            do i_ftuple = 1, sregion%nregions
                call ftuples(i_ftuple)%get (i, j)
                map%pseudo_isr = ftuples(i_ftuple)%pseudo_isr
                d = d + one / map%dij (p_real, i, j)
            end do
        end associate
        map%sumdij = d
    end subroutine fks_mapping_default_compute_sumdij

```

Computes

$$S_i = \frac{1}{\mathcal{D}d_{0i}}$$

or

$$S_{ij} = \frac{1}{\mathcal{D}d_{ij}},$$

respectively.

```

⟨fks regions: fks mapping default: TBP⟩+≡
  procedure :: svalue => fks_mapping_default_svalue

⟨fks regions: procedures⟩+≡
  function fks_mapping_default_svalue (map, p, i, j, i_res) result (value)
    real(default) :: value
    class(fks_mapping_default_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_res
    value = one / (map%di_j(p, i, j) * map%sumdi_j)
  end function fks_mapping_default_svalue

```

In the soft limit, our treatment of the divergencies requires a modification of the mapping functions. Recall that there, the ratios of the d -functions must approach either 1 or 0. This means

$$\frac{d_{lm}}{d_{0m}} = \frac{(2k_l \cdot k_m) [E_l E_m / (E_l + E_m)^2]}{E_m^2 (1 - y^2)} \Big|_{k_m = E_m \hat{k}} \frac{E_l E_m^2}{(E_l + E_m)^2} \frac{2k_l \cdot \hat{k}}{E_m^2 (1 - y^2)} \xrightarrow{E_m \rightarrow 0} \frac{2k_l \cdot \hat{k}}{E_l} (1 - y^2),$$

where we have written the gluon momentum in terms of the soft momentum \hat{k} .

In the same limit

$$\frac{d_{lm}}{d_{nm}} = \frac{k_l \cdot \hat{k}}{k_n \cdot \hat{k}} \frac{E_n}{E_l}.$$

From these equations we can deduce the soft limit of d :

$$\begin{aligned}
d_0^{\text{soft}} &= 1 - y^2, \\
d_1^{\text{soft}} &= 2(1 - y), \\
d_2^{\text{soft}} &= 2(1 + y), \\
d_i^{\text{soft}} &= \frac{2k_i \cdot \hat{k}}{E_i}.
\end{aligned}$$

```

⟨fks regions: fks mapping default: TBP⟩+≡
  procedure :: dij_soft => fks_mapping_default_dij_soft

⟨fks regions: procedures⟩+≡
  function fks_mapping_default_dij_soft (map, p_born, p_soft, em, i_con) result (d)
    real(default) :: d
    class(fks_mapping_default_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    integer, intent(in) :: em
    integer, intent(in), optional :: i_con
    if (map%pseudo_isr) then

```

```

        d = dij_soft_threshold_gluon_from_top (em, p_born, p_soft, map%exp_1)
    else if (em <= map%n_in) then
        d = dij_soft_isr (map%n_in, p_soft, map%exp_2)
    else
        d = dij_soft_fsr (p_born(em), p_soft, map%exp_1)
    end if
contains

function dij_soft_threshold_gluon_from_top (em, p_born, p_soft, expo) result (dij_soft)
    real(default) :: dij_soft
    integer, intent(in) :: em
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    real(default), intent(in) :: expo
    type(vector4_t) :: p_top
    if (em == THR_POS_B) then
        p_top = p_born(THR_POS_WP) + p_born(THR_POS_B)
    else
        p_top = p_born(THR_POS_WM) + p_born(THR_POS_BBAR)
    end if
    dij_soft = dij_soft_fsr (p_top, p_soft, expo)
end function dij_soft_threshold_gluon_from_top

function dij_soft_fsr (p_em, p_soft, expo) result (dij_soft)
    real(default) :: dij_soft
    type(vector4_t), intent(in) :: p_em, p_soft
    real(default), intent(in) :: expo
    dij_soft = (two * p_em * p_soft / p_em%p(0))**expo
end function dij_soft_fsr

function dij_soft_isr (n_in, p_soft, expo) result (dij_soft)
    real(default) :: dij_soft
    integer, intent(in) :: n_in
    type(vector4_t), intent(in) :: p_soft
    real(default), intent(in) :: expo
    real(default) :: y
    y = polar_angle_ct (p_soft)
    select case (n_in)
    case (1)
        dij_soft = one - y**2
    case (2)
        select case (em)
        case (0)
            dij_soft = one - y**2
        case (1)
            dij_soft = two * (one - y)
        case (2)
            dij_soft = two * (one + y)
        case default
            dij_soft = zero
            call msg_fatal ("fks_mappings_default_dij_soft: n_in > 2")
        end select
    case default
        dij_soft = zero

```

```

        call msg_fatal ("fks_mappings_default_dij_soft: n_in > 2")
    end select
    dij_soft = dij_soft**expo
end function dij_soft_isr
end function fks_mapping_default_dij_soft

```

Computes the sum of all soft dijs required to normalize the soft S functions `s_alpha_soft` similar to `fks_mapping_default_compute_sumdij`. In the soft limit however, we need to skip all ftuples (i, j) in which j does not correspond to the emitted particle because those d_{ij} s are finite and thus their contribution to the soft S function vanishes in the limit of soft radiation. Technically, they would not vanish if computed here because the fixed `p_soft` at this point would not fit their actual emitter.

```

<fks regions: fks mapping default: TBP>+≡
    procedure :: compute_sumdij_soft => fks_mapping_default_compute_sumdij_soft

<fks regions: procedures>+≡
    subroutine fks_mapping_default_compute_sumdij_soft (map, sregion, p_born, p_soft)
        class(fks_mapping_default_t), intent(inout) :: map
        type(singular_region_t), intent(in) :: sregion
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(in) :: p_soft
        real(default) :: d
        integer :: i_ftuple, i, j
        integer :: nlegs
        d = zero
        nlegs = size (sregion%flst_real%flst)
        associate (ftuples => sregion%ftuples)
            do i_ftuple = 1, sregion%nregions
                call ftuples(i_ftuple)%get (i ,j)
                if (j == nlegs) then
                    map%pseudo_isr = ftuples(i_ftuple)%pseudo_isr
                    d = d + one / map%dij_soft (p_born, p_soft, i)
                end if
            end do
        end associate
        map%sumdij_soft = d
    end subroutine fks_mapping_default_compute_sumdij_soft

<fks regions: fks mapping default: TBP>+≡
    procedure :: svalue_soft => fks_mapping_default_svalue_soft

<fks regions: procedures>+≡
    function fks_mapping_default_svalue_soft (map, p_born, p_soft, em, i_res) result (value)
        real(default) :: value
        class(fks_mapping_default_t), intent(in) :: map
        type(vector4_t), intent(in), dimension(:) :: p_born
        type(vector4_t), intent(in) :: p_soft
        integer, intent(in) :: em
        integer, intent(in), optional :: i_res
        value = one / (map%sumdij_soft * map%dij_soft (p_born, p_soft, em))
    end function fks_mapping_default_svalue_soft

```

```

<fks regions: interfaces>+≡
  interface assignment(=)
    module procedure fks_mapping_default_assign
  end interface

```

```

<fks regions: procedures>+≡
  subroutine fks_mapping_default_assign (fks_map_out, fks_map_in)
    type(fks_mapping_default_t), intent(out) :: fks_map_out
    type(fks_mapping_default_t), intent(in) :: fks_map_in
    fks_map_out%exp_1 = fks_map_in%exp_1
    fks_map_out%exp_2 = fks_map_in%exp_2
    fks_map_out%n_in = fks_map_in%n_in
  end subroutine fks_mapping_default_assign

```

The $d_{ij,k}$ -functions for the resonance mapping are basically the same as in the default case, but the kinematical values here must be evaluated in the resonance frame of reference. The energy of parton i in a given resonance frame with momentum p_{res} is

$$E_i = \frac{p_i^0 \cdot p_{res}}{m_{res}}.$$

However, since the expressions only depend on ratios of four-momenta, we leave out the denominator because it will cancel out anyway.

```

<fks regions: fks mapping resonances: TBP>≡
  procedure :: dij => fks_mapping_resonances_dij

<fks regions: procedures>+≡
  function fks_mapping_resonances_dij (map, p, i, j, i_con) result (d)
    real(default) :: d
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    integer, intent(in) :: i, j
    integer, intent(in), optional :: i_con
    real(default) :: E1, E2
    integer :: ii_con
    if (present (i_con)) then
      ii_con = i_con
    else
      call msg_fatal ("Resonance mappings require resonance index as input!")
    end if
    d = 0
    if (i /= j) then
      if (i > 2 .and. j > 2) then
        associate (p_res => map%res_map%p_res (ii_con))
          E1 = p(i) * p_res
          E2 = p(j) * p_res
          d = two * p(i) * p(j) * E1 * E2 / (E1 + E2)**2
        end associate
      else
        call msg_fatal ("Resonance mappings are not implemented for ISR")
      end if
    end if
  end function fks_mapping_resonances_dij

```

Computes

$$S_{\alpha} = \frac{P^{f_r(\alpha)} d^{-1}(\alpha)}{\sum_{f'_r \in T(F_r(\alpha))} P^{f'_r} \sum_{\alpha' \in S_r(f'_r)} d^{-1}(\alpha')}.$$

(fks regions: fks mapping resonances: TBP) +=

procedure :: compute_sumdij => fks_mapping_resonances_compute_sumdij

(fks regions: procedures) +=

```
subroutine fks_mapping_resonances_compute_sumdij (map, sregion, p_real)
  class(fks_mapping_resonances_t), intent(inout) :: map
  type(singular_region_t), intent(in) :: sregion
  type(vector4_t), intent(in), dimension(:) :: p_real
  real(default) :: d, pfr
  integer :: i_res, i_reg, i, j, i_con
  integer :: nlegreal

  nlegreal = size (p_real)
  d = zero
  do i_reg = 1, sregion%nregions
    associate (ftuple => sregion%ftuples(i_reg))
      call ftuple%get (i, j)
      i_res = ftuple%i_res
    end associate
    pfr = map%res_map%get_resonance_value (i_res, p_real, nlegreal)
    i_con = sregion%i_reg_to_i_con (i_reg)
    d = d + pfr / map%dij (p_real, i, j, i_con)
  end do
  map%sumdij = d
end subroutine fks_mapping_resonances_compute_sumdij
```

(fks regions: fks mapping resonances: TBP) +=

procedure :: svalue => fks_mapping_resonances_svalue

(fks regions: procedures) +=

```
function fks_mapping_resonances_svalue (map, p, i, j, i_res) result (value)
  real(default) :: value
  class(fks_mapping_resonances_t), intent(in) :: map
  type(vector4_t), intent(in), dimension(:) :: p
  integer, intent(in) :: i, j
  integer, intent(in), optional :: i_res
  real(default) :: pfr
  integer :: i_gluon
  i_gluon = size (p)
  pfr = map%res_map%get_resonance_value (i_res, p, i_gluon)
  value = pfr / (map%dij (p, i, j, map%i_con) * map%sumdij)
end function fks_mapping_resonances_svalue
```

(fks regions: fks mapping resonances: TBP) +=

procedure :: get_resonance_weight => fks_mapping_resonances_get_resonance_weight

(fks regions: procedures) +=

```
function fks_mapping_resonances_get_resonance_weight (map, alr, p) result (pfr)
  real(default) :: pfr
  class(fks_mapping_resonances_t), intent(in) :: map
  integer, intent(in) :: alr
```

```

    type(vector4_t), intent(in), dimension(:) :: p
    pfr = map%res_map%get_weight (alr, p)
end function fks_mapping_resonances_get_resonance_weight

```

As above, the soft limit of $d_{ij,k}$ must be computed in the resonance frame of reference.

```

(fks regions: fks mapping resonances: TBP)+≡
  procedure :: dij_soft => fks_mapping_resonances_dij_soft

(fks regions: procedures)+≡
  function fks_mapping_resonances_dij_soft (map, p_born, p_soft, em, i_con) result (d)
    real(default) :: d
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    integer, intent(in) :: em
    integer, intent(in), optional :: i_con
    real(default) :: E1, E2
    integer :: ii_con
    type(vector4_t) :: pb
    if (present (i_con)) then
      ii_con = i_con
    else
      call msg_fatal ("fks_mapping_resonances requires resonance index")
    end if
    associate (p_res => map%res_map%p_res(ii_con))
      pb = p_born(em)
      E1 = pb * p_res
      E2 = p_soft * p_res
      d = two * pb * p_soft * E1 * E2 / E1**2
    end associate
  end function fks_mapping_resonances_dij_soft

```

```

(fks regions: fks mapping resonances: TBP)+≡
  procedure :: compute_sumdij_soft => fks_mapping_resonances_compute_sumdij_soft

(fks regions: procedures)+≡
  subroutine fks_mapping_resonances_compute_sumdij_soft (map, sregion, p_born, p_soft)
    class(fks_mapping_resonances_t), intent(inout) :: map
    type(singular_region_t), intent(in) :: sregion
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    real(default) :: d
    real(default) :: pfr
    integer :: i_res, i, j, i_reg, i_con
    integer :: nlegs

    d = zero
    nlegs = size (sregion%flst_real%flst)
    do i_reg = 1, sregion%nregions
      associate (ftuple => sregion%ftuples(i_reg))
        call ftuple%get(i, j)
        i_res = ftuple%i_res
      end associate
    end do
  end subroutine fks_mapping_resonances_compute_sumdij_soft

```

```

        pfr = map%res_map%get_resonance_value (i_res, p_born)
        i_con = sregion%i_reg_to_i_con (i_reg)
        if (j == nlegs) d = d + pfr / map%dij_soft (p_born, p_soft, i, i_con)
    end do
    map%sumdij_soft = d
end subroutine fks_mapping_resonances_compute_sumdij_soft

<fks regions: fks mapping resonances: TBP>+≡
procedure :: svalue_soft => fks_mapping_resonances_svalue_soft

<fks regions: procedures>+≡
function fks_mapping_resonances_svalue_soft (map, p_born, p_soft, em, i_res) result (value)
    real(default) :: value
    class(fks_mapping_resonances_t), intent(in) :: map
    type(vector4_t), intent(in), dimension(:) :: p_born
    type(vector4_t), intent(in) :: p_soft
    integer, intent(in) :: em
    integer, intent(in), optional :: i_res
    real(default) :: pfr
    pfr = map%res_map%get_resonance_value (i_res, p_born)
    value = pfr / (map%sumdij_soft * map%dij_soft (p_born, p_soft, em, map%i_con))
end function fks_mapping_resonances_svalue_soft

<fks regions: fks mapping resonances: TBP>+≡
procedure :: set_resonance_momentum => fks_mapping_resonances_set_resonance_momentum

<fks regions: procedures>+≡
subroutine fks_mapping_resonances_set_resonance_momentum (map, p)
    class(fks_mapping_resonances_t), intent(inout) :: map
    type(vector4_t), intent(in) :: p
    map%res_map%p_res = p
end subroutine fks_mapping_resonances_set_resonance_momentum

<fks regions: fks mapping resonances: TBP>+≡
procedure :: set_resonance_momenta => fks_mapping_resonances_set_resonance_momenta

<fks regions: procedures>+≡
subroutine fks_mapping_resonances_set_resonance_momenta (map, p)
    class(fks_mapping_resonances_t), intent(inout) :: map
    type(vector4_t), intent(in), dimension(:) :: p
    map%res_map%p_res = p
end subroutine fks_mapping_resonances_set_resonance_momenta

<fks regions: interfaces>+≡
interface assignment(=)
    module procedure fks_mapping_resonances_assign
end interface

<fks regions: procedures>+≡
subroutine fks_mapping_resonances_assign (fks_map_out, fks_map_in)
    type(fks_mapping_resonances_t), intent(out) :: fks_map_out
    type(fks_mapping_resonances_t), intent(in) :: fks_map_in
    fks_map_out%exp_1 = fks_map_in%exp_1

```



```

fks_map_out%exp_2 = fks_map_in%exp_2
fks_map_out%res_map = fks_map_in%res_map
end subroutine fks_mapping_resonances_assign

```

(fks regions: public)+≡

```

public :: create_resonance_histories_for_threshold

```

(fks regions: procedures)+≡

```

function create_resonance_histories_for_threshold () result (res_history)
  type(resonance_history_t) :: res_history
  res_history%n_resonances = 2
  allocate (res_history%resonances (2))
  allocate (res_history%resonances(1)%contributors%c(2))
  allocate (res_history%resonances(2)%contributors%c(2))
  res_history%resonances(1)%contributors%c = [THR_POS_WP, THR_POS_B]
  res_history%resonances(2)%contributors%c = [THR_POS_WM, THR_POS_BBAR]
end function create_resonance_histories_for_threshold

```

(fks regions: public)+≡

```

public :: setup_region_data_for_test

```

(fks regions: procedures)+≡

```

subroutine setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, nlo_corr_type, &
  alpha_pow, alphas_pow)
  integer, intent(in) :: n_in, alpha_pow, alphas_pow
  integer, intent(in), dimension(:,:) :: flv_born, flv_real
  type(string_t), intent(in) :: nlo_corr_type
  type(region_data_t), intent(out) :: reg_data
  type(model_t), pointer :: test_model => null ()
  call create_test_model (var_str ("SM"), test_model)
  call test_model%set_real (var_str ("me"), 0._default)
  call test_model%set_real (var_str ("mmu"), 0._default)
  call test_model%set_real (var_str ("mtau"), 0._default)
  call test_model%set_real (var_str ("ms"), 0._default)
  call test_model%set_real (var_str ("mc"), 0._default)
  call test_model%set_real (var_str ("mb"), 0._default)
  call reg_data%init (n_in, test_model, flv_born, flv_real, nlo_corr_type, alpha_pow, &
    alphas_pow)
end subroutine setup_region_data_for_test

```

27.3.1 Unit tests

```

<fks_regions_ut.f90>≡
  <File header>

  module fks_regions_ut
    use unit_tests
    use fks_regions_util

    <Standard module head>

    <fks regions: public test>

    contains

    <fks regions: test driver>

  end module fks_regions_ut
<fks_regions_util.f90>≡
  <File header>

  module fks_regions_util

    <Use strings>
    use format_utils, only: write_separator
    use os_interface
    use models

    use fks_regions

    <Standard module head>

    <fks regions: test declarations>

    contains

    <fks regions: tests>

  end module fks_regions_util
<fks regions: public test>≡
  public :: fks_regions_test
<fks regions: test driver>≡
  subroutine fks_regions_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    call test(fks_regions_1, "fks_regions_1", &
      "Test flavor structure utilities", u, results)
    call test(fks_regions_2, "fks_regions_2", &
      "Test singular regions for final-state radiation for n = 2", &
      u, results)
    call test(fks_regions_3, "fks_regions_3", &
      "Test singular regions for final-state radiation for n = 3", &
      u, results)
    call test(fks_regions_4, "fks_regions_4", &
      "Test singular regions for final-state radiation for n = 4", &

```

```

        u, results)
call test(fks_regions_5, "fks_regions_5", &
        "Test singular regions for final-state radiation for n = 5", &
        u, results)
call test(fks_regions_6, "fks_regions_6", &
        "Test singular regions for initial-state radiation", &
        u, results)
call test(fks_regions_7, "fks_regions_7", &
        "Check Latex output", u, results)
call test(fks_regions_8, "fks_regions_8", &
        "Test singular regions for initial-state photon contributions", &
        u, results)
end subroutine fks_regions_test

```

(fks regions: test declarations)≡
public :: fks_regions_1

(fks regions: tests)≡

```

subroutine fks_regions_1 (u)
    integer, intent(in) :: u
    type(flv_structure_t) :: flv_born, flv_real
    type(model_t), pointer :: test_model => null ()
    write (u, "(A)") "* Test output: fks_regions_1"
    write (u, "(A)") "* Purpose: Test utilities of flavor structure manipulation"
    write (u, "(A)")

    call create_test_model (var_str ("SM"), test_model)

    flv_born = [11, -11, 2, -2]
    flv_real = [11, -11, 2, -2, 21]
    flv_born%n_in = 2; flv_real%n_in = 2
    write (u, "(A)") "* Valid splittings of ee -> uu"
    write (u, "(A)") "Born Flavors: "
    call flv_born%write (u)
    write (u, "(A)") "Real Flavors: "
    call flv_real%write (u)
    write (u, "(A,L1)") "3, 4 (2, -2) : ", flv_real%valid_pair (3, 4, flv_born, test_model)
    write (u, "(A,L1)") "4, 3 (-2, 2) : ", flv_real%valid_pair (4, 3, flv_born, test_model)
    write (u, "(A,L1)") "3, 5 (2, 21) : ", flv_real%valid_pair (3, 5, flv_born, test_model)
    write (u, "(A,L1)") "5, 3 (21, 2) : ", flv_real%valid_pair (5, 3, flv_born, test_model)
    write (u, "(A,L1)") "4, 5 (-2, 21): ", flv_real%valid_pair (4, 5, flv_born, test_model)
    write (u, "(A,L1)") "5, 4 (21, -2): ", flv_real%valid_pair (5, 4, flv_born, test_model)
    call write_separator (u)

    call flv_born%final ()
    call flv_real%final ()

    flv_born = [2, -2, 11, -11]
    flv_real = [2, -2, 11, -11, 21]
    flv_born%n_in = 2; flv_real%n_in = 2
    write (u, "(A)") "* Valid splittings of uu -> ee"
    write (u, "(A)") "Born Flavors: "
    call flv_born%write (u)
    write (u, "(A)") "Real Flavors: "

```

```

call flv_real%write (u)
write (u, "(A,L1)") "1, 2 (2, -2) : " , flv_real%valid_pair (1, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 1 (-2, 2) : " , flv_real%valid_pair (2, 1, flv_born, test_model)
write (u, "(A,L1)") "5, 2 (21, -2): " , flv_real%valid_pair (5, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 5 (-2, 21): " , flv_real%valid_pair (2, 5, flv_born, test_model)
write (u, "(A,L1)") "1, 5 (21, 2) : " , flv_real%valid_pair (5, 1, flv_born, test_model)
write (u, "(A,L1)") "5, 1 (2, 21) : " , flv_real%valid_pair (1, 5, flv_born, test_model)
call flv_real%final ()
flv_real = [21, -2, 11, -11, -2]
flv_real%n_in = 2
write (u, "(A)") "Real Flavors: "
call flv_real%write (u)
write (u, "(A,L1)") "1, 2 (21, -2): " , flv_real%valid_pair (1, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 1 (-2, 21): " , flv_real%valid_pair (2, 1, flv_born, test_model)
write (u, "(A,L1)") "5, 2 (-2, -2): " , flv_real%valid_pair (5, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 5 (-2, -2): " , flv_real%valid_pair (2, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 1 (-2, 21): " , flv_real%valid_pair (5, 1, flv_born, test_model)
write (u, "(A,L1)") "1, 5 (21, -2): " , flv_real%valid_pair (1, 5, flv_born, test_model)
call flv_real%final ()
flv_real = [2, 21, 11, -11, 2]
flv_real%n_in = 2
write (u, "(A)") "Real Flavors: "
call flv_real%write (u)
write (u, "(A,L1)") "1, 2 (2, 21) : " , flv_real%valid_pair (1, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 1 (21, 2) : " , flv_real%valid_pair (2, 1, flv_born, test_model)
write (u, "(A,L1)") "5, 2 (2, 21) : " , flv_real%valid_pair (5, 2, flv_born, test_model)
write (u, "(A,L1)") "2, 5 (21, 2) : " , flv_real%valid_pair (2, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 1 (2, 2) : " , flv_real%valid_pair (5, 1, flv_born, test_model)
write (u, "(A,L1)") "1, 5 (2, 2) : " , flv_real%valid_pair (1, 5, flv_born, test_model)
call write_separator (u)

call flv_born%final ()
call flv_real%final ()

flv_born = [11, -11, 2, -2, 21]
flv_real = [11, -11, 2, -2, 21, 21]
flv_born%n_in = 2; flv_real%n_in = 2
write (u, "(A)") "* Valid splittings of ee -> uug"
write (u, "(A)") "Born Flavors: "
call flv_born%write (u)
write (u, "(A)") "Real Flavors: "
call flv_real%write (u)
write (u, "(A,L1)") "3, 4 (2, -2) : " , flv_real%valid_pair (3, 4, flv_born, test_model)
write (u, "(A,L1)") "4, 3 (-2, 2) : " , flv_real%valid_pair (4, 3, flv_born, test_model)
write (u, "(A,L1)") "3, 5 (2, 21) : " , flv_real%valid_pair (3, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 3 (21, 2) : " , flv_real%valid_pair (5, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 5 (-2, 21): " , flv_real%valid_pair (4, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 4 (21, -2): " , flv_real%valid_pair (5, 4, flv_born, test_model)
write (u, "(A,L1)") "3, 6 (2, 21) : " , flv_real%valid_pair (3, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 3 (21, 2) : " , flv_real%valid_pair (6, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 6 (-2, 21): " , flv_real%valid_pair (4, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 4 (21, -2): " , flv_real%valid_pair (6, 4, flv_born, test_model)
write (u, "(A,L1)") "5, 6 (21, 21): " , flv_real%valid_pair (5, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 5 (21, 21): " , flv_real%valid_pair (6, 5, flv_born, test_model)

```

```

call flv_real%final ()
flv_real = [11, -11, 2, -2, 1, -1]
flv_real%n_in = 2
write (u, "(A)") "Real Flavours (exemplary g -> dd splitting): "
call flv_real%write (u)
write (u, "(A,L1)") "3, 4 (2, -2) : " , flv_real%valid_pair (3, 4, flv_born, test_model)
write (u, "(A,L1)") "4, 3 (-2, 2) : " , flv_real%valid_pair (4, 3, flv_born, test_model)
write (u, "(A,L1)") "3, 5 (2, 1) : " , flv_real%valid_pair (3, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 3 (1, 2) : " , flv_real%valid_pair (5, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 5 (-2, 1) : " , flv_real%valid_pair (4, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 4 (1, -2) : " , flv_real%valid_pair (5, 4, flv_born, test_model)
write (u, "(A,L1)") "3, 6 (2, -1) : " , flv_real%valid_pair (3, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 3 (-1, 2) : " , flv_real%valid_pair (6, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 6 (-2, -1) : " , flv_real%valid_pair (4, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 4 (-1, -2) : " , flv_real%valid_pair (6, 4, flv_born, test_model)
write (u, "(A,L1)") "5, 6 (1, -1) : " , flv_real%valid_pair (5, 6, flv_born, test_model)
write (u, "(A,L1)") "6, 5 (-1, 1) : " , flv_real%valid_pair (6, 5, flv_born, test_model)
call write_separator (u)

call flv_born%final ()
call flv_real%final ()

flv_born = [6, -5, 2, -1 ]
flv_real = [6, -5, 2, -1, 21]
flv_born%n_in = 1; flv_real%n_in = 1
write (u, "(A)") "* Valid splittings of t -> b u d~"
write (u, "(A)") "Born Flavours: "
call flv_born%write (u)
write (u, "(A)") "Real Flavours: "
call flv_real%write (u)
write (u, "(A,L1)") "1, 2 (6, -5) : " , flv_real%valid_pair (1, 2, flv_born, test_model)
write (u, "(A,L1)") "1, 3 (6, 2) : " , flv_real%valid_pair (1, 3, flv_born, test_model)
write (u, "(A,L1)") "1, 4 (6, -1) : " , flv_real%valid_pair (1, 4, flv_born, test_model)
write (u, "(A,L1)") "2, 1 (-5, 6) : " , flv_real%valid_pair (2, 1, flv_born, test_model)
write (u, "(A,L1)") "3, 1 (2, 6) : " , flv_real%valid_pair (3, 1, flv_born, test_model)
write (u, "(A,L1)") "4, 1 (-1, 6) : " , flv_real%valid_pair (4, 1, flv_born, test_model)
write (u, "(A,L1)") "2, 3 (-5, 2) : " , flv_real%valid_pair (2, 3, flv_born, test_model)
write (u, "(A,L1)") "2, 4 (-5, -1) : " , flv_real%valid_pair (2, 4, flv_born, test_model)
write (u, "(A,L1)") "3, 2 (2, -5) : " , flv_real%valid_pair (3, 2, flv_born, test_model)
write (u, "(A,L1)") "4, 2 (-1, -5) : " , flv_real%valid_pair (4, 2, flv_born, test_model)
write (u, "(A,L1)") "3, 4 (2, -1) : " , flv_real%valid_pair (3, 4, flv_born, test_model)
write (u, "(A,L1)") "4, 3 (-1, 2) : " , flv_real%valid_pair (4, 3, flv_born, test_model)
write (u, "(A,L1)") "1, 5 (6, 21) : " , flv_real%valid_pair (1, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 1 (21, 6) : " , flv_real%valid_pair (5, 1, flv_born, test_model)
write (u, "(A,L1)") "2, 5 (-5, 21) : " , flv_real%valid_pair (2, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 2 (21, 5) : " , flv_real%valid_pair (5, 2, flv_born, test_model)
write (u, "(A,L1)") "3, 5 (2, 21) : " , flv_real%valid_pair (3, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 3 (21, 2) : " , flv_real%valid_pair (5, 3, flv_born, test_model)
write (u, "(A,L1)") "4, 5 (-1, 21) : " , flv_real%valid_pair (4, 5, flv_born, test_model)
write (u, "(A,L1)") "5, 4 (21, -1) : " , flv_real%valid_pair (5, 4, flv_born, test_model)

call flv_born%final ()
call flv_real%final ()

```

```

end subroutine fks_regions_1

<fks regions: test declarations>+=
public :: fks_regions_2

<fks regions: tests>+=
subroutine fks_regions_2 (u)
  integer, intent(in) :: u
  integer :: n_flv_born, n_flv_real
  integer :: n_legs_born, n_legs_real
  integer :: n_in
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(region_data_t) :: reg_data
  write (u, "(A)") "* Test output: fks_regions_2"
  write (u, "(A)") "* Create singular regions for processes with up to four singular regions"
  write (u, "(A)") "* ee -> qq with QCD corrections"
  write (u, "(A)")

  n_flv_born = 1; n_flv_real = 1
  n_legs_born = 4; n_legs_real = 5
  n_in = 2

  allocate (flv_born (n_legs_born, n_flv_born))
  allocate (flv_real (n_legs_real, n_flv_real))
  flv_born (:, 1) = [11, -11, 2, -2]
  flv_real (:, 1) = [11, -11, 2, -2, 21]
  call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 0)
  call reg_data%check_consistency (.false., u)
  call reg_data%write (u)

  deallocate (flv_born, flv_real)
  call reg_data%final ()
  call write_separator (u)

  write (u, "(A)") "* ee -> qq with EW corrections"
  write (u, "(A)")

  allocate (flv_born (n_legs_born, n_flv_born))
  allocate (flv_real (n_legs_real, n_flv_real))
  flv_born (:, 1) = [11, -11, 2, -2]
  flv_real (:, 1) = [11, -11, 2, -2, 22]

  call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("EW"), 2, 0)
  call reg_data%check_consistency (.false., u)
  call reg_data%write (u)

  deallocate (flv_born, flv_real)
  call reg_data%final ()
  call write_separator (u)

  write (u, "(A)") "* ee -> tt"
  write (u, "(A)")
  write (u, "(A)") "* This process has four singular regions because they are not equivalent."

```

```

n_flv_born = 1; n_flv_real = 1
n_legs_born = 6; n_legs_real = 7
n_in = 2

allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))
flv_born (:, 1) = [11, -11, 6, -6, 6, -6]
flv_real (:, 1) = [11, -11, 6, -6, 6, -6, 21]
call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 4, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()
end subroutine fks_regions_2

```

<fks regions: test declarations>+≡

```
public :: fks_regions_3
```

<fks regions: tests>+≡

```

subroutine fks_regions_3 (u)
  integer, intent(in) :: u
  integer :: n_flv_born, n_flv_real
  integer :: n_legs_born, n_legs_real
  integer :: n_in, i, j
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(region_data_t) :: reg_data
  write (u, "(A)") "* Test output: fks_regions_3"
  write (u, "(A)") "* Create singular regions for processes with three final-state particles"

  write (u, "(A)") "* ee -> qqg"
  write (u, "(A)")
  n_flv_born = 1; n_flv_real = 2
  n_legs_born = 5; n_legs_real = 6
  n_in = 2
  allocate (flv_born (n_legs_born, n_flv_born))
  allocate (flv_real (n_legs_real, n_flv_real))

  flv_born (:, 1) = [11, -11, 2, -2, 21]
  flv_real (:, 1) = [11, -11, 2, -2, 21, 21]
  flv_real (:, 2) = [11, -11, 2, -2, 1, -1]

  call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 1)
  call reg_data%check_consistency (.false., u)
  call reg_data%write (u)

  deallocate (flv_born, flv_real)
  call reg_data%final ()
  call write_separator (u)

  write (u, "(A)") "* ee -> qqA"
  write (u, "(A)")
  n_flv_born = 1; n_flv_real = 2
  n_legs_born = 5; n_legs_real = 6

```



```

n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, 2, -2, 22]
flv_real (:, 1) = [11, -11, 2, -2, 22, 22]
flv_real (:, 2) = [11, -11, 2, -2, 11, -11]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("EW"), 3, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()
call write_separator (u)

write (u, "(A)") "* ee -> jet jet jet"
write (u, "(A)") "* with jet = u:U:d:D:s:S:c:C:b:B:gl"
write (u, "(A)")
n_flv_born = 5; n_flv_real = 22
n_legs_born = 5; n_legs_real = 6
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -4, 4, 21]
flv_born (:, 2) = [11, -11, -2, 2, 21]
flv_born (:, 3) = [11, -11, -5, 5, 21]
flv_born (:, 4) = [11, -11, -3, 3, 21]
flv_born (:, 5) = [11, -11, -1, 1, 21]
flv_real (:, 1) = [11, -11, -4, -4, 4, 4]
flv_real (:, 2) = [11, -11, -4, -2, 2, 4]
flv_real (:, 3) = [11, -11, -4, 4, 21, 21]
flv_real (:, 4) = [11, -11, -4, -5, 4, 5]
flv_real (:, 5) = [11, -11, -4, -3, 4, 3]
flv_real (:, 6) = [11, -11, -4, -1, 2, 3]
flv_real (:, 7) = [11, -11, -4, -1, 4, 1]
flv_real (:, 8) = [11, -11, -2, -2, 2, 2]
flv_real (:, 9) = [11, -11, -2, 2, 21, 21]
flv_real (:, 10) = [11, -11, -2, -5, 2, 5]
flv_real (:, 11) = [11, -11, -2, -3, 2, 3]
flv_real (:, 12) = [11, -11, -2, -3, 4, 1]
flv_real (:, 13) = [11, -11, -2, -1, 2, 1]
flv_real (:, 14) = [11, -11, -5, -5, 5, 5]
flv_real (:, 15) = [11, -11, -5, -3, 3, 5]
flv_real (:, 16) = [11, -11, -5, -1, 1, 5]
flv_real (:, 17) = [11, -11, -5, 5, 21, 21]
flv_real (:, 18) = [11, -11, -3, -3, 3, 3]
flv_real (:, 19) = [11, -11, -3, -1, 1, 3]
flv_real (:, 20) = [11, -11, -3, 3, 21, 21]
flv_real (:, 21) = [11, -11, -1, -1, 1, 1]
flv_real (:, 22) = [11, -11, -1, 1, 21, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 1)

```

```

call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()
call write_separator (u)

write (u, "(A)") "* ee -> L L A"
write (u, "(A)") "* with L = e2:E2:e3:E3"
write (u, "(A)")
n_flv_born = 2; n_flv_real = 6
n_legs_born = 5; n_legs_real = 6
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -15, 15, 22]
flv_born (:, 2) = [11, -11, -13, 13, 22]

flv_real (:, 1) = [11, -11, -15, -15, 15, 15]
flv_real (:, 2) = [11, -11, -15, -13, 13, 13]
flv_real (:, 3) = [11, -11, -13, -15, 13, 15]
flv_real (:, 4) = [11, -11, -15, 15, 22, 22]
flv_real (:, 5) = [11, -11, -13, -13, 13, 13]
flv_real (:, 6) = [11, -11, -13, 13, 22, 22]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("EW"), 3, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

end subroutine fks_regions_3

<fks regions: test declarations>+≡
public :: fks_regions_4

<fks regions: tests>+≡
subroutine fks_regions_4 (u)
  integer, intent(in) :: u
  integer :: n_flv_born, n_flv_real
  integer :: n_legs_born, n_legs_real
  integer :: n_in
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(region_data_t) :: reg_data
  write (u, "(A)") "* Test output: fks_regions_4"
  write (u, "(A)") "* Create singular regions for processes with four final-state particles"
  write (u, "(A)") "* ee -> 4 jet"
  write (u, "(A)") "* with jet = u:U:d:D:s:S:c:C:b:B:gl"
  write (u, "(A)")
  n_flv_born = 22; n_flv_real = 22
  n_legs_born = 6; n_legs_real = 7
  n_in = 2

```

```

allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -4, -4, 4, 4]
flv_born (:, 2) = [11, -11, -4, -2, 2, 4]
flv_born (:, 3) = [11, -11, -4, 4, 21, 21]
flv_born (:, 4) = [11, -11, -4, -5, 4, 5]
flv_born (:, 5) = [11, -11, -4, -3, 4, 3]
flv_born (:, 6) = [11, -11, -4, -1, 2, 3]
flv_born (:, 7) = [11, -11, -4, -1, 4, 1]
flv_born (:, 8) = [11, -11, -2, -2, 2, 2]
flv_born (:, 9) = [11, -11, -2, 2, 21, 21]
flv_born (:, 10) = [11, -11, -2, -5, 2, 5]
flv_born (:, 11) = [11, -11, -2, -3, 2, 3]
flv_born (:, 12) = [11, -11, -2, -3, 4, 1]
flv_born (:, 13) = [11, -11, -2, -1, 2, 1]
flv_born (:, 14) = [11, -11, -5, -5, 5, 5]
flv_born (:, 15) = [11, -11, -5, -3, 3, 5]
flv_born (:, 16) = [11, -11, -5, -1, 1, 5]
flv_born (:, 17) = [11, -11, -5, 5, 21, 21]
flv_born (:, 18) = [11, -11, -3, -3, 3, 3]
flv_born (:, 19) = [11, -11, -3, -1, 1, 3]
flv_born (:, 20) = [11, -11, -3, -3, 21, 21]
flv_born (:, 21) = [11, -11, -1, -1, 1, 1]
flv_born (:, 22) = [11, -11, -1, 1, 21, 21]
flv_real (:, 1) = [11, -11, -4, -4, 4, 4, 21]
flv_real (:, 2) = [11, -11, -4, -2, 2, 4, 21]
flv_real (:, 3) = [11, -11, -4, 4, 21, 21, 21]
flv_real (:, 4) = [11, -11, -4, -5, 4, 5, 21]
flv_real (:, 5) = [11, -11, -4, -3, 4, 3, 21]
flv_real (:, 6) = [11, -11, -4, -1, 2, 3, 21]
flv_real (:, 7) = [11, -11, -4, -1, 4, 1, 21]
flv_real (:, 8) = [11, -11, -2, -2, 2, 2, 21]
flv_real (:, 9) = [11, -11, -2, 2, 21, 21, 21]
flv_real (:, 10) = [11, -11, -2, -5, 2, 5, 21]
flv_real (:, 11) = [11, -11, -2, -3, 2, 3, 21]
flv_real (:, 12) = [11, -11, -2, -3, 4, 1, 21]
flv_real (:, 13) = [11, -11, -2, -1, 2, 1, 21]
flv_real (:, 14) = [11, -11, -5, -5, 5, 5, 21]
flv_real (:, 15) = [11, -11, -5, -3, 3, 5, 21]
flv_real (:, 16) = [11, -11, -5, -1, 1, 5, 21]
flv_real (:, 17) = [11, -11, -5, 5, 21, 21, 21]
flv_real (:, 18) = [11, -11, -3, -3, 3, 3, 21]
flv_real (:, 19) = [11, -11, -3, -1, 1, 3, 21]
flv_real (:, 20) = [11, -11, -3, 3, 21, 21, 21]
flv_real (:, 21) = [11, -11, -1, -1, 1, 1, 21]
flv_real (:, 22) = [11, -11, -1, 1, 21, 21, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 2)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

```

```

call write_separator (u)

write (u, "(A)") "* ee -> bbmumu with QCD corrections"
write (u, "(A)")
n_flv_born = 1; n_flv_real = 1
n_legs_born = 6; n_legs_real = 7
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -5, 5, -13, 13]
flv_real (:, 1) = [11, -11, -5, 5, -13, 13, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 4, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()
call write_separator (u)

write (u, "(A)") "* ee -> bbmumu with EW corrections"
write (u, "(A)")
n_flv_born = 1; n_flv_real = 1
n_legs_born = 6; n_legs_real = 7
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [11, -11, -5, 5, -13, 13]
flv_real (:, 1) = [11, -11, -5, 5, -13, 13, 22]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 4, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

end subroutine fks_regions_4

```

<fks regions: test declarations>+≡

```
public :: fks_regions_5
```

<fks regions: tests>+≡

```

subroutine fks_regions_5 (u)
  integer, intent(in) :: u
  integer :: n_flv_born, n_flv_real
  integer :: n_legs_born, n_legs_real
  integer :: n_in
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(region_data_t) :: reg_data
  write (u, "(A)") "* Test output: fks_regions_5"
  write (u, "(A)") "* Create singular regions for processes with five final-state particles"

```

```

write (u, "(A)") "* ee -> 5 jet"
write (u, "(A)") "* with jet = u:U:d:D:s:S:c:C:b:B:gl"
write (u, "(A)")
n_flv_born = 22; n_flv_real = 67
n_legs_born = 7; n_legs_real = 8
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

```

```

flv_born (:,1) = [11,-11,-4,-4,4,4,21]
flv_born (:,2) = [11,-11,-4,-2,2,4,21]
flv_born (:,3) = [11,-11,-4,4,21,21,21]
flv_born (:,4) = [11,-11,-4,-5,4,5,21]
flv_born (:,5) = [11,-11,-4,-3,4,3,21]
flv_born (:,6) = [11,-11,-4,-1,2,3,21]
flv_born (:,7) = [11,-11,-4,-1,4,1,21]
flv_born (:,8) = [11,-11,-2,-2,2,2,21]
flv_born (:,9) = [11,-11,-2,2,21,21,21]
flv_born (:,10) = [11,-11,-2,-5,2,5,21]
flv_born (:,11) = [11,-11,-2,-3,2,3,21]
flv_born (:,12) = [11,-11,-2,-3,4,1,21]
flv_born (:,13) = [11,-11,-2,-1,2,1,21]
flv_born (:,14) = [11,-11,-5,-5,5,5,21]
flv_born (:,15) = [11,-11,-5,-3,3,5,21]
flv_born (:,16) = [11,-11,-5,-1,1,5,21]
flv_born (:,17) = [11,-11,-5,5,21,21,21]
flv_born (:,18) = [11,-11,-3,-3,3,3,21]
flv_born (:,19) = [11,-11,-3,-1,1,3,21]
flv_born (:,20) = [11,-11,-3,3,21,21,21]
flv_born (:,21) = [11,-11,-1,-1,1,1,21]
flv_born (:,22) = [11,-11,-1,1,21,21,21]

```

```

flv_real (:,1) = [11,-11,-4,-4,-4,4,4]
flv_real (:,2) = [11,-11,-4,-4,-2,2,4]
flv_real (:,3) = [11,-11,-4,-4,4,4,21]
flv_real (:,4) = [11,-11,-4,-4,-5,4,4]
flv_real (:,5) = [11,-11,-4,-4,-3,4,4]
flv_real (:,6) = [11,-11,-4,-4,-1,2,4]
flv_real (:,7) = [11,-11,-4,-4,-1,4,4]
flv_real (:,8) = [11,-11,-4,-2,-2,2,4]
flv_real (:,9) = [11,-11,-4,-2,2,4,21]
flv_real (:,10) = [11,-11,-4,-2,-5,2,4]
flv_real (:,11) = [11,-11,-4,-2,-3,2,4]
flv_real (:,12) = [11,-11,-4,-2,-3,4,4]
flv_real (:,13) = [11,-11,-4,-2,-1,2,4]
flv_real (:,14) = [11,-11,-4,-2,-1,2,4]
flv_real (:,15) = [11,-11,-4,4,21,21,21]
flv_real (:,16) = [11,-11,-4,-5,4,5,21]
flv_real (:,17) = [11,-11,-4,-5,-5,4,5]
flv_real (:,18) = [11,-11,-4,-5,-3,4,5]
flv_real (:,19) = [11,-11,-4,-5,-1,2,5]
flv_real (:,20) = [11,-11,-4,-5,-1,4,5]
flv_real (:,21) = [11,-11,-4,-3,4,3,21]

```

```

flv_real (:,22) = [11,-11,-4,-3,-3,4,3,3]
flv_real (:,23) = [11,-11,-4,-3,-1,2,3,3]
flv_real (:,24) = [11,-11,-4,-3,-1,4,1,3]
flv_real (:,25) = [11,-11,-4,-1,2,3,21,21]
flv_real (:,26) = [11,-11,-4,-1,4,1,21,21]
flv_real (:,27) = [11,-11,-4,-1,-1,2,1,3]
flv_real (:,28) = [11,-11,-4,-1,-1,4,1,1]
flv_real (:,29) = [11,-11,-2,-2,-2,2,2,2]
flv_real (:,30) = [11,-11,-2,-2,2,2,21,21]
flv_real (:,31) = [11,-11,-2,-2,-5,2,2,5]
flv_real (:,32) = [11,-11,-2,-2,-3,2,2,3]
flv_real (:,33) = [11,-11,-2,-2,-3,2,4,1]
flv_real (:,34) = [11,-11,-2,-2,-1,2,2,1]
flv_real (:,35) = [11,-11,-2,2,21,21,21,21]
flv_real (:,36) = [11,-11,-2,-5,2,5,21,21]
flv_real (:,37) = [11,-11,-2,-5,-5,2,5,5]
flv_real (:,38) = [11,-11,-2,-5,-3,2,3,5]
flv_real (:,39) = [11,-11,-2,-5,-3,4,1,5]
flv_real (:,40) = [11,-11,-2,-5,-1,2,1,5]
flv_real (:,41) = [11,-11,-2,-3,2,3,21,21]
flv_real (:,42) = [11,-11,-2,-3,4,1,21,21]
flv_real (:,43) = [11,-11,-2,-3,-3,2,3,3]
flv_real (:,44) = [11,-11,-2,-3,-3,4,1,3]
flv_real (:,45) = [11,-11,-2,-3,-1,2,1,3]
flv_real (:,46) = [11,-11,-2,-3,-1,4,1,1]
flv_real (:,47) = [11,-11,-2,-1,2,1,21,21]
flv_real (:,48) = [11,-11,-2,-1,-1,2,1,1]
flv_real (:,49) = [11,-11,-5,-5,-5,5,5,5]
flv_real (:,50) = [11,-11,-5,-5,-3,3,5,5]
flv_real (:,51) = [11,-11,-5,-5,-1,1,5,5]
flv_real (:,52) = [11,-11,-5,-5,5,5,21,21]
flv_real (:,53) = [11,-11,-5,-3,-3,3,3,5]
flv_real (:,54) = [11,-11,-5,-3,-1,1,3,5]
flv_real (:,55) = [11,-11,-5,-3,3,5,21,21]
flv_real (:,56) = [11,-11,-5,-1,-1,1,1,5]
flv_real (:,57) = [11,-11,-5,-1,1,5,21,21]
flv_real (:,58) = [11,-11,-5,5,21,21,21,21]
flv_real (:,59) = [11,-11,-3,-3,-3,3,3,3]
flv_real (:,60) = [11,-11,-3,-3,-1,1,3,3]
flv_real (:,61) = [11,-11,-3,-3,3,3,21,21]
flv_real (:,62) = [11,-11,-3,-1,-1,1,1,3]
flv_real (:,63) = [11,-11,-3,-1,1,3,21,21]
flv_real (:,64) = [11,-11,-3,3,21,21,21,21]
flv_real (:,65) = [11,-11,-1,-1,-1,1,1,1]
flv_real (:,66) = [11,-11,-1,-1,1,1,21,21]
flv_real (:,67) = [11,-11,-1,1,21,21,21,21]

```

```

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 3)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

```

```

end subroutine fks_regions_5

<fks regions: test declarations>+≡
public :: fks_regions_6

<fks regions: tests>+≡
subroutine fks_regions_6 (u)
  integer, intent(in) :: u
  integer :: n_flv_born, n_flv_real
  integer :: n_legs_born, n_legs_real
  integer :: n_in
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(region_data_t) :: reg_data
  integer :: i, j
  integer, dimension(10) :: flavors
  write (u, "(A)") "* Test output: fks_regions_6"
  write (u, "(A)") "* Create table of singular regions for Drell Yan"
  write (u, "(A)")

  n_flv_born = 10; n_flv_real = 30
  n_legs_born = 4; n_legs_real = 5
  n_in = 2
  allocate (flv_born (n_legs_born, n_flv_born))
  allocate (flv_real (n_legs_real, n_flv_real))
  flavors = [-5, -4, -3, -2, -1, 1, 2, 3, 4, 5]
  do i = 1, n_flv_born
    flv_born (3:4, i) = [11, -11]
  end do
  do j = 1, n_flv_born
    flv_born (1, j) = flavors (j)
    flv_born (2, j) = -flavors (j)
  end do

  do i = 1, n_flv_real
    flv_real (3:4, i) = [11, -11]
  end do
  i = 1
  do j = 1, n_flv_real
    if (mod (j, 3) == 1) then
      flv_real (1, j) = flavors (i)
      flv_real (2, j) = -flavors (i)
      flv_real (5, j) = 21
    else if (mod (j, 3) == 2) then
      flv_real (1, j) = flavors (i)
      flv_real (2, j) = 21
      flv_real (5, j) = flavors (i)
    else
      flv_real (1, j) = 21
      flv_real (2, j) = -flavors (i)
      flv_real (5, j) = -flavors (i)
      i = i + 1
    end if
  end do
end do

```

```

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

call write_separator (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

write (u, "(A)") "* Create table of singular regions for hadronic top decay"
write (u, "(A)")
n_flv_born = 1; n_flv_real = 1
n_legs_born = 4; n_legs_real = 5
n_in = 1
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))

flv_born (:, 1) = [6, -5, 2, -1]
flv_real (:, 1) = [6, -5, 2, -1, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 0, 2)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

call write_separator (u)

deallocate (flv_born, flv_real)
call reg_data%final ()

write (u, "(A)") "* Create table of singular regions for dijet s sbar -> jet jet"
write (u, "(A)") "* With jet = u:d:gl"
write (u, "(A)")

n_flv_born = 3; n_flv_real = 3
n_legs_born = 4; n_legs_real = 5
n_in = 2
allocate (flv_born (n_legs_born, n_flv_born))
allocate (flv_real (n_legs_real, n_flv_real))
do i = 1, n_flv_born
    flv_born (1:2, i) = [3, -3]
end do
flv_born (3, :) = [1, 2, 21]
flv_born (4, :) = [-1, -2, 21]

do i = 1, n_flv_real
    flv_real (1:2, i) = [3, -3]
end do
flv_real (3, :) = [1, 2, 21]
flv_real (4, :) = [-1, -2, 21]
flv_real (5, :) = [21, 21, 21]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 0, 2)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)

```



```

        call reg_data%final ()

    end subroutine fks_regions_6

<fks regions: test declarations>+≡
    public :: fks_regions_7

<fks regions: tests>+≡
    subroutine fks_regions_7 (u)
        integer, intent(in) :: u
        integer :: n_flv_born, n_flv_real
        integer :: n_legs_born, n_legs_real
        integer :: n_in
        integer, dimension(:,:), allocatable :: flv_born, flv_real
        type(region_data_t) :: reg_data
        write (u, "(A)") "* Test output: fks_regions_7"
        write (u, "(A)") "* Create table of singular regions for ee -> qq"
        write (u, "(A)")

        n_flv_born = 1; n_flv_real = 1
        n_legs_born = 4; n_legs_real = 5
        n_in = 2

        allocate (flv_born (n_legs_born, n_flv_born))
        allocate (flv_real (n_legs_real, n_flv_real))
        flv_born (:, 1) = [11, -11, 2, -2]
        flv_real (:, 1) = [11, -11, 2, -2, 21]
        call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("QCD"), 2, 0)
        call reg_data%write_latex (u)
        call reg_data%final ()

    end subroutine fks_regions_7

<fks regions: test declarations>+≡
    public :: fks_regions_8

<fks regions: tests>+≡
    subroutine fks_regions_8 (u)
        integer, intent(in) :: u
        integer :: n_flv_born, n_flv_real
        integer :: n_legs_born, n_legs_real
        integer :: n_in
        integer, dimension(:,:), allocatable :: flv_born, flv_real
        type(region_data_t) :: reg_data
        integer :: i, j
        integer, dimension(10) :: flavors
        write (u, "(A)") "* Test output: fks_regions_8"
        write (u, "(A)") "* Create table of singular regions for ee -> ee"
        write (u, "(A)")

        n_flv_born = 1; n_flv_real = 3
        n_legs_born = 4; n_legs_real = 5
        n_in = 2
        allocate (flv_born (n_legs_born, n_flv_born))

```

```

allocate (flv_real (n_legs_real, n_flv_real))
flv_born (:, 1) = [11, -11, -11, 11]

flv_real (:, 1) = [11, -11, -11, 11, 22]
flv_real (:, 2) = [11, 22, -11, 11, 11]
flv_real (:, 3) = [22, -11, 11, -11, -11]

call setup_region_data_for_test (n_in, flv_born, flv_real, reg_data, var_str ("EW"), 2, 0)
call reg_data%check_consistency (.false., u)
call reg_data%write (u)
call reg_data%final ()

end subroutine fks_regions_8

```

27.4 Virtual contribution to the cross section

```

<virtual.f90>≡
  <File header>

  module virtual

    <Use kinds>
    <Use strings>
    <Use debug>
    use numeric_utils
    use constants
    use diagnostics
    use pdg_arrays
    use models
    use model_data, only: model_data_t, field_data_t
    use physics_defs
    use sm_physics
    use lorentz
    use flavors
    use nlo_data, only: get_threshold_momenta, nlo_settings_t
    use nlo_data, only: ASSOCIATED_LEG_PAIR
    use fks_regions

    <Standard module head>

    <virtual: public>

    <virtual: parameters>

    <virtual: types>

    contains

    <virtual: procedures>

  end module virtual

```

```

<virtual: public>≡
    public :: virtual_t

<virtual: types>≡
    type :: virtual_t
        type(nlo_settings_t) :: settings
        real(default), dimension(:,:,:), allocatable :: gamma_0, gamma_p, c_flv
        real(default) :: ren_scale2, fac_scale, es_scale2
        integer, dimension(:), allocatable :: n_is_neutrinos
        integer :: n_in, n_legs, n_flv
        logical :: bad_point = .false.
        type(string_t) :: selection
        real(default), dimension(:), allocatable :: sqme_born
        real(default), dimension(:), allocatable :: sqme_virt_fin
        real(default), dimension(:,:,:), allocatable :: sqme_color_c
        real(default), dimension(:,:,:), allocatable :: sqme_charge_c
        logical :: has_pdfs = .false.
    contains
        <virtual: virtual: TBP>
    end type virtual_t

<virtual: virtual: TBP>≡
    procedure :: init => virtual_init

<virtual: procedures>≡
    subroutine virtual_init (virt, flv_born, n_in, settings, model, has_pdfs)
        class(virtual_t), intent(inout) :: virt
        integer, intent(in), dimension(:,:) :: flv_born
        integer, intent(in) :: n_in
        type(nlo_settings_t), intent(in) :: settings
        class(model_data_t), intent(in) :: model
        logical, intent(in) :: has_pdfs
        integer :: i_flv, n_corr
        n_corr = 2
        virt%n_legs = size (flv_born, 1); virt%n_flv = size (flv_born, 2)
        virt%n_in = n_in
        allocate (virt%sqme_born (virt%n_flv))
        allocate (virt%sqme_virt_fin (virt%n_flv))
        allocate (virt%sqme_color_c (virt%n_legs, virt%n_legs, virt%n_flv))
        allocate (virt%sqme_charge_c (virt%n_legs, virt%n_legs, virt%n_flv))
        allocate (virt%gamma_0 (virt%n_legs, virt%n_flv, n_corr), &
            virt%gamma_p (virt%n_legs, virt%n_flv, n_corr), &
            virt%c_flv (virt%n_legs, virt%n_flv, n_corr))
        call virt%init_constants (flv_born, settings%fks_template%n_f, model)
        allocate (virt%n_is_neutrinos (virt%n_flv))
        virt%n_is_neutrinos = 0
        do i_flv = 1, virt%n_flv
            if (is_neutrino (flv_born(1, i_flv))) &
                virt%n_is_neutrinos(i_flv) = virt%n_is_neutrinos(i_flv) + 1
            if (is_neutrino (flv_born(2, i_flv))) &
                virt%n_is_neutrinos(i_flv) = virt%n_is_neutrinos(i_flv) + 1
        end do
        select case (char (settings%virtual_selection))
        case ("Full", "OLP", "Subtraction")
            virt%selection = settings%virtual_selection

```

```

case default
  call msg_fatal ('Virtual selection: Possible values are "Full", "OLP" or "Subtraction')
end select
virt%settings = settings
virt%has_pdfs = has_pdfs
contains

function is_neutrino (flv) result (neutrino)
  integer, intent(in) :: flv
  logical :: neutrino
  neutrino = (abs(flv) == 12 .or. abs(flv) == 14 .or. abs(flv) == 16)
end function is_neutrino

end subroutine virtual_init

```

The virtual subtraction terms contain Casimir operators and derived constants, listed below:

$$C(q) = C(\bar{q}) = C_F, \quad (27.2)$$

$$C(g) = C_A, \quad (27.3)$$

$$\gamma(q) = \gamma(\bar{q}) = \frac{3}{2}C_F, \quad (27.4)$$

$$\gamma(g) = \frac{11}{6}C_A - \frac{2}{3}T_F N_f, \quad (27.5)$$

$$\gamma'(q) = \gamma'(\bar{q}) = \left(\frac{13}{2} - \frac{2\pi^2}{3} \right) C_F, \quad (27.6)$$

$$\gamma'(g) = \left(\frac{67}{9} - \frac{2\pi^2}{3} \right) C_A - \frac{23}{9}T_F N_f. \quad (27.7)$$

For uncolored particles, `virtual_init_constants` sets C , γ and γ' to zero.

```

<virtual: virtual: TBP>+≡
  procedure :: init_constants => virtual_init_constants

<virtual: procedures>+≡
  subroutine virtual_init_constants (virt, flv_born, nf_input, model)
    class(virtual_t), intent(inout) :: virt
    integer, intent(in), dimension(:,:) :: flv_born
    integer, intent(in) :: nf_input
    type(string_t), dimension(2) :: corr_type
    class(model_data_t), intent(in) :: model
    type(field_data_t), pointer :: field
    integer :: i_part, i_flv, pdg, i_corr
    real(default) :: nf, CA_factor, TR_sum
    real(default), dimension(:,:), allocatable :: CF_factor, TR_factor
    type(flavor_t) :: flv
    allocate (CF_factor (size (flv_born, 1), size (flv_born, 2)), &
              TR_factor (size (flv_born, 1), size (flv_born, 2)))
    TR_sum = 0
    corr_type (1) = "QCD"; corr_type (2) = "EW"
    do i_corr = 1, 2
      if (i_corr == 1) then
        CA_factor = CA; CF_factor = CF; TR_factor = TR

```

```

        nf = real(nf_input, default)
        TR_sum = nf * TR
    else
        CA_factor = zero
        do i_flv = 1, size (flv_born, 2)
            do i_part = 1, size (flv_born, 1)
                call flv%init (flv_born(i_part, i_flv), model)
                CF_factor(i_part, i_flv) = (flv%get_charge ())**2
                TR_factor(i_part, i_flv) = (flv%get_charge ())**2
                if (is_quark (flv_born (i_part, i_flv))) &
                    TR_factor(i_part, i_flv) = NC * TR_factor(i_part, i_flv)
            end do
        end do
        do pdg = 1, nf_input
            field => model%get_field_ptr (pdg)
            TR_sum = TR_sum + NC*field%get_charge()**2
        end do
        do pdg = 11, 15, 2
            field => model%get_field_ptr (pdg)
            if (field%get_mass() > 0) exit
            TR_sum = TR_sum + field%get_charge()**2
        end do
    end if
    do i_flv = 1, size (flv_born, 2)
        do i_part = 1, size (flv_born, 1)
            if (is_massless_vectorboson (flv_born(i_part, i_flv), corr_type (i_corr))) then
                virt%gamma_0(i_part, i_flv, i_corr) = 11._default / 6._default * CA_factor &
                    - two / three * TR_sum
                virt%gamma_p(i_part, i_flv, i_corr) = (67._default / 9._default &
                    - two * pi**2 / three) * CA_factor &
                    - 23._default / 9._default * TR_sum
                virt%c_flv(i_part, i_flv, i_corr) = CA_factor
            else if (is_corresponding_fermion (flv_born(i_part, i_flv), corr_type (i_corr))) then
                virt%gamma_0(i_part, i_flv, i_corr) = 1.5_default * CF_factor(i_part, i_flv)
                virt%gamma_p(i_part, i_flv, i_corr) = (6.5_default - two * pi**2 / three) * CF_fac
                virt%c_flv(i_part, i_flv, i_corr) = CF_factor(i_part, i_flv)
            else if (is_massive_vectorboson (flv_born(i_part, i_flv), corr_type (i_corr))) then
                virt%gamma_0(i_part, i_flv, i_corr) = zero
                virt%gamma_p(i_part, i_flv, i_corr) = zero
                virt%c_flv(i_part, i_flv, i_corr) = CF_factor(i_part, i_flv)
            else
                virt%gamma_0(i_part, i_flv, i_corr) = zero
                virt%gamma_p(i_part, i_flv, i_corr) = zero
                virt%c_flv(i_part, i_flv, i_corr) = zero
            end if
        end do
    end do
end do
contains
function is_massless_vectorboson (pdg_nr, nlo_corr_type)
    logical :: is_massless_vectorboson
    integer, intent(in) :: pdg_nr
    type(string_t), intent(in) :: nlo_corr_type
    is_massless_vectorboson = .false.

```

```

        if (nlo_corr_type == "QCD") then
            is_massless_vectorboson = is_gluon (pdg_nr)
        else if (nlo_corr_type == "EW") then
            is_massless_vectorboson = is_photon (pdg_nr)
        end if
    end function is_massless_vectorboson
function is_corresponding_fermion (pdg_nr, nlo_corr_type)
    logical :: is_corresponding_fermion
    integer, intent(in) :: pdg_nr
    type(string_t), intent(in) :: nlo_corr_type
    is_corresponding_fermion = .false.
    if (nlo_corr_type == "QCD") then
        is_corresponding_fermion = is_quark (pdg_nr)
    else if (nlo_corr_type == "EW") then
        is_corresponding_fermion = is_fermion (pdg_nr)
    end if
end function is_corresponding_fermion
function is_massive_vectorboson (pdg_nr, nlo_corr_type)
    logical :: is_massive_vectorboson
    integer, intent(in) :: pdg_nr
    type(string_t), intent(in) :: nlo_corr_type
    is_massive_vectorboson = .false.
    if (nlo_corr_type == "EW") then
        is_massive_vectorboson = is_massive_vector (pdg_nr)
    end if
end function is_massive_vectorboson
end subroutine virtual_init_constants

```

Set the renormalization scale. If the input is zero, use the center-of-mass energy.

```

<virtual: virtual: TBP>+≡
    procedure :: set_ren_scale => virtual_set_ren_scale

<virtual: procedures>+≡
    subroutine virtual_set_ren_scale (virt, p, ren_scale)
        class(virtual_t), intent(inout) :: virt
        type(vector4_t), intent(in), dimension(:) :: p
        real(default), intent(in) :: ren_scale
        if (ren_scale > 0) then
            virt%ren_scale2 = ren_scale**2
        else
            virt%ren_scale2 = (p(1) + p(2))**2
        end if
    end subroutine virtual_set_ren_scale

<virtual: virtual: TBP>+≡
    procedure :: set_fac_scale => virtual_set_fac_scale

<virtual: procedures>+≡
    subroutine virtual_set_fac_scale (virt, p, fac_scale)
        class(virtual_t), intent(inout) :: virt
        type(vector4_t), dimension(:), intent(in) :: p
        real(default), optional :: fac_scale
        if (present (fac_scale)) then
            virt%fac_scale = fac_scale
        end if
    end subroutine virtual_set_fac_scale

```

```

else
  virt%fac_scale = (p(1) + p(2))*1
end if
end subroutine virtual_set_fac_scale

```

```

<virtual: virtual: TBP>+=
  procedure :: set_ellis_sexton_scale => virtual_set_ellis_sexton_scale
<virtual: procedures>+=
  subroutine virtual_set_ellis_sexton_scale (virt, Q)
    class(virtual_t), intent(inout) :: virt
    real(default), intent(in) :: Q
    virt%es_scale2 = Q * Q
  end subroutine virtual_set_ellis_sexton_scale

```

The virtual-subtracted matrix element is given by the equation

$$\mathcal{V} = \frac{\alpha_s}{2\pi} \left(\mathcal{Q}\mathcal{B} + \sum \mathcal{I}_{ij} \mathcal{B}_{ij} + \mathcal{V}_{fin} \right), \quad (27.8)$$

The expressions for \mathcal{Q} can be found in equations 27.9 and 27.11. The expressions for \mathcal{I}_{ij} can be found in equations (27.13), (27.14), (27.29), depending on whether the particles involved in the radiation process are massive or massless.

If two or more flavor structures would produce the same amplitude we only compute one and use the `eqv_index` to copy the result to the others (if `reuse_amplitudes_fks` is true).

```

<virtual: virtual: TBP>+=
  procedure :: evaluate => virtual_evaluate
<virtual: procedures>+=
  subroutine virtual_evaluate (virt, reg_data, alpha_coupling, &
    p_born, separate_uborns, sqme_virt)
    class(virtual_t), intent(inout) :: virt
    type(region_data_t), intent(in) :: reg_data
    real(default), dimension(2), intent(in) :: alpha_coupling
    type(vector4_t), intent(in), dimension(:) :: p_born
    logical, intent(in) :: separate_uborns
    real(default), dimension(:), intent(inout) :: sqme_virt
    integer, dimension(:), allocatable :: eqv_flv_index
    real(default), dimension(:), allocatable :: sqme_virt_arr
    real(default) :: s, s_o_Q2
    real(default), dimension(reg_data%n_flv_born) :: QB, BI
    integer :: i_flv, ii_flv, alr, i_corr
    logical, dimension(:), allocatable :: flv_evaluated
    integer, dimension(:), allocatable :: corr_index
    logical :: alr_qcd, alr_ew
    QB = zero; BI = zero
    allocate (flv_evaluated(reg_data%n_flv_born))
    allocate (sqme_virt_arr(reg_data%n_flv_born))
    sqme_virt_arr = zero
    flv_evaluated = .false.
    if (virt%bad_point) return
    if (debug2_active (D_VIRTUAL)) then
      print *, 'Compute virtual component using alpha = ', alpha_coupling
    end if
  end subroutine virtual_evaluate

```

```

        print *, 'Virtual selection: ', char (virt%selection)
        print *, 'virt%es_scale2 = ', virt%es_scale2 !!! Debugging
    end if
    s = sum (p_born(1 : virt%n_in))*2
    if (virt%settings%factorization_mode == FACTORIZATION_THRESHOLD) &
        call set_s_for_threshold ()
    s_o_Q2 = s / virt%es_scale2 * virt%settings%fks_template%xi_cut**2
    eqv_flv_index = reg_data%eqv_flv_index_born
    do i_flv = 1, reg_data%n_flv_born
        alr_qcd = .false.; alr_ew = .false.
        do alr = 1, reg_data%n_regions
            if (i_flv == reg_data%regions(alr)%uborn_index) then
                if (reg_data%regions(alr)%nlo_correction_type == "QCD") then
                    alr_qcd = .true.
                else if (reg_data%regions(alr)%nlo_correction_type == "EW") then
                    alr_ew = .true.
                end if
            end if
        end do
        if (alr_qcd .and. alr_ew) then
            allocate (corr_index (2))
            corr_index (1) = 1; corr_index (2) = 2
        else
            allocate (corr_index (1))
            corr_index (1) = 0
            if (alr_qcd) then
                corr_index (1) = 1
            else if (alr_ew) then
                corr_index (1) = 2
            end if
        end if
        if (.not. flv_evaluated(eqv_flv_index(i_flv)) .and. corr_index(1) > 0) then
            if (virt%selection == var_str ("Full") .or. virt%selection == var_str ("OLP")) then
                !!! A factor of alpha_coupling/twopi is assumed to be included in vfin
                sqme_virt_arr(i_flv) = sqme_virt_arr(i_flv) + virt%sqme_virt_fin(i_flv)
            end if
            do i_corr = 1, size (corr_index)
                if (virt%selection == var_str ("Full") .or. &
                    virt%selection == var_str ("Subtraction")) then
                    call virt%evaluate_initial_state (i_flv, corr_index (i_corr), reg_data, QB)
                    call virt%compute_collinear_contribution &
                        (i_flv, corr_index (i_corr), p_born, sqrt(s), reg_data, QB)
                    select case (virt%settings%factorization_mode)
                    case (FACTORIZATION_THRESHOLD)
                        call virt%compute_eikonals_threshold (i_flv, p_born, s_o_Q2, QB, BI)
                    case default
                        call virt%compute_massive_self_eikonals &
                            (i_flv, corr_index (i_corr), p_born, s_o_Q2, reg_data, QB)
                        call virt%compute_eikonals &
                            (i_flv, corr_index (i_corr), p_born, s_o_Q2, reg_data, BI)
                    end select
                if (debug2_active (D_VIRTUAL)) then
                    if (corr_index (i_corr) == 1) then
                        print *, 'Correction type: QCD'
                    end if
                end if
            end do
        end if
    end do
end do

```



```

        else
            print *, 'Correction type: EW'
        end if
        print *, 'Evaluate i_flv: ', i_flv
        print *, 'sqme_born: ', virt%sqme_born (i_flv)
        print *, 'Q * sqme_born: ', alpha_coupling / twopi * QB(i_flv)
        print *, 'BI: ', alpha_coupling / twopi * BI(i_flv)
        print *, 'vfin: ', virt%sqme_virt_fin (i_flv)
    end if
    sqme_virt_arr(i_flv) = sqme_virt_arr(i_flv) &
        + alpha_coupling (corr_index (i_corr))/ twopi * (QB(i_flv) + BI(i_flv))
    end if
end do
if (.not. (debug_active (D_VIRTUAL) .or. &
    debug2_active (D_VIRTUAL))) flv_evaluated(eqv_flv_index(i_flv)) = .true.
else
    sqme_virt_arr(i_flv) = sqme_virt_arr(eqv_flv_index(i_flv))
end if
if (separate_uborns) then
    sqme_virt(i_flv) = sqme_virt(i_flv) + sqme_virt_arr(i_flv)
else
    sqme_virt(1) = sqme_virt(1) + sqme_virt_arr(i_flv)
end if
deallocate (corr_index)
end do
if (debug2_active (D_VIRTUAL)) then
    call msg_debug2 (D_VIRTUAL, "virtual-subtracted matrix element(s): ")
    print *, sqme_virt
end if
do i_flv = 1, reg_data%n_flv_born
    if (virt%n_is_neutrinos(i_flv) > 0) &
        sqme_virt = sqme_virt * virt%n_is_neutrinos(i_flv) * two
end do
contains
subroutine set_s_for_threshold ()
    use ttv_formfactors, only: m1s_to_mpole
    real(default) :: mtop2
    mtop2 = m1s_to_mpole (sqrt(s))*2
    if (s < four * mtop2) s = four * mtop2
end subroutine set_s_for_threshold

end subroutine virtual_evaluate

```

<virtual: virtual: TBP>+≡

procedure :: compute_eikonals => virtual_compute_eikonals

<virtual: procedures>+≡

```

subroutine virtual_compute_eikonals (virtual, i_flv, i_corr, &
    p_born, s_o_Q2, reg_data, BI)
    class(virtual_t), intent(inout) :: virtual
    integer, intent(in) :: i_flv, i_corr
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in) :: s_o_Q2
    type(region_data_t), intent(in) :: reg_data

```

```

real(default), intent(inout), dimension(:) :: BI
integer :: i, j
real(default) :: I_ij, BI_tmp
BI_tmp = zero
! TODO vincent_r: Split the procedure into one computing QCD eikonals and one computing QED ei
! TODO vincent_r: In the best case, remove the dependency on reg_data completely.
associate (flst_born => reg_data%flv_born(i_flv))
  do i = 1, virtual%n_legs
    do j = 1, virtual%n_legs
      if (i /= j) then
        if (i_corr == 1) then
          if (flst_born%colored(i) .and. flst_born%colored(j)) then
            I_ij = compute_eikonal_factor (p_born, flst_born%massive, &
              i, j, s_o_Q2)
            BI_tmp = BI_tmp + virtual%sqme_color_c (i, j, i_flv) * I_ij
            if (debug2_active (D_VIRTUAL)) &
              print *, 'b-ij: ', i, j, virtual%sqme_color_c (i, j, i_flv), 'I-ij: ',
            end if
          else if (i_corr == 2) then
            I_ij = compute_eikonal_factor (p_born, flst_born%massive, &
              i, j, s_o_Q2)
            BI_tmp = BI_tmp + virtual%sqme_charge_c (i, j, i_flv) * I_ij
            if (debug2_active (D_VIRTUAL)) &
              print *, 'b-ij: ', virtual%sqme_charge_c (i, j, i_flv), 'I-ij: ', I_ij
            end if
          else if (debug2_active (D_VIRTUAL)) then
            if (i_corr == 1) then
              print *, 'b-ij: ', i, j, virtual%sqme_color_c (i, j, i_flv), 'I-ij: ', I_ij
            else if (i_corr == 2) then
              print *, 'b-ij: ', i, j, virtual%sqme_charge_c (i, j, i_flv), 'I-ij: ', I_ij
            end if
          end if
        end if
      end do
    end do
    if (virtual%settings%use_internal_color_correlations .or. i_corr == 2) &
      BI_tmp = BI_tmp * virtual%sqme_born (i_flv)
    end associate
    BI(i_flv) = BI(i_flv) + BI_tmp
end subroutine virtual_compute_eikonals

```

<virtual: virtual: TBP>+≡
 procedure :: compute_eikonals_threshold => virtual_compute_eikonals_threshold

<virtual: procedures>+≡
 subroutine virtual_compute_eikonals_threshold (virtual, i_flv, &
 p_born, s_o_Q2, QB, BI)
 class(virtual_t), intent(in) :: virtual
 integer, intent(in) :: i_flv
 type(vector4_t), intent(in), dimension(:) :: p_born
 real(default), intent(in) :: s_o_Q2
 real(default), intent(inout), dimension(:) :: QB
 real(default), intent(inout), dimension(:) :: BI
 type(vector4_t), dimension(4) :: p_thr
 integer :: leg

```

BI = zero; p_thr = get_threshold_momenta (p_born)
call compute_massive_self_eikonals (virtual%sqme_born(i_flg), QB(i_flg))
do leg = 1, 2
  BI(i_flg) = BI(i_flg) + evaluate_leg_pair (ASSOCIATED_LEG_PAIR(leg), i_flg)
end do
contains
subroutine compute_massive_self_eikonals (sqme_born, QB)
  real(default), intent(in) :: sqme_born
  real(default), intent(inout) :: QB
  integer :: i
  if (debug_on) call msg_debug2 (D_VIRTUAL, "compute_massive_self_eikonals")
  if (debug_on) call msg_debug2 (D_VIRTUAL, "s_o_Q2", s_o_Q2)
  if (debug_on) call msg_debug2 (D_VIRTUAL, "log (s_o_Q2)", log (s_o_Q2))
  do i = 1, 4
    QB = QB - (cf * (log (s_o_Q2) - 0.5_default * I_m_eps (p_thr(i)))) &
      * sqme_born
  end do
end subroutine compute_massive_self_eikonals

function evaluate_leg_pair (i_start, i_flg) result (b_ij_times_I)
  real(default) :: b_ij_times_I
  integer, intent(in) :: i_start, i_flg
  real(default) :: I_ij
  integer :: i, j
  b_ij_times_I = zero
  do i = i_start, i_start + 1
    do j = i_start, i_start + 1
      if (i /= j) then
        I_ij = compute_eikonal_factor &
          (p_thr, [.true., .true., .true., .true.], i, j, s_o_Q2)
        b_ij_times_I = b_ij_times_I + &
          virtual%sqme_color_c (i, j, i_flg) * I_ij
        if (debug2_active (D_VIRTUAL)) &
          print *, 'b_ij: ', virtual%sqme_color_c (i, j, i_flg), 'I_ij: ', I_ij
      end if
    end do
  end do
  if (virtual%settings%use_internal_color_correlations) &
    b_ij_times_I = b_ij_times_I * virtual%sqme_born (i_flg)
  if (debug2_active (D_VIRTUAL)) then
    print *, 'internal color: ', virtual%settings%use_internal_color_correlations
    print *, 'b_ij_times_I = ', b_ij_times_I
    print *, 'QB = ', QB
  end if
end function evaluate_leg_pair
end subroutine virtual_compute_eikonals_threshold

<virtual: virtual: TBP>+=
  procedure :: set_bad_point => virtual_set_bad_point

<virtual: procedures>+=
  subroutine virtual_set_bad_point (virt, value)
    class(virtual_t), intent(inout) :: virt
    logical, intent(in) :: value

```

```

virt%bad_point = value
end subroutine virtual_set_bad_point

```

The collinear limit of $\tilde{\mathcal{R}}$ can be integrated over the radiation degrees of freedom, giving the collinear contribution to the virtual component. Its general structure is $\mathcal{Q} \cdot \mathcal{B}$. The initial-state contribution to \mathcal{Q} is simply given by

$$\mathcal{Q} = -\log \frac{\mu_F^2}{Q^2} (\gamma(\mathcal{I}_1) + 2C(\mathcal{I}_1) \log(\xi_{\text{cut}}) + \gamma(\mathcal{I}_2) + 2C(\mathcal{I}_2) \log(\xi_{\text{cut}})), \quad (27.9)$$

where Q^2 is the Ellis-Sexton scale and γ is as in eqns. 27.4 and 27.5.

`virtual_evaluate_initial_state` computes this quantity. The loop over the initial-state particles is only executed if we are dealing with a scattering process, because for decays there are no virtual initial-initial interactions.

```

<virtual: virtual: TBP>+=
  procedure :: evaluate_initial_state => virtual_evaluate_initial_state

<virtual: procedures>+=
  subroutine virtual_evaluate_initial_state (virt, i_flv, i_corr, reg_data, QB)
    class(virtual_t), intent(inout) :: virt
    type(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: i_flv, i_corr
    real(default), intent(inout), dimension(:) :: QB
    real(default) :: sqme_born_virt
    integer :: i
    sqme_born_virt = zero
    if (reg_data%nlo_correction_type == "EW" .and. i_corr == 1 &
        .and. qcd_ew_interferences (reg_data%flv_born(i_flv)%flst)) then
      do i = 1, size (reg_data%flv_born(i_flv)%flst)
        if (is_quark (reg_data%flv_born(i_flv)%flst (i))) then
          sqme_born_virt = -virt%sqme_color_c (i, i, i_flv)/CF
          exit
        end if
      end do
    else
      sqme_born_virt = virt%sqme_born (i_flv)
    end if
    if (virt%n_in == 2) then
      do i = 1, virt%n_in
        QB(i_flv) = QB(i_flv) - (virt%gamma_0 (i, i_flv, i_corr) &
          + two * virt%c_flv(i, i_flv, i_corr) &
          * log (virt%settings%fks_template%xi_cut)) &
          * log(virt%fac_scale**2 / virt%es_scale2) * sqme_born_virt
      end do
    end if
  end subroutine virtual_evaluate_initial_state

```

Same as above, but for final-state particles. The collinear limit for final-state particles follows from the integral

$$I_{+,\alpha_r} = \int d\Phi_{n+1} \frac{\xi_+^{-1-2\epsilon}}{\xi_-^{-1-2\epsilon}} \mathcal{R}_{\alpha_r}.$$

We can distinguish three situations:

1. α_r contains a massive emitter. In this case, no collinear subtraction term is required and the integral above is irrelevant.
2. α_r contains a massless emitter, but resonances are not taken into account in the subtraction. Here, $\xi_{max} = \frac{2E_{em}}{\sqrt{s}}$ is the upper bound on ξ .
3. α_r contains a massless emitter and resonance-aware subtraction is used. Here, $\xi_{max} = \frac{2E_{em}}{\sqrt{k_{res}^2}}$.

Before version 2.4, only situations 1 and 2 were covered. The difference between situation 2 and 3 comes from the expansion of the plus-distribution in the integral above,

$$\xi_+^{-1-2\epsilon} = \xi^{-1-2\epsilon} + \frac{1}{2\epsilon} \delta(\xi) = \xi_{max}^{-1-2\epsilon} \left[(1-z)^{-1-2\epsilon} + \frac{\xi_{max}^{2\epsilon}}{2\epsilon} \delta(1-z) \right].$$

The expression from the standard FKS literature is given by \mathcal{Q} is given by

$$\mathcal{Q} = \sum_{k=n_{in}}^{n_L^{(B)}} \left[\gamma'(\mathcal{I}_k) - \log \frac{s\delta_o}{2Q^2} \left(\gamma(\mathcal{I}_k) - 2C(\mathcal{I}_k) \log \frac{2E_k}{\xi_{cut}\sqrt{s}} \right) + 2C(\mathcal{I}_k) \left(\log^2 \frac{2E_k}{\sqrt{s}} - \log^2 \xi_{cut} \right) - 2\gamma(\mathcal{I}_k) \log \frac{2E_k}{\sqrt{s}} \right]. \quad (27.10)$$

$n_L^{(B)}$ is the number of legs at Born level. Here, ξ_{max} is implicitly present in the ratios in the logarithms. Using the resonance-aware ξ_{max} yields

$$\mathcal{Q} = \sum_{k=n_{in}}^{n_L^{(B)}} \left[\gamma'(\mathcal{I}_k) + 2 \left(\log \frac{\sqrt{s}}{2E_{em}} + \log \xi_{max} \right) \left(\log \frac{\sqrt{s}}{2E_{em}} + \log \xi_{max} + \log \frac{Q^2}{s} \right) C(\mathcal{I}_k) + 2 \log \xi_{max} \left(\log \xi_{max} - \log \frac{Q^2}{k_{res}^2} \right) C(\mathcal{I}_k) + \left(\log \frac{Q^2}{k_{res}^2} - 2 \log \xi_{max} \right) \gamma(\mathcal{I}_k) \right]. \quad (27.11)$$

Equation 27.11 leads to 27.10 with the substitutions $\xi_{max} \rightarrow \frac{2E_{em}}{\sqrt{s}}$ and $k_{res}^2 \rightarrow s$. `virtual_compute_collinear_contribution` only implements the second one.

```

<virtual: virtual: TBP>+=
  procedure :: compute_collinear_contribution &
    => virtual_compute_collinear_contribution

<virtual: procedures>+=
  subroutine virtual_compute_collinear_contribution (virt, i_flg, i_corr, &
    p_born, sqrts, reg_data, QB)
    class(virtual_t), intent(inout) :: virt
    integer, intent(in) :: i_flg, i_corr
    type(vector4_t), dimension(:), intent(in) :: p_born
    real(default), intent(in) :: sqrts
    type(region_data_t), intent(in) :: reg_data
    real(default), intent(inout), dimension(:) :: QB
    real(default) :: s1, s2, s3, s4, s5
    real(default) :: sqme_born_virt
    integer :: alr, em, i

```

```

real(default) :: E_em, xi_max, log_xi_max, E_tot2
logical, dimension(virt%n_flv, virt%n_legs) :: evaluated
integer :: i_contr
type(vector4_t) :: k_res
type(lorentz_transformation_t) :: L_to_resonance
evaluated = .false.
sqme_born_virt = zero
if (reg_data%nlo_correction_type == "EW" .and. i_corr == 1 &
    .and. qcd_ew_interferences (reg_data%flv_born(i_flv)%flst)) then
  do i = 1, size (reg_data%flv_born(i_flv)%flst)
    if (is_quark (reg_data%flv_born(i_flv)%flst (i))) then
      sqme_born_virt = -virt%sqme_color_c (i, i, i_flv)/CF
      exit
    end if
  end do
else
  sqme_born_virt = virt%sqme_born (i_flv)
end if
do alr = 1, reg_data%n_regions
  if (i_flv /= reg_data%regions(alr)%uborn_index) cycle
  em = reg_data%regions(alr)%emitter
  if (em <= virt%n_in) cycle
  if (evaluated(i_flv, em)) cycle
  !!! Collinear terms only for massless particles
  if (reg_data%regions(alr)%flst_uborn%massive(em)) cycle
  E_em = p_born(em)%p(0)
  if (allocated (reg_data%alr_contributors)) then
    i_contr = reg_data%alr_to_i_contributor (alr)
    k_res = get_resonance_momentum (p_born, reg_data%alr_contributors(i_contr)%c)
    E_tot2 = k_res%p(0)**2
    L_to_resonance = inverse (boost (k_res, k_res**1))
    xi_max = two * space_part_norm (L_to_resonance * p_born(em)) / k_res%p(0)
  else
    E_tot2 = sqrts**2
    xi_max = two * E_em / sqrts
  end if
  log_xi_max = log (xi_max)
  associate (xi_cut => virt%settings%fks_template%xi_cut, delta_o => virt%settings%fks_templ
    if (virt%settings%virtual_resonance_aware_collinear) then
      if (debug_active (D_VIRTUAL)) &
        call msg_debug (D_VIRTUAL, "Using resonance-aware collinear subtraction")
      s1 = virt%gamma_p(em, i_flv, i_corr)
      s2 = two * (log (sqrts / (two * E_em)) + log_xi_max) * &
        (log (sqrts / (two * E_em)) + log_xi_max + log (virt%es_scale2 / sqrts**2)) &
        * virt%c_flv(em, i_flv, i_corr)
      s3 = two * log_xi_max * &
        (log_xi_max - log (virt%es_scale2 / E_tot2)) * virt%c_flv(em, i_flv, i_corr)
      s4 = (log (virt%es_scale2 / E_tot2) - two * log_xi_max) &
        * virt%gamma_0(em, i_flv, i_corr)
      QB(i_flv) = QB(i_flv) + (s1 + s2 + s3 + s4) * sqme_born_virt
    else
      if (debug_active (D_VIRTUAL)) &
        call msg_debug (D_VIRTUAL, "Using old-fashioned collinear subtraction")
      s1 = virt%gamma_p(em, i_flv, i_corr)

```

```

s2 = log (delta_o * sqrts**2 / (two * virt%es_scale2)) &
    * virt%gamma_0(em,i_flv, i_corr)
s3 = log (delta_o * sqrts**2 / (two * virt%es_scale2)) * two &
    * virt%c_flv(em,i_flv, i_corr) * log (two * E_em / (xi_cut * sqrts))
! s4 = two * virt%c_flv(em,i_flv, i_corr) * (log (two * E_em / sqrts)**2 - log (xi_cut
s4 = two * virt%c_flv(em,i_flv, i_corr) * & ! a**2 - b**2 = (a - b) * (a + b), for bet
    (log (two * E_em / sqrts) + log (xi_cut)) * (log (two * E_em / sqrts) - log (xi_c
s5 = two * virt%gamma_0(em,i_flv, i_corr) * log (two * E_em / sqrts)
QB(i_flv) = QB(i_flv) + (s1 - s2 + s3 + s4 - s5) * sqme_born_virt
end if
end associate
evaluated(i_flv, em) = .true.
end do
end subroutine virtual_compute_collinear_contribution

```

For the massless-massive case and $i = j$ we get the massive self-eikonal of (A.10) in arXiv:0908.4272, given as

$$\mathcal{I}_{ii} = \log \frac{\xi_{\text{cut}}^2 s}{Q^2} - \frac{1}{\beta} \log \frac{1 + \beta}{1 - \beta}. \quad (27.12)$$

```

<virtual: virtual: TBP>+=
  procedure :: compute_massive_self_eikonals => virtual_compute_massive_self_eikonals
<virtual: procedures>+=
  subroutine virtual_compute_massive_self_eikonals (virt, i_flv, i_corr, &
    p_born, s_over_Q2, reg_data, QB)
    class(virtual_t), intent(inout) :: virt
    integer, intent(in) :: i_flv, i_corr
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in) :: s_over_Q2
    type(region_data_t), intent(in) :: reg_data
    real(default), intent(inout), dimension(:) :: QB
    real(default) :: sqme_born_virt
    integer :: i
    logical :: massive
    sqme_born_virt = zero
    if (reg_data%nlo_correction_type == "EW" .and. i_corr == 1 &
      .and. qcd_ew_interferences (reg_data%flv_born(i_flv)%flst)) then
      do i = 1, size (reg_data%flv_born(i_flv)%flst)
        if (is_quark (reg_data%flv_born(i_flv)%flst (i))) then
          sqme_born_virt = -virt%sqme_color_c (i, i, i_flv)/CF
          exit
        end if
      end do
    else
      sqme_born_virt = virt%sqme_born (i_flv)
    end if
    do i = 1, virt%n_legs
      massive = reg_data%flv_born(i_flv)%massive(i)
      if (massive) then
        QB(i_flv) = QB(i_flv) - (virt%c_flv (i, i_flv, i_corr) &
          * (log (s_over_Q2) - 0.5_default * I_m_eps (p_born(i)))) &
          * sqme_born_virt
      end if
    end do
  end subroutine

```

```

end do
end subroutine virtual_compute_massive_self_eikonals

```

The following code implements the \mathcal{I}_{ij} -function. The complete formulas can be found in arXiv:0908.4272 (A.1-A.17) and are also discussed in arXiv:1002.2581 in Appendix A. The implementation may differ in the detail from the formulas presented in the above paper. The parameter ξ_{cut} is unphysically and cancels with appropriate factors in the real subtraction. We keep the additional parameter for debug usage. The implemented formulas are then defined as follows:

massless-massless case $p^2 = 0, k^2 = 0$,

$$\begin{aligned} \mathcal{I}_{ij} = & \frac{1}{2} \log^2 \frac{\xi_{\text{cut}}^2 s}{Q^2} + \log \frac{\xi_{\text{cut}}^2 s}{Q^2} \log \frac{k_i k_j}{2E_i E_j} - \text{Li}_2 \left(\frac{k_i k_j}{2E_i E_j} \right) \\ & + \frac{1}{2} \log^2 \frac{k_i k_j}{2E_i E_j} - \log \left(1 - \frac{k_i k_j}{2E_i E_j} \right) \log \frac{k_i k_j}{2E_i E_j}. \end{aligned} \quad (27.13)$$

massive-massive case $p^2 \neq 0, k^2 \neq 0$,

$$\mathcal{I}_{ij} = \frac{1}{2} I_0(k_i, k_j) \log \frac{\xi_{\text{cut}}^2 s}{Q^2} - \frac{1}{2} I_\epsilon(k_i, k_j) \quad (27.14)$$

with

$$I_0(k_i, k_j) = \frac{1}{\beta} \log \frac{1 + \beta}{1 - \beta}, \quad \beta = \sqrt{1 - \frac{k_i^2 k_j^2}{(k_i \cdot k_j)^2}} \quad (27.15)$$

and a rather involved expression for I_ϵ :

$$I_\epsilon(k_i, k_j) = (K(z_j) - K(z_i)) \frac{1 - \vec{\beta}_i \cdot \vec{\beta}_j}{\sqrt{a(1-b)}}, \quad (27.16)$$

$$\vec{\beta}_i = \frac{\vec{k}_i}{k_i^0}, \quad (27.17)$$

$$a = \beta_i^2 + \beta_j^2 - 2\vec{\beta}_i \cdot \vec{\beta}_j, \quad (27.18)$$

$$x_i = \frac{\beta_i^2 - \vec{\beta}_i \cdot \vec{\beta}_j}{a}, \quad (27.19)$$

$$x_j = \frac{\beta_j^2 - \vec{\beta}_i \cdot \vec{\beta}_j}{a} = 1 - x_i, \quad (27.20)$$

$$b = \frac{\beta_i^2 \beta_j^2 - (\vec{\beta}_i \cdot \vec{\beta}_j)^2}{a}, \quad (27.21)$$

$$c = \sqrt{\frac{b}{4a}}, \quad (27.22)$$

$$z_+ = \frac{1 + \sqrt{1-b}}{\sqrt{b}}, \quad (27.23)$$

$$z_- = \frac{1 - \sqrt{1-b}}{\sqrt{b}}, \quad (27.24)$$

$$z_i = \frac{\sqrt{x_i^2 + 4c^2} - x_i}{2c}, \quad (27.25)$$

$$z_j = \frac{\sqrt{x_j^2 + 4c^2} + x_j}{2c}, \quad (27.26)$$

$$K(z) = -\frac{1}{2} \log^2 \frac{(z - z_-)(z_+ - z)}{(z_+ + z)(z_- + z)} - 2Li_2 \left(\frac{2z_-(z_+ - z)}{(z_+ - z_-)(z_- + z)} \right) \quad (27.27)$$

$$- 2Li_2 \left(-\frac{2z_+(z_- + z)}{(z_+ - z_-)(z_+ - z)} \right) \quad (27.28)$$

massless-massive case $p^2 = 0, k^2 \neq 0$,

$$\mathcal{I}_{ij} = \frac{1}{2} \left[\frac{1}{2} \log^2 \frac{\xi_{\text{cut}}^2 s}{Q^2} - \frac{\pi^2}{6} \right] + \frac{1}{2} I_0(k_i, k_j) \log \frac{\xi_{\text{cut}}^2 s}{Q^2} - \frac{1}{2} I_\epsilon(k_i, k_j) \quad (27.29)$$

with

$$I_0(p, k) = \log \frac{(\hat{p} \cdot \hat{k})^2}{\hat{k}^2}, \quad (27.30)$$

$$I_\epsilon(p, k) = -2 \left[\frac{1}{4} \log^2 \frac{1-\beta}{1+\beta} + \log \frac{\hat{p} \cdot \hat{k}}{1+\beta} \log \frac{\hat{p} \cdot \hat{k}}{1-\beta} + Li_2 \left(1 - \frac{\hat{p} \cdot \hat{k}}{1+\beta} \right) + Li_2 \left(1 - \frac{\hat{p} \cdot \hat{k}}{1-\beta} \right) \right], \quad (27.31)$$

using

$$\hat{p} = \frac{p}{p^0}, \quad \hat{k} = \frac{k}{k^0}, \quad \beta = \frac{|\vec{k}|}{k_0}, \quad (27.32)$$

$$\text{Li}_2(1-x) + \text{Li}_2(1-x^{-1}) = -\frac{1}{2} \log^2 x. \quad (27.33)$$

(virtual: procedures)+≡

```
function compute_eikonal_factor (p_born, massive, i, j, s_o_Q2) result (I_ij)
  real(default) :: I_ij
  type(vector4_t), intent(in), dimension(:) :: p_born
  logical, dimension(:), intent(in) :: massive
  integer, intent(in) :: i, j
  real(default), intent(in) :: s_o_Q2
  if (massive(i) .and. massive(j)) then
    I_ij = compute_Imm (p_born(i), p_born(j), s_o_Q2)
  else if (.not. massive(i) .and. massive(j)) then
    I_ij = compute_I0m (p_born(i), p_born(j), s_o_Q2)
  else if (massive(i) .and. .not. massive(j)) then
    I_ij = compute_I0m (p_born(j), p_born(i), s_o_Q2)
  else
    I_ij = compute_I00 (p_born(i), p_born(j), s_o_Q2)
  end if
end function compute_eikonal_factor
```

```
function compute_I00 (pi, pj, s_o_Q2) result (I)
  type(vector4_t), intent(in) :: pi, pj
  real(default), intent(in) :: s_o_Q2
  real(default) :: I
  real(default) :: Ei, Ej
  real(default) :: pij, Eij
  real(default) :: s1, s2, s3, s4, s5
  real(default) :: arglog
  real(default), parameter :: tiny_value = epsilon(1.0)
  s1 = 0; s2 = 0; s3 = 0; s4 = 0; s5 = 0
  Ei = pi%p(0); Ej = pj%p(0)
  pij = pi * pj; Eij = Ei * Ej
  s1 = 0.5_default * log(s_o_Q2)**2
  s2 = log(s_o_Q2) * log(pij / (two * Eij))
  s3 = Li2 (pij / (two * Eij))
  s4 = 0.5_default * log (pij / (two * Eij))**2
  arglog = one - pij / (two * Eij)
  if (arglog > tiny_value) then
    s5 = log(arglog) * log(pij / (two * Eij))
  else
    s5 = zero
  end if
  I = s1 + s2 - s3 + s4 - s5
end function compute_I00
```

```
function compute_I0m (ki, kj, s_o_Q2) result (I)
  type(vector4_t), intent(in) :: ki, kj
  real(default), intent(in) :: s_o_Q2
  real(default) :: I
```

```

real(default) :: logsomu
real(default) :: s1, s2, s3
s1 = 0; s2 = 0; s3 = 0
logsomu = log(s_o_Q2)
s1 = 0.5 * (0.5 * logsomu**2 - pi**2 / 6)
s2 = 0.5 * I_0m_0 (ki, kj) * logsomu
s3 = 0.5 * I_0m_eps (ki, kj)
I = s1 + s2 - s3
end function compute_I0m

function compute_Imm (pi, pj, s_o_Q2) result (I)
  type(vector4_t), intent(in) :: pi, pj
  real(default), intent(in) :: s_o_Q2
  real(default) :: I
  real(default) :: s1, s2
  s1 = 0.5 * log(s_o_Q2) * I_mm_0(pi, pj)
  s2 = 0.5 * I_mm_eps(pi, pj)
  I = s1 - s2
end function compute_Imm

function I_m_eps (p) result (I)
  type(vector4_t), intent(in) :: p
  real(default) :: I
  real(default) :: beta
  beta = space_part_norm (p)/p%p(0)
  if (beta < tiny_07) then
    I = four * (one + beta**2/3 + beta**4/5 + beta**6/7)
  else
    I = two * log((one + beta) / (one - beta)) / beta
  end if
end function I_m_eps

function I_0m_eps (p, k) result (I)
  type(vector4_t), intent(in) :: p, k
  real(default) :: I
  type(vector4_t) :: pp, kp
  real(default) :: beta

  pp = p / p%p(0); kp = k / k%p(0)

  beta = sqrt (one - kp*kp)
  I = -2*(log((one - beta) / (one + beta))**2/4 + log((pp*kp) / (one + beta))*log((pp*kp) / (one
    + Li2(one - (pp*kp) / (one + beta)) + Li2(one - (pp*kp) / (one - beta)))
end function I_0m_eps

function I_0m_0 (p, k) result (I)
  type(vector4_t), intent(in) :: p, k
  real(default) :: I
  type(vector4_t) :: pp, kp

  pp = p / p%p(0); kp = k / k%p(0)
  I = log((pp*kp)**2 / kp**2)
end function I_0m_0

```

```

function I_mm_eps (p1, p2) result (I)
  type(vector4_t), intent(in) :: p1, p2
  real(default) :: I
  type(vector3_t) :: beta1, beta2
  real(default) :: a, b, b2
  real(default) :: zp, zm, z1, z2, x1, x2
  real(default) :: zmb, z1b
  real(default) :: K1, K2

  beta1 = space_part (p1) / energy(p1)
  beta2 = space_part (p2) / energy(p2)
  a = beta1**2 + beta2**2 - 2 * beta1 * beta2
  b = beta1**2 * beta2**2 - (beta1 * beta2)**2
  if (beta1**1 > beta2**1) call switch_beta (beta1, beta2)
  if (beta1 == vector3_null) then
    b2 = beta2**1
    I = (-0.5 * log ((one - b2) / (one + b2))**2 - two * Li2 (-two * b2 / (one - b2))) &
      * one / sqrt (a - b)
    return
  end if
  x1 = beta1**2 - beta1 * beta2
  x2 = beta2**2 - beta1 * beta2
  zp = sqrt (a) + sqrt (a - b)
  zm = sqrt (a) - sqrt (a - b)
  zmb = one / zp
  z1 = sqrt (x1**2 + b) - x1
  z2 = sqrt (x2**2 + b) + x2
  z1b = one / (sqrt (x1**2 + b) + x1)
  K1 = - 0.5 * log (((z1b - zmb) * (zp - z1)) / ((zp + z1) * (z1b + zmb)))**2 &
    - two * Li2 ((two * zmb * (zp - z1)) / ((zp - zm) * (zmb + z1b))) &
    - two * Li2 ((-two * zp * (zm + z1)) / ((zp - zm) * (zp - z1)))
  K2 = - 0.5 * log (((z2 - zm) * (zp - z2)) / ((zp + z2) * (z2 + zm)))**2 &
    - two * Li2 ((two * zm * (zp - z2)) / ((zp - zm) * (zm + z2))) &
    - two * Li2 ((-two * zp * (zm + z2)) / ((zp - zm) * (zp - z2)))
  I = (K2 - K1) * (one - beta1 * beta2) / sqrt (a - b)
contains
  subroutine switch_beta (beta1, beta2)
    type(vector3_t), intent(inout) :: beta1, beta2
    type(vector3_t) :: beta_tmp
    beta_tmp = beta1
    beta1 = beta2
    beta2 = beta_tmp
  end subroutine switch_beta
end function I_mm_eps

function I_mm_0 (k1, k2) result (I)
  type(vector4_t), intent(in) :: k1, k2
  real(default) :: I
  real(default) :: beta
  beta = sqrt (one - k1**2 * k2**2 / (k1 * k2)**2)
  I = log ((one + beta) / (one - beta)) / beta
end function I_mm_0

```

$\langle virtual: virtual: TBP \rangle \equiv$

```

    procedure :: final => virtual_final
<virtual: procedures>+≡
    subroutine virtual_final (virtual)
        class(virtual_t), intent(inout) :: virtual
        if (allocated (virtual%gamma_0)) deallocate (virtual%gamma_0)
        if (allocated (virtual%gamma_p)) deallocate (virtual%gamma_p)
        if (allocated (virtual%c_flv)) deallocate (virtual%c_flv)
        if (allocated (virtual%n_is_neutrinos)) deallocate (virtual%n_is_neutrinos)
    end subroutine virtual_final

```

27.5 Real Subtraction

```
<real_subtraction.f90>≡  
  <File header>  
  
  module real_subtraction  
  
    <Use kinds with double>  
    <Use strings>  
    <Use debug>  
    use io_units  
    use format_defs, only: FMT_15  
    use string_utils  
    use constants  
    use numeric_utils  
    use diagnostics  
    use pdg_arrays  
    use models  
    use physics_defs  
    use sm_physics  
    use lorentz  
    use flavors  
    use phs_fks, only: real_kinematics_t, isr_kinematics_t  
    use phs_fks, only: I_PLUS, I_MINUS  
    use phs_fks, only: SQRTS_VAR, SQRTS_FIXED  
    use phs_fks, only: phs_point_set_t  
    use ttv_formfactors, only: mis_to_mpole  
  
    use fks_regions  
    use nlo_data  
  
    <Standard module head>  
  
    <real subtraction: public>  
  
    <real subtraction: parameters>  
  
    <real subtraction: types>  
  
    <real subtraction: interfaces>  
  
    contains  
  
    <real subtraction: procedures>  
  
  end module real_subtraction
```

Soft subtraction terms

```
<real subtraction: parameters>≡  
  integer, parameter, public :: INTEGRATION = 0  
  integer, parameter, public :: FIXED_ORDER_EVENTS = 1  
  integer, parameter, public :: POWHEG = 2
```

Translates the purpose into a string.

```

⟨real subtraction: public⟩≡
  public :: this_purpose

⟨real subtraction: procedures⟩≡
  function this_purpose (purpose)
    type(string_t) :: this_purpose
    integer, intent(in) :: purpose
    select case (purpose)
    case (INTEGRATION)
      this_purpose = var_str ("Integration")
    case (FIXED_ORDER_EVENTS)
      this_purpose = var_str ("Fixed order NLO events")
    case (POWHEG)
      this_purpose = var_str ("Powheg events")
    case default
      this_purpose = var_str ("Undefined!")
    end select
  end function this_purpose

```

In the soft limit, the real matrix element behaves as

$$\mathcal{R}_{\text{soft}} = 4\pi\alpha_s \left[\sum_{i \neq j} \mathcal{B}_{ij} \frac{k_i \cdot k_j}{(k_i \cdot k)(k_j \cdot k)} - \mathcal{B} \sum_i \frac{k_i^2}{(k_i \cdot k)^2} C_i \right],$$

where k denotes the momentum of the emitted parton. The quantity \mathcal{B}_{ij} is called the color-correlated Born matrix element defined as

$$\mathcal{B}_{ij} = \frac{1}{2s} \sum_{\substack{\text{colors} \\ \text{spins}}} \mathcal{M}_{\{c_k\}} \left(\mathcal{M}_{\{c_k\}}^\dagger \right)_{\substack{c_i \rightarrow c'_i \\ c_j \rightarrow c'_j}} T_{c_i, c'_i}^a T_{c_j, c'_j}^a.$$

```

⟨real subtraction: types⟩≡
  type :: soft_subtraction_t
    type(region_data_t), pointer :: reg_data => null ()
    real(default), dimension(:,:), allocatable :: momentum_matrix
    logical :: use_resonance_mappings = .false.
    type(vector4_t) :: p_soft = vector4_null
    logical :: use_internal_color_correlations = .true.
    logical :: use_internal_spin_correlations = .false.
    logical :: xi2_expanded = .true.
    integer :: factorization_mode = NO_FACTORIZATION
  contains
    ⟨real subtraction: soft sub: TBP⟩
  end type soft_subtraction_t

```

```

⟨real subtraction: soft sub: TBP⟩≡
  procedure :: init => soft_subtraction_init

```

```

⟨real subtraction: procedures⟩+=
  subroutine soft_subtraction_init (sub_soft, reg_data)
    class(soft_subtraction_t), intent(inout) :: sub_soft
    type(region_data_t), intent(in), target :: reg_data
  end subroutine

```

```

sub_soft%reg_data => reg_data
allocate (sub_soft%momentum_matrix (reg_data%n_legs_born, &
    reg_data%n_legs_born))
end subroutine soft_subtraction_init

<real subtraction: soft sub: TBP>+≡
procedure :: requires_boost => soft_subtraction_requires_boost

<real subtraction: procedures>+≡
function soft_subtraction_requires_boost (sub_soft, sqrts) result (requires_boost)
    logical :: requires_boost
    class(sub_soft), intent(in) :: sub_soft
    real(default), intent(in) :: sqrts
    real(default) :: mtop
    logical :: above_threshold
    if (sub_soft%factorization_mode == FACTORIZATION_THRESHOLD) then
        mtop = mis_to_mpole (sqrts)
        above_threshold = sqrts**2 - four * mtop**2 > zero
    else
        above_threshold = .false.
    end if
    requires_boost = sub_soft%use_resonance_mappings .or. above_threshold
end function soft_subtraction_requires_boost

```

The treatment of the momentum k follows the discussion about the soft limit of the partition functions (see [1002.2581], p. 29 and C. Weiss' PhD Thesis, p. 24). The parton momentum is pulled out, $k = E\hat{k}$. In fact, we will substitute \hat{k} for k throughout the code, because the energy will factor out of the equation when the soft \mathcal{S} -function is multiplied. The momentum $\mathbf{p_soft}$ represents the soft limit of the radiated particle divided by its energy. It is a unit vector, because $k^2 = (k^0)^2 - (\vec{k})^2 \hat{k}^2 = 0$.

The soft momentum is constructed by first creating a unit vector parallel to the emitter's Born momentum. This unit vector is then rotated about the corresponding angles y and ϕ to match the direction of the real radiation in the soft limit.

```

<real subtraction: soft sub: TBP>+≡
procedure :: create_softvec_fsr => soft_subtraction_create_softvec_fsr

<real subtraction: procedures>+≡
subroutine soft_subtraction_create_softvec_fsr &
    (sub_soft, p_born, y, phi, emitter, xi_ref_momentum)
    class(sub_soft), intent(inout) :: sub_soft
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in) :: y, phi
    integer, intent(in) :: emitter
    type(vector4_t), intent(in) :: xi_ref_momentum
    type(vector3_t) :: dir
    type(vector4_t) :: p_em
    type(lorentz_transformation_t) :: rot
    type(lorentz_transformation_t) :: boost_to_rest_frame
    logical :: requires_boost
    associate (p_soft => sub_soft%p_soft)
        p_soft%p(0) = one
    end associate
end subroutine soft_subtraction_create_softvec_fsr

```



```

requires_boost = sub_soft%requires_boost (two * p_born(1)%p(0))
if (requires_boost) then
  boost_to_rest_frame = inverse (boost (xi_ref_momentum, xi_ref_momentum**1))
  p_em = boost_to_rest_frame * p_born(emitter)
else
  p_em = p_born(emitter)
end if
p_soft%p(1:3) = p_em%p(1:3) / space_part_norm (p_em)
dir = create_orthogonal (space_part (p_em))
rot = rotation (y, sqrt(one - y**2), dir)
p_soft = rot * p_soft
if (.not. vanishes (phi)) then
  dir = space_part (p_em) / space_part_norm (p_em)
  rot = rotation (cos(phi), sin(phi), dir)
  p_soft = rot * p_soft
end if
if (requires_boost) p_soft = inverse (boost_to_rest_frame) * p_soft
end associate
end subroutine soft_subtraction_create_softvec_fsr

```

For initial-state emissions, the soft vector is just a unit vector with the same direction as the radiated particle. As y for ISR is defined independently of the emitter, also p_soft is the same for all initial state emitters.

```

<real subtraction: soft sub: TBP>+≡
  procedure :: create_softvec_isr => soft_subtraction_create_softvec_isr
<real subtraction: procedures>+≡
  subroutine soft_subtraction_create_softvec_isr (sub_soft, y, phi)
    class(soft_subtraction_t), intent(inout) :: sub_soft
    real(default), intent(in) :: y, phi
    real(default) :: sin_theta
    sin_theta = sqrt(one - y**2)
    associate (p => sub_soft%p_soft%p)
      p(0) = one
      p(1) = sin_theta * sin(phi)
      p(2) = sin_theta * cos(phi)
      p(3) = y
    end associate
  end subroutine soft_subtraction_create_softvec_isr

```

The soft vector for the real mismatch is basically the same as for usual FSR, except for the scaling with the total gluon energy. Moreover, the resulting vector is rotated into the frame where the 3-axis points along the direction of the emitter. This is necessary because in the collinear limit, the approximation

$$k_i = \frac{k_i^0}{\bar{k}_j^0} \bar{k}_j = \frac{\xi \sqrt{s}}{2\bar{k}_j^0} \bar{k}_j$$

is used. The collinear limit is not included in the soft mismatch yet, but we keep the rotation for future usage here already (the performance loss is negligible).

```

<real subtraction: soft sub: TBP>+≡
  procedure :: create_softvec_mismatch => &
    soft_subtraction_create_softvec_mismatch

```

<real subtraction: procedures>+≡

```

subroutine soft_subtraction_create_softvec_mismatch (sub_soft, E, y, phi, p_em)
  class(soft_subtraction_t), intent(inout) :: sub_soft
  real(default), intent(in) :: E, phi, y
  type(vector4_t), intent(in) :: p_em
  real(default) :: sin_theta
  type(lorentz_transformation_t) :: rot_em_off_3_axis
  sin_theta = sqrt (one - y**2)
  associate (p => sub_soft%p_soft%p)
    p(0) = E
    p(1) = E * sin_theta * sin(phi)
    p(2) = E * sin_theta * cos(phi)
    p(3) = E * y
  end associate
  rot_em_off_3_axis = rotation_to_2nd (3, space_part (p_em))
  sub_soft%p_soft = rot_em_off_3_axis * sub_soft%p_soft
end subroutine soft_subtraction_create_softvec_mismatch

```

Computation of the soft limit of R_α . Note that what we are actually integrating (in the case of final-state radiation) is the quantity $f(0, y)/\xi$, where

$$f(\xi, y) = \frac{J(\xi, y, \phi)}{\xi} \xi^2 R_\alpha.$$

J/ξ is computed by the phase space generator. The additional factor of ξ^{-1} is supplied in the `evaluate_region_fsr`-routine. Thus, we are left with a factor of ξ^2 . A look on the expression for the soft limit of R_α below reveals that we are factoring out the gluon energy E_i in the denominator. Therefore, we have a factor $\xi^2/E_i^2 = 4/q^2$.

Note that the same routine is used also for the computation of the soft mismatch. There, the gluon energy is not factored out from the soft vector, so that we are left with the ξ^2 -factor, which will eventually be cancelled out again. So, we just multiply with 1. Both cases are distinguished by the flag `xi2_expanded`.

Note that for the soft subtraction term, also the S functions are computed in the soft limit. The input momenta are thus the real momenta in the soft limit, i.e. the Born momenta given by `p_born`.

<real subtraction: soft sub: TBP>+≡

```

procedure :: compute => soft_subtraction_compute

```

<real subtraction: procedures>+≡

```

function soft_subtraction_compute (sub_soft, p_born, &
  born_ij, y, q2, alpha_coupling, alr, emitter, i_res) result (sqme)
  real(default) :: sqme
  class(soft_subtraction_t), intent(inout) :: sub_soft
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in), dimension(:, :) :: born_ij
  real(default), intent(in) :: y
  real(default), intent(in) :: q2, alpha_coupling
  integer, intent(in) :: alr, emitter, i_res
  real(default) :: s_alpha_soft
  real(default) :: kb
  real(default) :: xi2_factor

```

```

if (.not. vector_set_is_cms (p_born, sub_soft%reg_data%n_in)) then
  call vector4_write_set (p_born, show_mass = .true., &
    check_conservation = .true.)
  call msg_fatal ("Soft subtraction: phase space point must be in CMS")
end if
if (debug2_active (D_SUBTRACTION)) then
  select case (char (sub_soft%reg_data%regions(alr)%nlo_correction_type))
  case ("QCD")
    print *, 'Compute soft subtraction using alpha_s = ', alpha_coupling
  case ("EW")
    print *, 'Compute soft subtraction using alpha_qed = ', alpha_coupling
  end select
end if

s_alpha_soft = sub_soft%reg_data%get_svalue_soft (p_born, &
  sub_soft%p_soft, alr, emitter, i_res)
if (s_alpha_soft > one + tiny_07) call msg_fatal ("s_alpha_soft > 1!")
if (debug2_active (D_SUBTRACTION)) &
  call msg_print_color ('s_alpha_soft', s_alpha_soft, COL_YELLOW)
select case (sub_soft%factorization_mode)
case (NO_FACTORIZATION)
  kb = sub_soft%evaluate_factorization_default (p_born, born_ij)
case (FACTORIZATION_THRESHOLD)
  kb = sub_soft%evaluate_factorization_threshold (thr_leg(emitter), p_born, born_ij)
end select
if (debug_on) call msg_debug2 (D_SUBTRACTION, 'KB', kb)
sqme = four * pi * alpha_coupling * s_alpha_soft * kb
if (sub_soft%xi2_expanded) then
  xi2_factor = four / q2
else
  xi2_factor = one
end if
if (emitter <= sub_soft%reg_data%n_in) then
  sqme = xi2_factor * (one - y**2) * sqme
else
  sqme = xi2_factor * (one - y) * sqme
end if
if (sub_soft%reg_data%regions(alr)%double_fsr) sqme = sqme * two
end function soft_subtraction_compute

```

We loop over all external legs and do not take care to leave out non-colored ones because `born_ij` is constructed in such a way that it is only non-zero for colored entries.

```

<real subtraction: soft sub: TBP>+≡
  procedure :: evaluate_factorization_default => &
    soft_subtraction_evaluate_factorization_default

<real subtraction: procedures>+≡
  function soft_subtraction_evaluate_factorization_default &
    (sub_soft, p, born_ij) result (kb)
  real(default) :: kb
  class(sub_soft), intent(inout) :: sub_soft
  type(vector4_t), intent(in), dimension(:) :: p
  real(default), intent(in), dimension(:, :) :: born_ij

```

```

integer :: i, j
kb = zero
call sub_soft%compute_momentum_matrix (p)
do i = 1, size (p)
  do j = 1, size (p)
    kb = kb + sub_soft%momentum_matrix (i, j) * born_ij (i, j)
  end do
end do
end function soft_subtraction_evaluate_factorization_default

```

We have to multiply this with $\xi^2(1-y)$. Further, when applying the soft \mathcal{S} -function, the energy of the radiated particle is factored out. Thus we have $\xi^2/E_{em}^2(1-y) = 4/q_0^2(1-y)$. Computes the quantity $\mathcal{K}_{ij} = \frac{k_i \cdot k_j}{(k_i \cdot k)(k_j \cdot k)}$.

```

<real subtraction: soft sub: TBP>+≡
  procedure :: compute_momentum_matrix => &
    soft_subtraction_compute_momentum_matrix

<real subtraction: procedures>+≡
  subroutine soft_subtraction_compute_momentum_matrix &
    (sub_soft, p_born)
    class(sub_soft), intent(inout) :: sub_soft
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default) :: num, deno1, deno2
    integer :: i, j
    do i = 1, sub_soft%reg_data%n_legs_born
      do j = 1, sub_soft%reg_data%n_legs_born
        if (i <= j) then
          num = p_born(i) * p_born(j)
          deno1 = p_born(i) * sub_soft%p_soft
          deno2 = p_born(j) * sub_soft%p_soft
          sub_soft%momentum_matrix(i, j) = num / (deno1 * deno2)
        else
          !!! momentum matrix is symmetric.
          sub_soft%momentum_matrix(i, j) = sub_soft%momentum_matrix(j, i)
        end if
      end do
    end do
  end subroutine soft_subtraction_compute_momentum_matrix

<real subtraction: soft sub: TBP>+≡
  procedure :: evaluate_factorization_threshold => &
    soft_subtraction_evaluate_factorization_threshold

<real subtraction: procedures>+≡
  function soft_subtraction_evaluate_factorization_threshold &
    (sub_soft, leg, p_born, born_ij) result (kb)
    real(default) :: kb
    class(sub_soft), intent(inout) :: sub_soft
    integer, intent(in) :: leg
    type(vector4_t), intent(in), dimension(:) :: p_born
    real(default), intent(in), dimension(:, :) :: born_ij
    type(vector4_t), dimension(4) :: p
    p = get_threshold_momenta (p_born)

```

```

kb = evaluate_leg_pair (ASSOCIATED_LEG_PAIR (leg))
if (debug2_active (D_SUBTRACTION)) call show_debug ()

contains

function evaluate_leg_pair (i_start) result (kbb)
  real(default) :: kbb
  integer, intent(in) :: i_start
  integer :: i1, i2
  real(default) :: numerator, deno1, deno2
  kbb = zero
  do i1 = i_start, i_start + 1
    do i2 = i_start, i_start + 1
      numerator = p(i1) * p(i2)
      deno1 = p(i1) * sub_soft%p_soft
      deno2 = p(i2) * sub_soft%p_soft
      kbb = kbb + numerator * born_ij (i1, i2) / deno1 / deno2
    end do
  end do
  if (debug2_active (D_SUBTRACTION)) then
    do i1 = i_start, i_start + 1
      do i2 = i_start, i_start + 1
        call msg_print_color('i1', i1, COL_PEACH)
        call msg_print_color('i2', i2, COL_PEACH)
        call msg_print_color('born_ij (i1,i2)', born_ij (i1,i2), COL_PINK)
        print *, 'Top momentum: ', p(1)%p
      end do
    end do
  end if
end function evaluate_leg_pair

subroutine show_debug ()
  integer :: i
  call msg_print_color ('soft_subtraction_evaluate_factorization_threshold', COL_GREEN)
  do i = 1, 4
    print *, 'sqrt(p(i)**2) = ', sqrt(p(i)**2)
  end do
end subroutine show_debug

end function soft_subtraction_evaluate_factorization_threshold

<real subtraction: soft sub: TBP>+≡
  procedure :: i_xi_ref => soft_subtraction_i_xi_ref

<real subtraction: procedures>+≡
  function soft_subtraction_i_xi_ref (sub_soft, alr, i_phs) result (i_xi_ref)
    integer :: i_xi_ref
    class(soft_subtraction_t), intent(in) :: sub_soft
    integer, intent(in) :: alr, i_phs
    if (sub_soft%use_resonance_mappings) then
      i_xi_ref = sub_soft%reg_data%alr_to_i_contributor (alr)
    else if (sub_soft%factorization_mode == FACTORIZATION_THRESHOLD) then
      i_xi_ref = i_phs
    else

```

```

        i_xi_ref = 1
    end if
end function soft_subtraction_i_xi_ref

```

```

<real subtraction: soft sub: TBP>+=
    procedure :: final => soft_subtraction_final

<real subtraction: procedures>+=
    subroutine soft_subtraction_final (sub_soft)
        class(soft_subtraction_t), intent(inout) :: sub_soft
        if (associated (sub_soft%reg_data)) nullify (sub_soft%reg_data)
        if (allocated (sub_soft%momentum_matrix)) deallocate (sub_soft%momentum_matrix)
    end subroutine soft_subtraction_final

```

27.5.1 Soft mismatch

```

<real subtraction: public>+=
    public :: soft_mismatch_t

<real subtraction: types>+=
    type :: soft_mismatch_t
        type(region_data_t), pointer :: reg_data => null ()
        real(default), dimension(:), allocatable :: sqme_born
        real(default), dimension(:,:), allocatable :: sqme_born_color_c
        real(default), dimension(:,:), allocatable :: sqme_born_charge_c
        type(real_kinematics_t), pointer :: real_kinematics => null ()
        type(soft_subtraction_t) :: sub_soft
    contains
        <real subtraction: soft mismatch: TBP>
    end type soft_mismatch_t

<real subtraction: soft mismatch: TBP>=
    procedure :: init => soft_mismatch_init

<real subtraction: procedures>+=
    subroutine soft_mismatch_init (soft_mismatch, reg_data, &
        real_kinematics, factorization_mode)
        class(soft_mismatch_t), intent(inout) :: soft_mismatch
        type(region_data_t), intent(in), target :: reg_data
        type(real_kinematics_t), intent(in), target :: real_kinematics
        integer, intent(in) :: factorization_mode
        soft_mismatch%reg_data => reg_data
        allocate (soft_mismatch%sqme_born (reg_data%n_flv_born))
        allocate (soft_mismatch%sqme_born_color_c (reg_data%n_legs_born, &
            reg_data%n_legs_born, reg_data%n_flv_born))
        allocate (soft_mismatch%sqme_born_charge_c (reg_data%n_legs_born, &
            reg_data%n_legs_born, reg_data%n_flv_born))
        call soft_mismatch%sub_soft%init (reg_data)
        soft_mismatch%sub_soft%xi2_expanded = .false.
        soft_mismatch%real_kinematics => real_kinematics
        soft_mismatch%sub_soft%factorization_mode = factorization_mode
    end subroutine soft_mismatch_init

```

Main routine to compute the soft mismatch. Loops over all singular regions. There, it first creates the soft vector, then the necessary soft real matrix element. These inputs are then used to get the numerical value of the soft mismatch.

```

<real subtraction: soft mismatch: TBP>+≡
  procedure :: evaluate => soft_mismatch_evaluate

<real subtraction: procedures>+≡
function soft_mismatch_evaluate (soft_mismatch, alpha_s) result (sqme_mismatch)
  real(default) :: sqme_mismatch
  class(soft_mismatch_t), intent(inout) :: soft_mismatch
  real(default), intent(in) :: alpha_s
  integer :: alr, i_born, emitter, i_res, i_phs, i_con
  real(default) :: xi, y, q2, s
  real(default) :: E_gluon
  type(vector4_t) :: p_em
  real(default) :: sqme_alr, sqme_soft
  type(vector4_t), dimension(:), allocatable :: p_born
  sqme_mismatch = zero
  associate (real_kinematics => soft_mismatch%real_kinematics)
    xi = real_kinematics%xi_mismatch
    y = real_kinematics%y_mismatch
    s = real_kinematics%cms_energy2
    E_gluon = sqrt (s) * xi / two

    if (debug_active (D_MISMATCH)) then
      print *, 'Evaluating soft mismatch: '
      print *, 'Phase space: '
      call vector4_write_set (real_kinematics%p_born_cms%get_momenta(1), &
        show_mass = .true.)
      print *, 'xi: ', xi, 'y: ', y, 's: ', s, 'E_gluon: ', E_gluon
    end if

    allocate (p_born (soft_mismatch%reg_data%n_legs_born))

    do alr = 1, soft_mismatch%reg_data%n_regions

      i_phs = real_kinematics%alr_to_i_phs (alr)
      if (soft_mismatch%reg_data%has_pseudo_isr ()) then
        i_con = 1
        p_born = soft_mismatch%real_kinematics%p_born_onshell%get_momenta(1)
      else
        i_con = soft_mismatch%reg_data%alr_to_i_contributor (alr)
        p_born = soft_mismatch%real_kinematics%p_born_cms%get_momenta(1)
      end if
      q2 = real_kinematics%xi_ref_momenta(i_con)**2
      emitter = soft_mismatch%reg_data%regions(alr)%emitter
      p_em = p_born (emitter)
      i_res = soft_mismatch%reg_data%regions(alr)%i_res
      i_born = soft_mismatch%reg_data%regions(alr)%uborn_index

      call print_debug_alr ()

      call soft_mismatch%sub_soft%create_softvec_mismatch &
        (E_gluon, y, real_kinematics%phi, p_em)
    end do
  end associate
end function

```

```

    if (debug_active (D_MISMATCH)) &
        print *, 'Created soft vector: ', soft_mismatch%sub_soft%p_soft%p

    select type (fks_mapping => soft_mismatch%reg_data%fks_mapping)
    type is (fks_mapping_resonances_t)
        call fks_mapping%set_resonance_momentum &
            (real_kinematics%xi_ref_momenta(i_con))
    end select

    sqme_soft = soft_mismatch%sub_soft%compute &
        (p_born, soft_mismatch%sqme_born_color_c(:, :, i_born), y, &
        q2, alpha_s, alr, emitter, i_res)

    sqme_alr = soft_mismatch%compute (alr, xi, y, p_em, &
        real_kinematics%xi_ref_momenta(i_con), soft_mismatch%sub_soft%p_soft, &
        soft_mismatch%sqme_born(i_born), sqme_soft, &
        alpha_s, s)

    if (debug_on) call msg_debug (D_MISMATCH, 'sqme_alr: ', sqme_alr)
    sqme_mismatch = sqme_mismatch + sqme_alr

end do
end associate
contains
subroutine print_debug_alr ()
    if (debug_active (D_MISMATCH)) then
        print *, 'alr: ', alr
        print *, 'i_phs: ', i_phs, 'i_con: ', i_con, 'i_res: ', i_res
        print *, 'emitter: ', emitter, 'i_born: ', i_born
        print *, 'emitter momentum: ', p_em%p
        print *, 'resonance momentum: ', &
            soft_mismatch%real_kinematics%xi_ref_momenta(i_con)%p
        print *, 'q2: ', q2
    end if
end subroutine print_debug_alr
end function soft_mismatch_evaluate

```

Computes the soft mismatch in a given α_r ,

$$\begin{aligned}
 I_{s+, \alpha_r} = & \int d\Phi_B \int_0^\infty d\xi \int_{-1}^1 dy \int_0^{2\pi} d\phi \frac{s\xi}{(4\pi)^3} \\
 & \times \left\{ \tilde{R}_{\alpha_r} \left(e^{-\frac{2k_\gamma \cdot k_{res}}{k_{res}^2}} - e^{-\xi} \right) - \frac{32\pi\alpha_s C_{em}}{s\xi^2} B_{f_b(\alpha_r)}(1-y)^{-1} \left[e^{-\frac{2k_{em} \cdot k_{res}}{k_{res}^2} \frac{k_\gamma^0}{k_{em}^0}} - e^{-\xi} \right] \right\}.
 \end{aligned}$$

(real subtraction: soft mismatch: TBP)+≡

```
procedure :: compute => soft_mismatch_compute
```

(real subtraction: procedures)+≡

```

function soft_mismatch_compute (soft_mismatch, alr, xi, y, p_em, p_res, p_soft, &
    sqme_born, sqme_soft, alpha_s, s) result (sqme_mismatch)
    real(default) :: sqme_mismatch
    class(soft_mismatch_t), intent(in) :: soft_mismatch
    integer, intent(in) :: alr

```



```

real(default), intent(in) :: xi, y
type(vector4_t), intent(in) :: p_em, p_res, p_soft
real(default), intent(in) :: sqme_born, sqme_soft
real(default), intent(in) :: alpha_s, s
real(default) :: q2, expo, sm1, sm2, jacobian

q2 = p_res**2
expo = - two * p_soft * p_res / q2
!!! Divide by 1 - y to factor out the corresponding
!!! factor in the soft matrix element
sm1 = sqme_soft / (one - y) * ( exp(expo) - exp(- xi) )
if (debug_on) call msg_debug2 (D_MISMATCH, 'sqme_soft in mismatch ', sqme_soft)

sm2 = zero
if (soft_mismatch%reg_data%regions(alr)%has_collinear_divergence ()) then
    expo = - two * p_em * p_res / q2 * &
        p_soft%p(0) / p_em%p(0)
    sm2 = 32 * pi * alpha_s * cf / (s * xi**2) * sqme_born * &
        ( exp(expo) - exp(- xi) ) / (one - y)
end if

jacobian = soft_mismatch%real_kinematics%jac_mismatch * s * xi / (8 * twopi3)
sqme_mismatch = (sm1 - sm2) * jacobian

end function soft_mismatch_compute

<real subtraction: soft mismatch: TBP>+≡
procedure :: final => soft_mismatch_final

<real subtraction: procedures>+≡
subroutine soft_mismatch_final (soft_mismatch)
    class(soft_mismatch_t), intent(inout) :: soft_mismatch
    call soft_mismatch%sub_soft%final ()
    if (associated (soft_mismatch%reg_data)) nullify (soft_mismatch%reg_data)
    if (allocated (soft_mismatch%sqme_born)) deallocate (soft_mismatch%sqme_born)
    if (allocated (soft_mismatch%sqme_born_color_c)) deallocate (soft_mismatch%sqme_born_color_c)
    if (allocated (soft_mismatch%sqme_born_charge_c)) deallocate (soft_mismatch%sqme_born_charge_c)
    if (associated (soft_mismatch%real_kinematics)) nullify (soft_mismatch%real_kinematics)
end subroutine soft_mismatch_final

```

27.5.2 Collinear and soft-collinear subtraction terms

This data type deals with the calculation of the collinear and soft-collinear contribution to the cross section.

```

<real subtraction: public>+≡
public :: coll_subtraction_t

<real subtraction: types>+≡
type :: coll_subtraction_t
    integer :: n_in, n_alr
    logical :: use_resonance_mappings = .false.
    real(default) :: CA = 0, CF = 0, TR = 0
contains

```

```

⟨real subtraction: coll sub: TBP⟩
end type coll_subtraction_t

```

```

⟨real subtraction: coll sub: TBP⟩≡
  procedure :: init => coll_subtraction_init

⟨real subtraction: procedures⟩+≡
  subroutine coll_subtraction_init (coll_sub, n_alr, n_in)
    class(coll_subtraction_t), intent(inout) :: coll_sub
    integer, intent(in) :: n_alr, n_in
    coll_sub%n_in = n_in
    coll_sub%n_alr = n_alr
  end subroutine coll_subtraction_init

```

Set the corresponding algebra parameters of the underlying gauge group of the correction.

```

⟨real subtraction: coll sub: TBP⟩+≡
  procedure :: set_parameters => coll_subtraction_set_parameters

⟨real subtraction: procedures⟩+≡
  subroutine coll_subtraction_set_parameters (coll_sub, CA, CF, TR)
    class(coll_subtraction_t), intent(inout) :: coll_sub
    real(default), intent(in) :: CA, CF, TR
    coll_sub%CA = CA
    coll_sub%CF = CF
    coll_sub%TR = TR
  end subroutine coll_subtraction_set_parameters

```

This subroutine computes the collinear limit of $g^\alpha(\xi, y)$ introduced in eq. 27.34. Care is given to also enable the usage for the soft-collinear limit. This, we write all formulas in terms of soft-finite quantities.

We have to compute

$$\frac{J(\Phi_n, \xi, y, \phi)}{\xi} [(1-y)\xi^2 \mathcal{R}^\alpha(\Phi_{n+1})] |_{y=1}.$$

The Jacobian J is proportional to ξ , due to the d^3k_{n+1}/k_{n+1}^0 factor in the integration measure. It cancels the factor of ξ in the denominator. The remaining part of the Jacobian is multiplied in `evaluate_region_fsr` and is not relevant here. Inserting the splitting functions exemplarily for $q \rightarrow qg$ yields

$$g^\alpha = \frac{8\pi\alpha_s}{k_{\text{em}}^2} C_F (1-y) \xi^2 \frac{1+(1-z)^2}{z} \mathcal{B},$$

where we have chosen $z = E_{\text{rad}}/\bar{E}_{\text{em}}$ and \bar{E}_{em} denotes the emitter energy in the Born frame. The collinear final state imposes $\bar{k}_n = k_n + k_{n+1}$ for the connection between Φ_n - and Φ_{n+1} -phasepace and we get $1-z = E_{\text{em}}/\bar{E}_{\text{em}}$. The denominator can be rewritten by the constraint $\bar{k}_n^2 = (k_n + k_{n+1})^2 = 0$ to

$$k_{\text{em}}^2 = 2E_{\text{rad}}E_{\text{em}}(1-y)$$

which cancels the $(1-y)$ factor in the numerator, thus showing that the whole expression is indeed collinear-finite. We can further transform

$$E_{\text{rad}}E_{\text{em}} = z(1-z)\bar{E}_{\text{em}}^2$$

so that in total we have

$$g^\alpha = \frac{4\pi\alpha_s}{1-z} \frac{1}{\bar{k}_{\text{em}}^2} C_F \left(\frac{\xi}{z} \right)^2 (1 + (1-z)^2) \mathcal{B}$$

Follow up calculations give us

$$g^{\alpha, g \rightarrow gg} = \frac{4\pi\alpha_s}{1-z} \frac{1}{\bar{k}_{\text{em}}^2} C_A \frac{\xi}{z} \left\{ 2 \left(\frac{z}{1-z} \xi + \frac{1-z}{\xi} \right) \mathcal{B} + 4\xi z(1-z) \hat{k}_\perp^\mu \hat{k}_\perp^\nu \mathcal{B}_{\mu\nu} \right\},$$

$$g^{\alpha, g \rightarrow qq} = \frac{4\pi\alpha_s}{1-z} \frac{1}{\bar{k}_{\text{em}}^2} T_R \frac{\xi}{z} \left\{ \xi \mathcal{B} - 4\xi z(1-z) \hat{k}_\perp^\mu \hat{k}_\perp^\nu \mathcal{B}_{\mu\nu} \right\}.$$

The ratio z/ξ is finite in the soft limit

$$\frac{z}{\xi} = \frac{q^0}{2E_{\text{em}}}$$

so that ξ does not appear explicitly in the computation.

The argumentation above is valid for $q \rightarrow qg$ -splittings, but the general factorization is valid for general splittings, also for those involving spin correlations and QED splittings. Note that care has to be given to the definition of z . Further, we have factored out a factor of z to include in the ratio z/ξ , which has to be taken into account in the implementation of the splitting functions.

(real subtraction: coll sub: TBP)+≡

`procedure :: compute_fsr => coll_subtraction_compute_fsr`

(real subtraction: procedures)+≡

```
function coll_subtraction_compute_fsr &
  (coll_sub, emitter, flst, p_res, p_born, sqme_born, mom_times_sqme_spin_c, &
   xi, alpha_coupling, double_fsr) result (sqme)
real(default) :: sqme
class(coll_subtraction_t), intent(in) :: coll_sub
integer, intent(in) :: emitter
integer, dimension(:), intent(in) :: flst
type(vector4_t), intent(in) :: p_res
type(vector4_t), intent(in), dimension(:) :: p_born
real(default), intent(in) :: sqme_born, mom_times_sqme_spin_c
real(default), intent(in) :: xi, alpha_coupling
logical, intent(in) :: double_fsr
real(default) :: q0, z, p0, z_o_xi, onemz
integer :: nlegs, flv_em, flv_rad
nlegs = size (flst)
flv_rad = flst(nlegs); flv_em = flst(emitter)
q0 = p_res**1
p0 = p_res * p_born(emitter) / q0
!!! Here, z corresponds to 1-z in the formulas of arXiv:1002.2581;
!!! the integrand is symmetric under this variable change
z_o_xi = q0 / (two * p0)
z = xi * z_o_xi; onemz = one - z
if (is_gluon (flv_em) .and. is_gluon (flv_rad)) then
  sqme = coll_sub%CA * ( two * ( z / onemz * xi + onemz / z_o_xi ) * sqme_born &
    + four * xi * z * onemz * mom_times_sqme_spin_c )
else if (is_fermion (flv_em) .and. is_fermion (flv_rad)) then
```

```

    sqme = coll_sub%TR * xi * (sqme_born - four * z * onemz * mom_times_sqme_spin_c)
  else if (is_fermion (flv_em) .and. is_massless_vector (flv_rad)) then
    sqme = sqme_born * coll_sub%CF * (one + onemz**2) / z_o_xi
  else
    sqme = zero
  end if
  sqme = sqme / (p0**2 * onemz * z_o_xi)
  sqme = sqme * four * pi * alpha_coupling
  if (double_fsr) sqme = sqme * onemz * two
end function coll_subtraction_compute_fsr

```

Like in the context of `coll_subtraction_compute_fsr` we compute the quantity

$$\lim_{y \rightarrow \pm 1} \left\{ \frac{J(\Phi_n, \xi, y, \phi)}{\xi} [(1 - y^2) \xi^2 \mathcal{R}^\alpha(\Phi_{n+1})] \right\},$$

where the $(1 - y^2)$ accounts for both $y = \pm 1$. Again, the Jacobian is proportional to ξ , so we drop the J/ξ factor. Note that it is important to take into account this missing factor of ξ in the computation of the Jacobian during phase-space generation both for fixed-beam and structure ISR. We consider only a $q \rightarrow qg$ splitting arguing that other splittings are identical in terms of the factors which cancel. It is given by

$$g^\alpha = \frac{8\pi\alpha_s}{-k_{\text{em}}^2} C_F (1 - y^2) \xi^2 \frac{1 + z^2}{1 - z} \mathcal{B},$$

where g^α is defined akin to the one for FSR in eq. 27.34. Note the negative sign of k_{em}^2 to compensate the negative virtuality of the initial-state emitter. For ISR, z is defined with respect to the emitter energy entering the hard interaction, i.e.

$$z = \frac{E_{\text{beam}} - E_{\text{rad}}}{E_{\text{beam}}} = 1 - \frac{E_{\text{rad}}}{E_{\text{beam}}}.$$

Because $E_{\text{rad}} = E_{\text{beam}} \cdot \xi$, it is $z = 1 - \xi$, thus one factor of ξ is cancelled by $(1 - z)$ in the denominator of g^α . The factor k_{em}^2 in the denominator is rewritten as

$$k_{\text{em}}^2 = (p_{\text{beam}} - p_{\text{rad}})^2 = -2p_{\text{beam}} \cdot p_{\text{rad}} = -2E_{\text{beam}} E_{\text{rad}} (1 \pm y) = -2E_{\text{beam}}^2 (1 - z)(1 \pm y),$$

where we used

$$E_{\text{beam}} E_{\text{rad}} = E_{\text{beam}}^2 (1 - z).$$

This leads to the cancellation of the corresponding $(1 \pm y)$ factor in $(1 - y^2)$, with the other factor becoming a simple factor of 2, and the remaining factor of ξ in the numerator. We thus end up with

$$g^\alpha = \frac{8\pi\alpha_s}{E_{\text{beam}}^2} C_F (1 + z^2) \mathcal{B},$$

which is soft-finite.

Note that here in `compute_isr`, `sqme_born` is supposed to be the squared Born matrix element convoluted with the real PDF.

(real subtraction: coll sub: TBP) +=

```

  procedure :: compute_isr => coll_subtraction_compute_isr

```

<real subtraction: procedures>+≡

```

function coll_subtraction_compute_isr &
  (coll_sub, emitter, flst, p_born, sqme_born, mom_times_sqme_spin_c, &
   xi, alpha_coupling, isr_mode) result (sqme)
  real(default) :: sqme
  class(coll_subtraction_t), intent(in) :: coll_sub
  integer, intent(in) :: emitter
  integer, dimension(:), intent(in) :: flst
  type(vector4_t), intent(in), dimension(:) :: p_born
  real(default), intent(in) :: sqme_born
  real(default), intent(in) :: mom_times_sqme_spin_c
  real(default), intent(in) :: xi, alpha_coupling
  integer, intent(in) :: isr_mode
  real(default) :: z, onemz, p02
  integer :: nlegs, flv_em, flv_rad
  !!! p_born must be in lab frame.
  nlegs = size (flst)
  flv_rad = flst(nlegs); flv_em = flst(emitter)
  !!! No need to pay attention to n_in = 1, because this case always has a
  !!! massive initial-state particle and thus no collinear divergence.
  p02 = p_born(1)%p(0) * p_born(2)%p(0) / two
  z = one - xi; onemz = xi
  if (is_massless_vector (flv_em) .and. is_massless_vector (flv_rad)) then
    sqme = coll_sub%CA * (two * (z + z * onemz**2) * sqme_born + four * onemz**2 &
      / z * mom_times_sqme_spin_c)
  else if (is_fermion (flv_em) .and. is_massless_vector (flv_rad)) then
    sqme = coll_sub%CF * (one + z**2) * sqme_born
  else if (is_fermion (flv_em) .and. is_fermion (flv_rad)) then
    sqme = coll_sub%CF * (z * onemz * sqme_born + four * onemz**2 / z * mom_times_sqme_spin_c)
  else if (is_massless_vector (flv_em) .and. is_fermion (flv_rad)) then
    sqme = coll_sub%TR * (z**2 + onemz**2) * onemz * sqme_born
  else
    sqme = zero
  end if
  if (isr_mode == SQRTS_VAR) then
    sqme = sqme / p02 * z
  else
    !!! We have no idea why this seems to work as there should be no factor
    !!! of z for the fixed-beam settings. This should definitely be understood in the
    !!! future!
    sqme = sqme / p02 / z
  end if
  sqme = sqme * four * pi * alpha_coupling
end function coll_subtraction_compute_isr

```

<real subtraction: coll sub: TBP>+≡

```

procedure :: final => coll_subtraction_final

```

<real subtraction: procedures>+≡

```

subroutine coll_subtraction_final (sub_coll)
  class(coll_subtraction_t), intent(inout) :: sub_coll
  sub_coll%use_resonance_mappings = .false.
end subroutine coll_subtraction_final

```

27.5.3 Real Subtraction

We store a pointer to the `nlo_settings_t` object which holds tuning parameters, e.g. cutoffs for the subtraction terms.

```

<real subtraction: public>+≡
    public :: real_subtraction_t

<real subtraction: types>+≡
    type :: real_subtraction_t
        type(nlo_settings_t), pointer :: settings => null ()
        type(region_data_t), pointer :: reg_data => null ()
        type(real_kinematics_t), pointer :: real_kinematics => null ()
        type(isr_kinematics_t), pointer :: isr_kinematics => null ()
        type(real_scales_t) :: scales
        real(default), dimension(:,:), allocatable :: sqme_real_non_sub
        real(default), dimension(:), allocatable :: sqme_born
        real(default), dimension(:,:), allocatable :: sf_factors
        real(default), dimension(:,:,:), allocatable :: sqme_born_color_c
        real(default), dimension(:,:,:), allocatable :: sqme_born_charge_c
        real(default), dimension(:,:,:), allocatable :: sqme_born_spin_c
        type(soft_subtraction_t) :: sub_soft
        type(coll_subtraction_t) :: sub_coll
        logical, dimension(:), allocatable :: sc_required
        logical :: subtraction_deactivated = .false.
        integer :: purpose = INTEGRATION
        logical :: radiation_event = .true.
        logical :: subtraction_event = .false.
        integer, dimension(:), allocatable :: selected_alr
contains
<real subtraction: real subtraction: TBP>
end type real_subtraction_t

```

Initializer

```

<real subtraction: real subtraction: TBP>≡
    procedure :: init => real_subtraction_init

<real subtraction: procedures>+≡
    subroutine real_subtraction_init (rsub, reg_data, settings)
        class(real_subtraction_t), intent(inout), target :: rsub
        type(region_data_t), intent(in), target :: reg_data
        type(nlo_settings_t), intent(in), target :: settings
        integer :: alr
        if (debug_on) call msg_debug (D_SUBTRACTION, "real_subtraction_init")
        if (debug_on) call msg_debug (D_SUBTRACTION, "n_in", reg_data%n_in)
        if (debug_on) call msg_debug (D_SUBTRACTION, "nlegs_born", reg_data%n_legs_born)
        if (debug_on) call msg_debug (D_SUBTRACTION, "nlegs_real", reg_data%n_legs_real)
        if (debug_on) call msg_debug (D_SUBTRACTION, "reg_data%n_regions", reg_data%n_regions)
        if (debug2_active (D_SUBTRACTION)) call reg_data%write ()
        rsub%reg_data => reg_data
        allocate (rsub%sqme_born (reg_data%n_flv_born))
        rsub%sqme_born = zero
        allocate (rsub%sf_factors (reg_data%n_regions, 0:reg_data%n_in))
        rsub%sf_factors = zero
        allocate (rsub%sqme_born_color_c (reg_data%n_legs_born, reg_data%n_legs_born, &
            reg_data%n_flv_born))
    end subroutine

```

```

    rsub%sqme_born_color_c = zero
    allocate (rsub%sqme_born_charge_c (reg_data%n_legs_born, reg_data%n_legs_born, &
        reg_data%n_flv_born))
    rsub%sqme_born_charge_c = zero
    allocate (rsub%sqme_real_non_sub (reg_data%n_flv_real, reg_data%n_phs))
    rsub%sqme_real_non_sub = zero
    allocate (rsub%sc_required (reg_data%n_regions))
    do alr = 1, reg_data%n_regions
        rsub%sc_required(alr) = reg_data%regions(alr)%sc_required
    end do
    if (rsub%requires_spin_correlations ()) then
        allocate (rsub%sqme_born_spin_c (1:3, 1:3, reg_data%n_legs_born, reg_data%n_flv_born))
        rsub%sqme_born_spin_c = zero
    end if
    call rsub%sub_soft%init (reg_data)
    call rsub%sub_coll%init (reg_data%n_regions, reg_data%n_in)
    rsub%settings => settings
    rsub%sub_soft%use_resonance_mappings = settings%use_resonance_mappings
    rsub%sub_coll%use_resonance_mappings = settings%use_resonance_mappings
    rsub%sub_soft%factorization_mode = settings%factorization_mode
end subroutine real_subtraction_init

```

```

<real subtraction: real subtraction: TBP>+≡
    procedure :: set_real_kinematics => real_subtraction_set_real_kinematics

```

```

<real subtraction: procedures>+≡
    subroutine real_subtraction_set_real_kinematics (rsub, real_kinematics)
        class(real_subtraction_t), intent(inout) :: rsub
        type(real_kinematics_t), intent(in), target :: real_kinematics
        rsub%real_kinematics => real_kinematics
    end subroutine real_subtraction_set_real_kinematics

```

```

<real subtraction: real subtraction: TBP>+≡
    procedure :: set_isr_kinematics => real_subtraction_set_isr_kinematics

```

```

<real subtraction: procedures>+≡
    subroutine real_subtraction_set_isr_kinematics (rsub, fractions)
        class(real_subtraction_t), intent(inout) :: rsub
        type(isr_kinematics_t), intent(in), target :: fractions
        rsub%isr_kinematics => fractions
    end subroutine real_subtraction_set_isr_kinematics

```

```

<real subtraction: real subtraction: TBP>+≡
    procedure :: get_i_res => real_subtraction_get_i_res

```

```

<real subtraction: procedures>+≡
    function real_subtraction_get_i_res (rsub, alr) result (i_res)
        integer :: i_res
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr
        select type (fks_mapping => rsub%reg_data%fks_mapping)
            type is (fks_mapping_resonances_t)
                i_res = fks_mapping%res_map%alr_to_i_res (alr)
            class default

```

```

        i_res = 0
    end select
end function real_subtraction_get_i_res

```

27.5.4 The real contribution to the cross section

In each singular region α , the real contribution to σ is given by the second summand of eqn. ??,

$$\sigma_{\text{real}}^\alpha = \int d\Phi_n \int_0^{2\pi} d\phi \int_{-1}^1 dy \int_0^{\xi_{\text{max}}} d\xi \left(\frac{1}{\xi} \right)_+ \left(\frac{1}{1-y} \right)_+ \underbrace{\frac{J(\Phi_n, \xi, y, \phi)}{\xi} [(1-y)\xi^2 \mathcal{R}^\alpha(\Phi_{n+1})]}_{g^\alpha(\xi, y)} \quad (27.34)$$

Writing out the plus-distribution and introducing $\tilde{\xi} = \xi/\xi_{\text{max}}$ to set the upper integration limit to 1, this turns out to be equal to

$$\begin{aligned} \sigma_{\text{real}}^\alpha = \int d\Phi_n \int_0^{2\pi} d\phi \int_{-1}^1 \frac{dy}{1-y} \left\{ \int_0^1 d\tilde{\xi} \left[\frac{g^\alpha(\tilde{\xi}\xi_{\text{max}}, y)}{\tilde{\xi}} - \underbrace{\frac{g^\alpha(0, y)}{\tilde{\xi}}}_{\text{soft}} - \underbrace{\frac{g^\alpha(\tilde{\xi}\xi_{\text{max}}, 1)}{\tilde{\xi}}}_{\text{coll.}} + \underbrace{\frac{g^\alpha(0, 1)}{\tilde{\xi}}}_{\text{coll.+soft}} \right] \right. \\ \left. + [\log \xi_{\text{max}}(y)g^\alpha(0, y) - \log \xi_{\text{max}}(1)g^\alpha(0, 1)] \right\}. \end{aligned} \quad (27.35)$$

This formula is implemented in `compute_sqme_real_fin`

If two or more singular regions would produce the same amplitude we only compute one and use the `eqv_index` to copy the result to the others (if `reuse_amplitudes_fks` is true).

```

⟨real subtraction: real subtraction: TBP⟩+≡
  procedure :: compute => real_subtraction_compute

⟨real subtraction: procedures⟩+≡
  subroutine real_subtraction_compute (rsub, emitter, i_phs, alpha_s, &
    alpha_qed, separate_alrs, sqme)
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: emitter, i_phs
    logical, intent(in) :: separate_alrs
    real(default), intent(inout), dimension(:) :: sqme
    real(default), dimension(:), allocatable :: sqme_alr_arr
    real(default), intent(in) :: alpha_s, alpha_qed
    real(default) :: sqme_alr, alpha_coupling
    integer :: alr, i_con, i_res, this_emitter
    logical :: same_emitter
    logical, dimension(:), allocatable :: alr_evaluated
    allocate (alr_evaluated(rsub%reg_data%n_regions))
    allocate (sqme_alr_arr(rsub%reg_data%n_regions))
    sqme_alr_arr = zero
    alr_evaluated = .false.
    do alr = 1, rsub%reg_data%n_regions
      if (.not. alr_evaluated(rsub%reg_data%regions(alr)%eqv_index)) then
        if (allocated (rsub%selected_alr)) then

```



```

        if (.not. any (rsub%selected_alr == alr)) cycle
    end if
    sqme_alr = zero
    if (emitter > rsub%isr_kinematics%n_in) then
        same_emitter = emitter == rsub%reg_data%regions(alr)%emitter
    else
        same_emitter = rsub%reg_data%regions(alr)%emitter <= rsub%isr_kinematics%n_in
    end if
    select case (char(rsub%reg_data%regions(alr)%nlo_correction_type))
    case ("QCD")
        alpha_coupling = alpha_s
    case ("EW")
        alpha_coupling = alpha_qed
    end select
    if (same_emitter .and. i_phs == rsub%real_kinematics%alr_to_i_phs (alr)) then
        i_res = rsub%get_i_res (alr)
        this_emitter = rsub%reg_data%regions(alr)%emitter
        sqme_alr = rsub%evaluate_emitter_region (alr, this_emitter, i_phs, i_res, &
            alpha_coupling)
        if (rsub%purpose == INTEGRATION .or. rsub%purpose == FIXED_ORDER_EVENTS) then
            !!! (PS-2021-09-13) This is always executed as purpose is never set.
            i_con = rsub%get_i_contributor (alr)
            sqme_alr = sqme_alr * rsub%get_phs_factor (i_con)
        end if
    end if
    sqme_alr_arr(alr) = sqme_alr_arr(alr) + sqme_alr
    if (.not. (debug_active (D_SUBTRACTION) .or. debug2_active (D_SUBTRACTION))) then
        if (.not. allocated (rsub%selected_alr)) &
            alr_evaluated(rsub%reg_data%regions(alr)%eqv_index) = .true.
    end if
else
    sqme_alr_arr(alr) = sqme_alr_arr(rsub%reg_data%regions(alr)%eqv_index)
end if
if (separate_alrs) then
    sqme(alr) = sqme(alr) + sqme_alr_arr(alr)
else
    sqme(1) = sqme(1) + sqme_alr_arr(alr)
end if
end do
if (debug_on) then
    if (debug2_active (D_SUBTRACTION)) call check_s_alpha_consistency ()
end if
contains
subroutine check_s_alpha_consistency ()
    real(default) :: sum_s_alpha, sum_s_alpha_soft
    integer :: i_ftuple
    if (debug_on) call msg_debug2 (D_SUBTRACTION, "Check consistency of s_alpha: ")
    do alr = 1, rsub%reg_data%n_regions
        sum_s_alpha = rsub%sum_up_s_alpha(alr, i_phs)
        call msg_debug2 (D_SUBTRACTION, 'sum_s_alpha', sum_s_alpha)
        if (.not. nearly_equal(sum_s_alpha, one)) then
            call msg_bug ("The sum of all S functions should be equal to one!")
        end if
        sum_s_alpha_soft = rsub%sum_up_s_alpha_soft(alr, i_phs)
    end do
end subroutine

```

```

        call msg_debug2 (D_SUBTRACTION, 'sum_s_alpha_soft', sum_s_alpha_soft)
        if (.not. nearly_equal(sum_s_alpha_soft, one)) then
            call msg_bug ("The sum of all soft S functions should be equal to one!")
        end if
    end do
end subroutine check_s_alpha_consistency
end subroutine real_subtraction_compute

```

The emitter is fixed. We now have to decide whether we evaluate in ISR or FSR region, and also if resonances are used.

```

<real subtraction: real subtraction: TBP>+=
    procedure :: evaluate_emitter_region => real_subtraction_evaluate_emitter_region
<real subtraction: procedures>+=
    function real_subtraction_evaluate_emitter_region (rsub, alr, emitter, &
        i_phs, i_res, alpha_coupling) result (sqme)
        real(default) :: sqme
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, emitter, i_phs, i_res
        real(default), intent(in) :: alpha_coupling
        if (emitter <= rsub%isr_kinematics%n_in) then
            sqme = rsub%evaluate_region_isr (alr, emitter, i_phs, i_res, alpha_coupling)
        else
            select type (fks_mapping => rsub%reg_data%fks_mapping)
            type is (fks_mapping_resonances_t)
                call fks_mapping%set_resonance_momenta &
                    (rsub%real_kinematics%xi_ref_momenta)
            end select
            sqme = rsub%evaluate_region_fsr (alr, emitter, i_phs, i_res, alpha_coupling)
        end if
    end function real_subtraction_evaluate_emitter_region

```

Sums up $\sum_{i_1, i_2} S_{i_1 i_2}$ for the given alr.

```

<real subtraction: real subtraction: TBP>+=
    procedure :: sum_up_s_alpha => real_subtraction_sum_up_s_alpha
<real subtraction: procedures>+=
    function real_subtraction_sum_up_s_alpha (rsub, alr, i_phs) result (sum_s_alpha)
        real(default) :: sum_s_alpha
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, i_phs
        type(vector4_t), dimension(:), allocatable :: p_real
        integer :: i_res, i_ftuple, i1, i2
        allocate (p_real (rsub%reg_data%n_legs_real))
        if (rsub%reg_data%has_pseudo_isr ()) then
            p_real = rsub%real_kinematics%p_real_onshell(i_phs)%get_momenta (i_phs)
        else
            p_real = rsub%real_kinematics%p_real_cms%get_momenta (i_phs)
        end if
        i_res = rsub%get_i_res (alr)
        sum_s_alpha = zero
        do i_ftuple = 1, rsub%reg_data%regions(alr)%nregions
            call rsub%reg_data%regions(alr)%ftuples(i_ftuple)%get (i1, i2)
            sum_s_alpha = sum_s_alpha + rsub%reg_data%get_svalue (p_real, alr, i1, i2, i_res)
        end do
    end function real_subtraction_sum_up_s_alpha

```

```

end do
end function real_subtraction_sum_up_s_alpha

```

Sums up $\sum_{i_1, i_2} S_{i_1 i_2}$ for the given alr. The soft S functions take the real momenta in the soft limit, i.e. the Born momenta. For each summand of `sum_s_alpha_soft` we take `p_soft` constructed from the emitter of the given alpha region also for ftuples in which the first integer `i1` does not coincide with the emitter. This is necessary because only if we keep `p_soft` fixed, all soft S functions are computed with the same denominator and thus add up to 1.

```

<real subtraction: real subtraction: TBP>+=
  procedure :: sum_up_s_alpha_soft => real_subtraction_sum_up_s_alpha_soft
<real subtraction: procedures>+=
  function real_subtraction_sum_up_s_alpha_soft (rsub, alr, i_phs) result (sum_s_alpha_soft)
    real(default) :: sum_s_alpha_soft
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, i_phs
    type(vector4_t), dimension(:), allocatable :: p_born
    integer :: i_res, i_ftuple, i1, i2, emitter, nlegs
    allocate (p_born (rsub%reg_data%n_legs_born))
    if (rsub%reg_data%has_pseudo_isr ()) then
      p_born = rsub%real_kinematics%p_born_onshell%get_momenta (1)
    else
      p_born = rsub%real_kinematics%p_born_cms%get_momenta (1)
    end if
    i_res = rsub%get_i_res (alr)
    emitter = rsub%reg_data%regions(alr)%emitter
    associate (r => rsub%real_kinematics)
      if (emitter > rsub%sub_soft%reg_data%n_in) then
        call rsub%sub_soft%create_softvec_fsr (p_born, r%y_soft(i_phs), r%phi, &
          emitter, r%xi_ref_momenta(rsub%sub_soft%i_xi_ref (alr, i_phs)))
      else
        call rsub%sub_soft%create_softvec_isr (r%y_soft(i_phs), r%phi)
      end if
    end associate
    nlegs = rsub%reg_data%n_legs_real
    sum_s_alpha_soft = zero
    do i_ftuple = 1, rsub%reg_data%regions(alr)%nregions
      call rsub%reg_data%regions(alr)%ftuples(i_ftuple)%get (i1, i2)
      if (i2 == nlegs) then
        sum_s_alpha_soft = sum_s_alpha_soft + rsub%reg_data%get_svalue_soft &
          (p_born, rsub%sub_soft%p_soft, alr, i1, i_res)
      end if
    end do
  end function real_subtraction_sum_up_s_alpha_soft

```

This subroutine computes the finite part of the real matrix element in an individual singular region. First, the radiation variables are fetched and \mathcal{R} is multiplied by the appropriate S_α -factors, region multiplicities and double-FSR factors. Then, it computes the soft, collinear, soft-collinear and remnant matrix elements and supplies the corresponding factor $1/\xi/(1-y)$ as well as the corresponding Jacobians.

```

<real subtraction: real subtraction: TBP>+=

```

```

procedure :: evaluate_region_fsr => real_subtraction_evaluate_region_fsr
{real subtraction: procedures}+=
function real_subtraction_evaluate_region_fsr (rsub, alr, emitter, i_phs, &
    i_res, alpha_coupling) result (sqme_tot)
    real(default) :: sqme_tot
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, emitter, i_phs, i_res
    real(default), intent(in) :: alpha_coupling
    real(default) :: sqme_rad, sqme_soft, sqme_coll, sqme_cs, sqme_remn
    sqme_rad = zero; sqme_soft = zero; sqme_coll = zero
    sqme_cs = zero; sqme_remn = zero
    associate (region => rsub%reg_data%regions(alr), template => rsub%settings%fks_template)
        if (rsub%radiation_event) then
            sqme_rad = rsub%sqme_real_non_sub (rsub%reg_data%get_matrix_element_index (alr), i_phs)
            call evaluate_fks_factors (sqme_rad, rsub%reg_data, rsub%real_kinematics, &
                alr, i_phs, emitter, i_res)
            call apply_kinematic_factors_radiation (sqme_rad, rsub%purpose, &
                rsub%real_kinematics, i_phs, .false., rsub%reg_data%has_pseudo_isr (), &
                emitter)
        end if
        if (rsub%subtraction_event .and. .not. (rsub%subtraction_deactivated &
            .or. region%nlo_correction_type == "none")) then
            if (debug2_active (D_SUBTRACTION)) then
                print *, "[real_subtraction_evaluate_region_fsr]"
                print *, "xi: ", rsub%real_kinematics%xi_max(i_phs) * rsub%real_kinematics%xi_tilde
                print *, "y: ", rsub%real_kinematics%y(i_phs)
            end if
            call rsub%evaluate_subtraction_terms_fsr (alr, emitter, i_phs, i_res, alpha_coupling, &
                sqme_soft, sqme_coll, sqme_cs)
            call apply_kinematic_factors_subtraction_fsr (sqme_soft, sqme_coll, sqme_cs, &
                rsub%real_kinematics, i_phs)
            associate (symm_factor_fs => rsub%reg_data%born_to_real_symm_factor_fs (alr))
                sqme_soft = sqme_soft * symm_factor_fs
                sqme_coll = sqme_coll * symm_factor_fs
                sqme_cs = sqme_cs * symm_factor_fs
            end associate
            sqme_remn = compute_sqme_remnant_fsr (sqme_soft, sqme_cs, &
                rsub%real_kinematics%xi_max(i_phs), template%xi_cut, rsub%real_kinematics%xi_tilde)
            select case (rsub%purpose)
            case (INTEGRATION)
                sqme_tot = sqme_rad - sqme_soft - sqme_coll + sqme_cs + sqme_remn
            case (FIXED_ORDER_EVENTS)
                sqme_tot = - sqme_soft - sqme_coll + sqme_cs + sqme_remn
            case default
                sqme_tot = zero
                call msg_bug ("real_subtraction_evaluate_region_fsr: " // &
                    "Undefined rsub%purpose")
            end select
        else
            sqme_tot = sqme_rad
        end if
        sqme_tot = sqme_tot * rsub%real_kinematics%jac_rand(i_phs)
        sqme_tot = sqme_tot * rsub%reg_data%regions(alr)%mult
    end associate
end function

```

```

if (debug_active (D_SUBTRACTION) .and. .not. debug2_active (D_SUBTRACTION)) then
    call real_subtraction_register_debug_sqme (rsub, alr, emitter, i_phs, sqme_rad, sqme_soft,
        sqme_coll=sqme_coll, sqme_cs=sqme_cs)
else if (debug2_active (D_SUBTRACTION)) then
    call write_computation_status_fsr ()
end if
contains
<real subtraction: real subtraction evaluate region_fsr: procedures>
subroutine write_computation_status_fsr (passed, total, region_type, full)
    integer, intent(in), optional :: passed, total
    character(*), intent(in), optional :: region_type
    integer :: i_born
    integer :: u
    real(default) :: xi
    logical :: yorn
    logical, intent(in), optional :: full
    yorn = .true.
    if (present (full)) yorn = full
    if (debug_on) call msg_debug (D_SUBTRACTION, "real_subtraction_evaluate_region_fsr")
    u = given_output_unit (); if (u < 0) return
    i_born = rsub%reg_data%regions(alr)%uborn_index
    xi = rsub%real_kinematics%xi_max (i_phs) * rsub%real_kinematics%xi_tilde
    write (u,'(A,I2)') 'rsub%purpose: ', rsub%purpose
    write (u,'(A,I4)') 'alr: ', alr
    write (u,'(A,I3)') 'emitter: ', emitter
    write (u,'(A,I3)') 'i_phs: ', i_phs
    write (u,'(A,F6.4)') 'xi_max: ', rsub%real_kinematics%xi_max (i_phs)
    write (u,'(A,F6.4)') 'xi_cut: ', rsub%real_kinematics%xi_max(i_phs) * rsub%settings%fks_temp
    write (u,'(A,F6.4,2X,A,F6.4)') 'xi: ', xi, 'y: ', rsub%real_kinematics%y (i_phs)
    if (yorn) then
        write (u,'(A,ES16.9)') 'sqme_born: ', rsub%sqme_born(i_born)
        write (u,'(A,ES16.9)') 'sqme_real: ', sqme_rad
        write (u,'(A,ES16.9)') 'sqme_soft: ', sqme_soft
        write (u,'(A,ES16.9)') 'sqme_coll: ', sqme_coll
        write (u,'(A,ES16.9)') 'sqme_coll-soft: ', sqme_cs
        write (u,'(A,ES16.9)') 'sqme_remn: ', sqme_remn
        write (u,'(A,ES16.9)') 'sqme_tot: ', sqme_tot
        if (present (passed) .and. present (total) .and. &
            present (region_type)) &
            write (u,'(A)') char (str (passed) // " of " // str (total) // &
                " " // region_type // " points passed in total")
    end if
    write (u,'(A,ES16.9)') 'jacobian - real: ', rsub%real_kinematics%jac(i_phs)%jac(1)
    write (u,'(A,ES16.9)') 'jacobian - soft: ', rsub%real_kinematics%jac(i_phs)%jac(2)
    write (u,'(A,ES16.9)') 'jacobian - coll: ', rsub%real_kinematics%jac(i_phs)%jac(3)
end subroutine write_computation_status_fsr
end function real_subtraction_evaluate_region_fsr

```

Compares the real matrix element to the subtraction terms in the soft, the collinear or the soft-collinear limits. Used for debug purposes if `?test_anti_coll_limit`, `?test_coll_limit` and/or `?test_soft_limit` are set in the Sindarin. `sqme_soft` and `sqme_cs` need to be provided if called for FSR and `sqme_coll_plus`, `sqme_coll_minus`, `sqme_cs_plus` as well as `sqme_cs_minus` need to be provided if called for ISR.

<real subtraction: procedures>+≡

```

subroutine real_subtraction_register_debug_sqme (rsub, alr, emitter, i_phs, sqme_rad, sqme_soft,
      sqme_coll, sqme_cs, sqme_coll_plus, sqme_coll_minus, sqme_cs_plus, sqme_cs_minus)
  class(real_subtraction_t), intent(in) :: rsub
  integer, intent(in) :: alr, emitter, i_phs
  real(default), intent(in) :: sqme_rad, sqme_soft
  real(default), intent(in), optional :: sqme_coll, sqme_cs, sqme_coll_plus, sqme_coll_minus, sq
  real(default), dimension(:), allocatable, save :: sqme_rad_store
  logical :: is_soft, is_collinear_plus, is_collinear_minus, is_fsr
  real(default), parameter :: soft_threshold = 0.001_default
  real(default), parameter :: coll_threshold = 0.99_default
  real(default), parameter :: rel_smallness = 0.01_default
  real(default) :: sqme_dummy, this_sqme_rad, y, xi_tilde
  logical, dimension(:), allocatable, save :: count_alr

  if (.not. allocated (sqme_rad_store)) then
    allocate (sqme_rad_store (rsub%reg_data%n_regions))
    sqme_rad_store = zero
  end if
  if (rsub%radiation_event) then
    sqme_rad_store(alr) = sqme_rad
  else
    if (.not. allocated (count_alr)) then
      allocate (count_alr (rsub%reg_data%n_regions))
      count_alr = .false.
    end if

    if (is_massless_vector (rsub%reg_data%regions(alr)%flst_real%flst(rsub%reg_data%n_legs_real
      xi_tilde = rsub%real_kinematics%xi_tilde
      is_soft = xi_tilde < soft_threshold
    else
      is_soft = .false.
    end if
    y = rsub%real_kinematics%y(i_phs)
    is_collinear_plus = y > coll_threshold .and. &
      rsub%reg_data%regions(alr)%has_collinear_divergence()
    is_collinear_minus = -y > coll_threshold .and. &
      rsub%reg_data%regions(alr)%has_collinear_divergence()

    is_fsr = emitter > rsub%isr_kinematics%n_in

    if (is_fsr) then
      if (.not. present(sqme_coll) .or. .not. present(sqme_cs)) &
        call msg_error ("real_subtraction_register_debug_sqme: Wrong arguments for FSR")
    else
      if (.not. present(sqme_coll_plus) .or. .not. present(sqme_coll_minus) &
        .or. .not. present(sqme_cs_plus) .or. .not. present(sqme_cs_minus)) &
        call msg_error ("real_subtraction_register_debug_sqme: Wrong arguments for ISR")
    end if

    this_sqme_rad = sqme_rad_store(alr)
    if (is_soft .and. .not. is_collinear_plus .and. .not. is_collinear_minus) then
      if ( .not. nearly_equal (this_sqme_rad, sqme_soft, &
        abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then

```

```

        call msg_print_color (char ("Soft MEs do not match in region " // str (alr)), COL_RED)
    else
        call msg_print_color (char ("sqme_soft OK in region " // str (alr)), COL_GREEN)
    end if
    print *, 'this_sqme_rad, sqme_soft = ', this_sqme_rad, sqme_soft
end if

if (is_collinear_plus .and. .not. is_soft) then
    if (is_fsr) then
        if ( .not. nearly_equal (this_sqme_rad, sqme_coll, &
            abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
            call msg_print_color (char ("Collinear MEs do not match in region " // str (alr)), COL_RED)
        else
            call msg_print_color (char ("sqme_coll OK in region " // str (alr)), COL_GREEN)
        end if
        print *, 'this_sqme_rad, sqme_coll = ', this_sqme_rad, sqme_coll
    else
        if ( .not. nearly_equal (this_sqme_rad, sqme_coll_plus, &
            abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
            call msg_print_color (char ("Collinear MEs do not match in region " // str (alr)), COL_RED)
        else
            call msg_print_color (char ("sqme_coll_plus OK in region " // str (alr)), COL_GREEN)
        end if
        print *, 'this_sqme_rad, sqme_coll_plus = ', this_sqme_rad, sqme_coll_plus
    end if
end if

if (is_collinear_minus .and. .not. is_soft) then
    if (.not. is_fsr) then
        if ( .not. nearly_equal (this_sqme_rad, sqme_coll_minus, &
            abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
            call msg_print_color (char ("Collinear MEs do not match in region " // str (alr)), COL_RED)
        else
            call msg_print_color (char ("sqme_coll_minus OK in region " // str (alr)), COL_GREEN)
        end if
        print *, 'this_sqme_rad, sqme_coll_minus = ', this_sqme_rad, sqme_coll_minus
    end if
end if

if (is_soft .and. is_collinear_plus) then
    if (is_fsr) then
        if ( .not. nearly_equal (this_sqme_rad, sqme_cs, &
            abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
            call msg_print_color (char ("Soft-collinear MEs do not match in region " // str (alr)), COL_RED)
        else
            call msg_print_color (char ("sqme_cs OK in region " // str (alr)), COL_GREEN)
        end if
        print *, 'this_sqme_rad, sqme_cs = ', this_sqme_rad, sqme_cs
    else
        if ( .not. nearly_equal (this_sqme_rad, sqme_cs_plus, &
            abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
            call msg_print_color (char ("Soft-collinear MEs do not match in region " // str (alr)), COL_RED)
        else
            call msg_print_color (char ("sqme_cs_plus OK in region " // str (alr)), COL_GREEN)
        end if
    end if
end if

```

```

        end if
        print *, 'this_sqme_rad, sqme_cs_plus = ', this_sqme_rad, sqme_cs_plus
    end if
end if

if (is_soft .and. is_collinear_minus) then
    if (.not. is_fsr) then
        if ( .not. nearly_equal (this_sqme_rad, sqme_cs_minus, &
            abs_smallness=tiny(1._default), rel_smallness=rel_smallness)) then
            call msg_print_color (char ("Soft-collinear MEs do not match in region " // str (a
        else
            call msg_print_color (char ("sqme_cs_minus OK in region " // str (alr)), COL_GREEN
        end if
        print *, 'this_sqme_rad, sqme_cs_minus = ', this_sqme_rad, sqme_cs_minus
    end if
end if

count_alr (alr) = .true.
if (all (count_alr)) then
    deallocate (count_alr)
    deallocate (sqme_rad_store)
end if
end if
end subroutine real_subtraction_register_debug_sqme

```

For final state radiation, the subtraction remnant cross section is

$$\sigma_{\text{remn}} = (\sigma_{\text{soft}} - \sigma_{\text{soft-coll}}) \log(\xi_{\text{max}}) \cdot \frac{\tilde{\xi}}{\xi_{\text{cut}}}. \quad (27.36)$$

There is only one factor of $\log(\xi_{\text{max}})$ for both limits as ξ_{max} does not depend on y in the case of FSR. We use the already computed `sqme_soft` and `sqme_cs` with a factor of $\tilde{\xi}$ which we have to compensate. We also need a factor $1/\xi_{\text{cut}}$ here to assure that the cross section is independent of this free cutoff parameter. However, it still remains to be motivated analytically.

```

⟨real subtraction: real subtraction evaluate region fsr: procedures⟩≡
    function compute_sqme_remnant_fsr (sqme_soft, sqme_cs, xi_max, xi_cut, xi_tilde) result (sqme_re
        real(default) :: sqme_remn
        real(default), intent(in) :: sqme_soft, sqme_cs, xi_max, xi_cut, xi_tilde
        if (debug_on) call msg_debug (D_SUBTRACTION, "compute_sqme_remnant_fsr")
        sqme_remn = (sqme_soft - sqme_cs) * log (xi_max) * xi_tilde / xi_cut
    end function compute_sqme_remnant_fsr

```

```

⟨real subtraction: real subtraction: TBP⟩+≡
    procedure :: evaluate_region_isr => real_subtraction_evaluate_region_isr

```

```

⟨real subtraction: procedures⟩+≡
    function real_subtraction_evaluate_region_isr (rsub, alr, emitter, i_phs, i_res, alpha_coupling)
        result (sqme_tot)
        real(default) :: sqme_tot
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, emitter, i_phs, i_res
        real(default), intent(in) :: alpha_coupling
    end function

```



```

real(default) :: sqme_rad, sqme_soft, sqme_coll_plus, sqme_coll_minus
real(default) :: sqme_cs_plus, sqme_cs_minus
real(default) :: sqme_remn
sqme_rad = zero; sqme_soft = zero;
sqme_coll_plus = zero; sqme_coll_minus = zero
sqme_cs_plus = zero; sqme_cs_minus = zero
sqme_remn = zero
associate (region => rsub%reg_data%regions(alr), template => rsub%settings%fks_template)
  if (rsub%radiation_event) then
    sqme_rad = rsub%sqme_real_non_sub (rsub%reg_data%get_matrix_element_index (alr), i_phs)
    call evaluate_fks_factors (sqme_rad, rsub%reg_data, rsub%real_kinematics, &
      alr, i_phs, emitter, i_res)
    call apply_kinematic_factors_radiation (sqme_rad, rsub%purpose, rsub%real_kinematics, &
      i_phs, .true., .false.)
  end if
  if (rsub%subtraction_event .and. .not. (rsub%subtraction_deactivated &
    .or. region%nlo_correction_type == "none")) then
    call rsub%evaluate_subtraction_terms_isr (alr, emitter, i_phs, i_res, alpha_coupling, &
      sqme_soft, sqme_coll_plus, sqme_coll_minus, sqme_cs_plus, sqme_cs_minus)
    call apply_kinematic_factors_subtraction_isr (sqme_soft, sqme_coll_plus, &
      sqme_coll_minus, sqme_cs_plus, sqme_cs_minus, rsub%real_kinematics, i_phs)
    associate (symm_factor_fs => rsub%reg_data%born_to_real_symm_factor_fs (alr))
      sqme_soft = sqme_soft * symm_factor_fs
      sqme_coll_plus = sqme_coll_plus * symm_factor_fs
      sqme_coll_minus = sqme_coll_minus * symm_factor_fs
      sqme_cs_plus = sqme_cs_plus * symm_factor_fs
      sqme_cs_minus = sqme_cs_minus * symm_factor_fs
    end associate
    sqme_remn = compute_sqme_remnant_isr (rsub%isr_kinematics%isr_mode, &
      sqme_soft, sqme_cs_plus, sqme_cs_minus, &
      rsub%isr_kinematics, rsub%real_kinematics, i_phs, template%xi_cut)
    sqme_tot = sqme_rad - sqme_soft - sqme_coll_plus - sqme_coll_minus &
      + sqme_cs_plus + sqme_cs_minus + sqme_remn
  else
    sqme_tot = sqme_rad
  end if
end associate
sqme_tot = sqme_tot * rsub%real_kinematics%jac_rand (i_phs)
sqme_tot = sqme_tot * rsub%reg_data%regions(alr)%mult
if (debug_active (D_SUBTRACTION) .and. .not. debug2_active (D_SUBTRACTION)) then
  call real_subtraction_register_debug_sqme (rsub, alr, emitter, i_phs, sqme_rad,&
    sqme_soft, sqme_coll_plus=sqme_coll_plus, sqme_coll_minus=sqme_coll_minus,&
    sqme_cs_plus=sqme_cs_plus, sqme_cs_minus=sqme_cs_minus)
else if (debug2_active (D_SUBTRACTION)) then
  call write_computation_status_isr ()
end if
contains
<real subtraction: evaluate region isr: procedures>
subroutine write_computation_status_isr (unit)
  integer, intent(in), optional :: unit
  integer :: i_born
  integer :: u
  real(default) :: xi
  u = given_output_unit (unit); if (u < 0) return

```

```

i_born = rsub%reg_data%regions(alr)%uborn_index
xi = rsub%real_kinematics%xi_max (i_phs) * rsub%real_kinematics%xi_tilde
write (u,'(A,I4)') 'alr: ', alr
write (u,'(A,I2)') 'emitter: ', emitter
write (u,'(A,F4.2)') 'xi_max: ', rsub%real_kinematics%xi_max (i_phs)
print *, 'xi: ', xi, 'y: ', rsub%real_kinematics%y (i_phs)
print *, 'xb1: ', rsub%isr_kinematics%x(1), 'xb2: ', rsub%isr_kinematics%x(2)
print *, 'random jacobian: ', rsub%real_kinematics%jac_rand (i_phs)
write (u,'(A,ES16.9)') 'sqme_born: ', rsub%sqme_born(i_born)
write (u,'(A,ES16.9)') 'sqme_real: ', sqme_rad
write (u,'(A,ES16.9)') 'sqme_soft: ', sqme_soft
write (u,'(A,ES16.9)') 'sqme_coll_plus: ', sqme_coll_plus
write (u,'(A,ES16.9)') 'sqme_coll_minus: ', sqme_coll_minus
write (u,'(A,ES16.9)') 'sqme_cs_plus: ', sqme_cs_plus
write (u,'(A,ES16.9)') 'sqme_cs_minus: ', sqme_cs_minus
write (u,'(A,ES16.9)') 'sqme_remn: ', sqme_remn
write (u,'(A,ES16.9)') 'sqme_tot: ', sqme_tot
write (u,'(A,ES16.9)') 'jacobian - real: ', rsub%real_kinematics%jac(i_phs)%jac(1)
write (u,'(A,ES16.9)') 'jacobian - soft: ', rsub%real_kinematics%jac(i_phs)%jac(2)
write (u,'(A,ES16.9)') 'jacobian - collplus: ', rsub%real_kinematics%jac(i_phs)%jac(3)
write (u,'(A,ES16.9)') 'jacobian - collminus: ', rsub%real_kinematics%jac(i_phs)%jac(4)
end subroutine write_computation_status_isr
end function real_subtraction_evaluate_region_isr

```

Computes the soft remnant for ISR. The formulas can be found in arXiv:1002.2581, eq. 4.21. and arXiv:0709.2092, sec. 5.1.2. This results in

$$\sigma_{\text{remn}}^{\text{ISR}} = \log(\xi_{\text{max}}(y))\sigma_{\text{soft}} - \frac{1}{2} \log(\xi_{\text{max}}(1))\sigma_{\oplus}^{\text{soft-coll}} - \frac{1}{2} \log(\xi_{\text{max}}(-1))\sigma_{\ominus}^{\text{soft-coll}} \quad (27.37)$$

where for ISR, ξ_{max} does explicitly depend on y due to the rescaling of the x values from the Born to the real partonic system according to

$$x_{\oplus} = \frac{\bar{x}_{\oplus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1-y)}{2-\xi(1+y)}}, \quad x_{\ominus} = \frac{\bar{x}_{\ominus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1+y)}{2-\xi(1-y)}} \quad (27.38)$$

As ξ_{max} is determined by the fact that the real x_{\oplus}, x_{\ominus} have to stay in a physically meaningful regime, i.e. $x_{\oplus}, x_{\ominus} < 1$, this leads to

$$\xi_{\text{max}} = 1 - \max \left\{ \frac{2(1+y)\bar{x}_{\oplus}^2}{\sqrt{(1+\bar{x}_{\oplus}^2)^2(1-y)^2 + 16y\bar{x}_{\oplus}^2} + (1-y)(1-\bar{x}_{\oplus}^2)}, \quad (27.39) \right.$$

$$\left. \frac{2(1-y)\bar{x}_{\oplus}^2}{\sqrt{(1+\bar{x}_{\oplus}^2)^2(1+y)^2 - 16y\bar{x}_{\oplus}^2} + (1+y)(1-\bar{x}_{\oplus}^2)} \right\} \quad (27.40)$$

and thus

$$\xi_{\text{max}}(y=1) = 1 - \bar{x}_{\oplus} \quad (27.41)$$

$$\xi_{\text{max}}(y=-1) = 1 - \bar{x}_{\ominus} \quad (27.42)$$

So we need to use the unrescaled $\bar{x}_{\oplus}, \bar{x}_{\ominus}$ here. Factors of $\frac{1}{2}$ and $\frac{1}{\xi}$ are already included in the matrix elements from `apply_kinematic_factors_subtraction_isr`.

We keep the former and remove the latter by multiplying with $\tilde{\xi}$. The factor $1/\xi_{\text{cut}}$ is probably needed to assure that the cross section is independent of this free cutoff parameter in analogy to the FSR case. However, it still remains to be motivated analytically and to be validated.

(real subtraction: evaluate region isr: procedures) \equiv

```
function compute_sqme_remnant_isr (isr_mode, sqme_soft, sqme_cs_plus, sqme_cs_minus, &
    isr_kinematics, real_kinematics, i_phs, xi_cut) result (sqme_remn)
    real(default) :: sqme_remn
    integer, intent(in) :: isr_mode
    real(default), intent(in) :: sqme_soft, sqme_cs_plus, sqme_cs_minus
    type(isr_kinematics_t), intent(in) :: isr_kinematics
    type(real_kinematics_t), intent(in) :: real_kinematics
    integer, intent(in) :: i_phs
    real(default), intent(in) :: xi_cut
    real(default) :: xi_tilde, xi_max, xi_max_plus, xi_max_minus, xb_plus, xb_minus
    xi_max = real_kinematics%xi_max (i_phs)
    xi_tilde = real_kinematics%xi_tilde
    select case (isr_mode)
    case (SQRTS_VAR)
        xb_plus = isr_kinematics%x(I_PLUS)
        xb_minus = isr_kinematics%x(I_MINUS)
        xi_max_plus = one - xb_plus
        xi_max_minus = one - xb_minus
    case (SQRTS_FIXED)
        xi_max_plus = real_kinematics%xi_max (i_phs)
        xi_max_minus = real_kinematics%xi_max (i_phs)
    end select
    sqme_remn = log (xi_max) * xi_tilde * sqme_soft &
        - log (xi_max_plus) * xi_tilde * sqme_cs_plus &
        - log (xi_max_minus) * xi_tilde * sqme_cs_minus
    sqme_remn = sqme_remn / xi_cut
end function compute_sqme_remnant_isr
```

(real subtraction: real subtraction: TBP) \equiv

```
procedure :: evaluate_subtraction_terms_fsr => &
    real_subtraction_evaluate_subtraction_terms_fsr
```

(real subtraction: procedures) \equiv

```
subroutine real_subtraction_evaluate_subtraction_terms_fsr (rsub, &
    alr, emitter, i_phs, i_res, alpha_coupling, sqme_soft, sqme_coll, sqme_cs)
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, emitter, i_phs, i_res
    real(default), intent(in) :: alpha_coupling
    real(default), intent(out) :: sqme_soft, sqme_coll, sqme_cs
    if (debug_on) call msg_debug (D_SUBTRACTION, "real_subtraction_evaluate_subtraction_terms_fsr")
    sqme_soft = zero; sqme_coll = zero; sqme_cs = zero
    associate (xi_tilde => rsub%real_kinematics%xi_tilde, &
        y => rsub%real_kinematics%y(i_phs), template => rsub%settings%fks_template)
    if (template%xi_cut > xi_tilde) &
        sqme_soft = rsub%compute_sub_soft (alr, emitter, i_phs, i_res, alpha_coupling)
    if (y - 1 + template%delta_o > 0) &
        sqme_coll = rsub%compute_sub_coll (alr, emitter, i_phs, alpha_coupling)
    if (template%xi_cut > xi_tilde .and. y - 1 + template%delta_o > 0) &
        sqme_cs = rsub%compute_sub_coll_soft (alr, emitter, i_phs, alpha_coupling)
```

```

    if (debug2_active (D_SUBTRACTION)) then
      print *, "FSR Cutoff:"
      print *, "sub_soft: ", template%xi_cut > xi_tilde, "(ME: ", sqme_soft, ")"
      print *, "sub_coll: ", (y - 1 + template%delta_o) > 0, "(ME: ", sqme_coll, ")"
      print *, "sub_coll_soft: ", template%xi_cut > xi_tilde .and. (y - 1 + template%delta_o) >
        "(ME: ", sqme_cs, ")"
    end if
  end associate
end subroutine real_subtraction_evaluate_subtraction_terms_fsr

```

(real subtraction: procedures)+≡

```

subroutine evaluate_fks_factors (sqme, reg_data, real_kinematics, &
  alr, i_phs, emitter, i_res)
  real(default), intent(inout) :: sqme
  type(region_data_t), intent(inout) :: reg_data
  type(real_kinematics_t), intent(in), target :: real_kinematics
  integer, intent(in) :: alr, i_phs, emitter, i_res
  real(default) :: s_alpha
  type(phs_point_set_t), pointer :: p_real => null ()
  if (reg_data%has_pseudo_isr ()) then
    p_real => real_kinematics%p_real_onshell (i_phs)
  else
    p_real => real_kinematics%p_real_cms
  end if
  s_alpha = reg_data%get_svalue (p_real%get_momenta(i_phs), alr, emitter, i_res)
  if (debug2_active (D_SUBTRACTION)) call msg_print_color('s_alpha', s_alpha, COL_YELLOW)
  if (s_alpha > one + tiny_07) call msg_fatal ("s_alpha > 1!")
  sqme = sqme * s_alpha
  associate (region => reg_data%regions(alr))
    if (emitter > reg_data%n_in) then
      if (debug2_active (D_SUBTRACTION)) &
        print *, 'Double FSR: ', region%double_fsr_factor (p_real%get_momenta(i_phs))
      sqme = sqme * region%double_fsr_factor (p_real%get_momenta(i_phs))
    end if
  end associate
end subroutine evaluate_fks_factors

```

(real subtraction: procedures)+≡

```

subroutine apply_kinematic_factors_radiation (sqme, purpose, real_kinematics, &
  i_phs, isr, threshold, emitter)
  real(default), intent(inout) :: sqme
  integer, intent(in) :: purpose
  type(real_kinematics_t), intent(in) :: real_kinematics
  integer, intent(in) :: i_phs
  logical, intent(in) :: isr, threshold
  integer, intent(in), optional :: emitter
  real(default) :: xi, xi_tilde, s
  xi_tilde = real_kinematics%xi_tilde
  xi = xi_tilde * real_kinematics%xi_max (i_phs)
  select case (purpose)
    case (INTEGRATION, FIXED_ORDER_EVENTS)
      sqme = sqme * xi**2 / xi_tilde * real_kinematics%jac(i_phs)%jac(1)
    case (POWHEG)

```

```

!!! (PS 2021-09-21) This has been implemented but is never executed so far.
if (.not. isr) then
  s = real_kinematics%cms_energy2
  sqme = sqme * real_kinematics%jac(i_phs)%jac(1) * s / (8 * twopi3) * xi
else
  call msg_fatal ("POWHEG with initial-state radiation not implemented yet")
end if
end select
end subroutine apply_kinematic_factors_radiation

```

This routine applies the factors in the integrand of eq. 4.20 in arXiv:1002.2581 to the matrix elements.

```

<real subtraction: procedures>+≡
subroutine apply_kinematic_factors_subtraction_fsr &
  (sqme_soft, sqme_coll, sqme_cs, real_kinematics, i_phs)
real(default), intent(inout) :: sqme_soft, sqme_coll, sqme_cs
type(real_kinematics_t), intent(in) :: real_kinematics
integer, intent(in) :: i_phs
real(default) :: xi_tilde, onemy
xi_tilde = real_kinematics%xi_tilde
onemy = one - real_kinematics%y(i_phs)
sqme_soft = sqme_soft / onemy / xi_tilde
sqme_coll = sqme_coll / onemy / xi_tilde
sqme_cs = sqme_cs / onemy / xi_tilde
associate (jac => real_kinematics%jac(i_phs)%jac)
  sqme_soft = sqme_soft * jac(2)
  sqme_coll = sqme_coll * jac(3)
  sqme_cs = sqme_cs * jac(2)
end associate
end subroutine apply_kinematic_factors_subtraction_fsr

```

This routine applies the factors in the integrand of eq. 4.21 in arXiv:1002.2581 to the matrix elements.

```

<real subtraction: procedures>+≡
subroutine apply_kinematic_factors_subtraction_isr &
  (sqme_soft, sqme_coll_plus, sqme_coll_minus, sqme_cs_plus, &
   sqme_cs_minus, real_kinematics, i_phs)
real(default), intent(inout) :: sqme_soft, sqme_coll_plus, sqme_coll_minus
real(default), intent(inout) :: sqme_cs_plus, sqme_cs_minus
type(real_kinematics_t), intent(in) :: real_kinematics
integer, intent(in) :: i_phs
real(default) :: xi_tilde, y, onemy, onepy
xi_tilde = real_kinematics%xi_tilde
y = real_kinematics%y(i_phs)
onemy = one - y; onepy = one + y
associate (jac => real_kinematics%jac(i_phs)%jac)
  sqme_soft = sqme_soft / (one - y**2) / xi_tilde * jac(2)
  sqme_coll_plus = sqme_coll_plus / onemy / xi_tilde / two * jac(3)
  sqme_coll_minus = sqme_coll_minus / onepy / xi_tilde / two * jac(4)
  sqme_cs_plus = sqme_cs_plus / onemy / xi_tilde / two * jac(2)
  sqme_cs_minus = sqme_cs_minus / onepy / xi_tilde / two * jac(2)
end associate
end subroutine apply_kinematic_factors_subtraction_isr

```

This subroutine evaluates the soft and collinear subtraction terms for ISR. References:

- arXiv:0709.2092, sec. 2.4.2
- arXiv:0908.4272, sec. 4.2

For the collinear terms, the procedure is as follows:

If the emitter is 0, then a gluon was radiated from one of the incoming partons. Gluon emissions require two counter terms: One for emission in the direction of the first incoming parton \oplus and a second for emission in the direction of the second incoming parton \ominus because in both cases, there are divergent diagrams contributing to the matrix element. So in this case both, `sqme_coll_plus` and `sqme_coll_minus`, are non-zero.

If the emitter is 1 or 2, then a quark was emitted instead of a gluon. This only leads to a divergence collinear to the emitter because for anti-collinear quark emission, there are simply no divergent diagrams in the same region as two collinear quarks that cannot originate in the same splitting are non-divergent. This means that in case the emitter is 1, we need non-zero `sqme_coll_plus` and in case the emitter is 2, we need non-zero `sqme_coll_minus`.

At this point, we want to remind ourselves that in case of initial state divergences, y is just the polar angle, so the `sqme_coll_minus` terms are there to counter emissions in the direction of the second incoming parton \ominus and **not** to counter in general anti-collinear divergences.

```

<real subtraction: real subtraction: TBP>+=
  procedure :: evaluate_subtraction_terms_isr => &
    real_subtraction_evaluate_subtraction_terms_isr

<real subtraction: procedures>+=
  subroutine real_subtraction_evaluate_subtraction_terms_isr (rsub, &
    alr, emitter, i_phs, i_res, alpha_coupling, sqme_soft, sqme_coll_plus, &
    sqme_coll_minus, sqme_cs_plus, sqme_cs_minus)
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, emitter, i_phs, i_res
    real(default), intent(in) :: alpha_coupling
    real(default), intent(out) :: sqme_soft
    real(default), intent(out) :: sqme_coll_plus, sqme_coll_minus
    real(default), intent(out) :: sqme_cs_plus, sqme_cs_minus
    sqme_coll_plus = zero; sqme_cs_plus = zero
    sqme_coll_minus = zero; sqme_cs_minus = zero
    associate (xi_tilde => rsub%real_kinematics%xi_tilde, &
      y => rsub%real_kinematics%y(i_phs), template => rsub%settings%fks_template)
      if (template%xi_cut > xi_tilde) &
        sqme_soft = rsub%compute_sub_soft (alr, emitter, i_phs, i_res, alpha_coupling)
      if (emitter /= 2) then
        if (y - 1 + template%delta_i > 0) then
          sqme_coll_plus = rsub%compute_sub_coll (alr, 1, i_phs, alpha_coupling)
          if (template%xi_cut > xi_tilde) then
            sqme_cs_plus = rsub%compute_sub_coll_soft (alr, 1, i_phs, alpha_coupling)
          end if
        end if
      end if
    end if
  end if
end if

```

```

    if (emitter /= 1) then
      if (-y - 1 + template%delta_i > 0) then
        sqme_coll_minus = rsub%compute_sub_coll (alr, 2, i_phs, alpha_coupling)
        if (template%xi_cut > xi_tilde) then
          sqme_cs_minus = rsub%compute_sub_coll_soft (alr, 2, i_phs, alpha_coupling)
        end if
      end if
    end if
    if (debug2_active (D_SUBTRACTION)) then
      print *, "ISR Cutoff:"
      print *, "y: ", y
      print *, "delta_i: ", template%delta_i
      print *, "emitter: ", emitter
      print *, "sub_soft: ", template%xi_cut > xi_tilde, "(ME: ", sqme_soft, ")"
      print *, "sub_coll_plus: ", (-y - 1 + template%delta_i) > 0, "(ME: ", sqme_coll_plus, ")"
      print *, "sub_coll_minus: ", (-y - 1 + template%delta_i) > 0, "(ME: ", sqme_coll_minus, ")"
      print *, "sub_coll_soft_plus: ", template%xi_cut > xi_tilde .and. (-y - 1 + template%delta_i) > 0, "(ME: ", sqme_cs_plus, ")"
      print *, "sub_coll_soft_minus: ", template%xi_cut > xi_tilde .and. (-y - 1 + template%delta_i) > 0, "(ME: ", sqme_cs_minus, ")"
    end if
  end associate
end subroutine real_subtraction_evaluate_subtraction_terms_isr

```

This is basically the global part of the real Jacobian corresponding to

$$\frac{q^2}{8(2\pi)^3}.$$

We interpret it as the additional phase space factor of the real component, to be more consistent with the evaluation of the Born phase space.

We specifically use the Born center-of-mass energy here. The real center-of-mass energy is only different from the Born center-of-mass energy in case of ISR. The missing factor $\frac{1}{1-\xi}$ for this conversion is supplied in `apply_kinematic_factors_radiation` and `phs_fks_generator_generate_isr`.

```

<real subtraction: real subtraction: TBP>+≡
  procedure :: get_phs_factor => real_subtraction_get_phs_factor

<real subtraction: procedures>+≡
  function real_subtraction_get_phs_factor (rsub, i_con) result (factor)
    real(default) :: factor
    class(real_subtraction_t), intent(in) :: rsub
    integer, intent(in) :: i_con
    real(default) :: s
    s = rsub%real_kinematics%xi_ref_momenta (i_con)**2
    factor = s / (8 * twopi3)
  end function real_subtraction_get_phs_factor

<real subtraction: real subtraction: TBP>+≡
  procedure :: get_i_contributor => real_subtraction_get_i_contributor

<real subtraction: procedures>+≡
  function real_subtraction_get_i_contributor (rsub, alr) result (i_con)
    integer :: i_con

```

```

class(real_subtraction_t), intent(in) :: rsub
integer, intent(in) :: alr
if (allocated (rsub%reg_data%alr_to_i_contributor)) then
    i_con = rsub%reg_data%alr_to_i_contributor (alr)
else
    i_con = 1
end if
end function real_subtraction_get_i_contributor

```

Computes the soft subtraction term. If there is an initial state emission having a soft divergence, then a gluon has to have been emitted. A gluon can always be emitted from both IS partons and thus, we can take the `sf_factor` for emitter 0 in this case. Be aware that this approach will not work for *pe* collisions.

```

<real subtraction: real subtraction: TBP>+=
    procedure :: compute_sub_soft => real_subtraction_compute_sub_soft

<real subtraction: procedures>+=
    function real_subtraction_compute_sub_soft (rsub, alr, emitter, &
        i_phs, i_res, alpha_coupling) result (sqme_soft)
        real(default) :: sqme_soft
        class(real_subtraction_t), intent(inout) :: rsub
        integer, intent(in) :: alr, emitter, i_phs, i_res
        real(default), intent(in) :: alpha_coupling
        integer :: i_xi_ref, i_born
        real(default) :: q2, sf_factor
        type(vector4_t), dimension(:), allocatable :: p_born
        associate (real_kinematics => rsub%real_kinematics, &
            nlo_corr_type => rsub%reg_data%regions(alr)%nlo_correction_type, &
            sregion => rsub%reg_data%regions(alr))
            sqme_soft = zero
            if (sregion%has_soft_divergence ()) then
                i_xi_ref = rsub%sub_soft%i_xi_ref (alr, i_phs)
                q2 = real_kinematics%xi_ref_momenta (i_xi_ref)**2
                allocate (p_born (rsub%reg_data%n_legs_born))
                if (rsub%reg_data%has_pseudo_isr ()) then
                    p_born = real_kinematics%p_born_onshell%get_momenta (1)
                else
                    p_born = real_kinematics%p_born_cms%get_momenta (1)
                end if
                if (emitter > rsub%sub_soft%reg_data%n_in) then
                    call rsub%sub_soft%create_softvec_fsr &
                        (p_born, real_kinematics%y_soft(i_phs), &
                            real_kinematics%phi, emitter, &
                            real_kinematics%xi_ref_momenta(i_xi_ref))
                    sf_factor = one
                else
                    call rsub%sub_soft%create_softvec_isr &
                        (real_kinematics%y_soft(i_phs), real_kinematics%phi)
                    sf_factor = rsub%sf_factors(alr, 0)
                end if
                i_born = sregion%uborn_index
                select case (char (nlo_corr_type))
                case ("QCD")
                    sqme_soft = rsub%sub_soft%compute &

```



```

        (p_born, rsub%sqme_born_color_c(:, :, i_born) * &
sf_factor, real_kinematics%y(i_phs), &
q2, alpha_coupling, alr, emitter, i_res)
    case ("EW")
        sqme_soft = rsub%sub_soft%compute &
        (p_born, rsub%sqme_born_charge_c(:, :, i_born) * &
sf_factor, real_kinematics%y(i_phs), &
q2, alpha_coupling, alr, emitter, i_res)
    end select
end if
end associate
if (debug2_active(D_SUBTRACTION)) call check_soft_vector ()
contains
subroutine check_soft_vector ()
    !!! p_soft = p_gluon / E_gluon only in the soft limit
    !!! This check only has to be passed for ISR or for FSR if ?test_soft_limit = true is set.
    type(vector4_t) :: p_gluon
    if (debug_on) call msg_debug2 (D_SUBTRACTION, "Compare soft vector: ")
    print *, 'p_soft: ', rsub%sub_soft%p_soft%p
    print *, 'Normalized gluon momentum: '
    if (rsub%reg_data%has_pseudo_isr ()) then
        p_gluon = rsub%real_kinematics%p_real_onshell(thr_leg(emitter))%get_momentum &
        (i_phs, rsub%reg_data%n_legs_real)
    else
        p_gluon = rsub%real_kinematics%p_real_cms%get_momentum &
        (i_phs, rsub%reg_data%n_legs_real)
    end if
    call vector4_write (p_gluon / p_gluon%p(0), show_mass = .true.)
end subroutine check_soft_vector
end function real_subtraction_compute_sub_soft

```

```

<real subtraction: real subtraction: TBP>+≡
    procedure :: get_spin_correlation_term => real_subtraction_get_spin_correlation_term

<real subtraction: procedures>+≡
    function real_subtraction_get_spin_correlation_term (rsub, alr, i_born, emitter) &
        result (mom_times_sqme)
        real(default) :: mom_times_sqme
        class(real_subtraction_t), intent(in) :: rsub
        integer, intent(in) :: alr, i_born, emitter
        real(default), dimension(0:3) :: k_perp
        integer :: mu, nu
        if (rsub%sc_required(alr)) then
            if (debug2_active(D_SUBTRACTION)) call check_me_consistency ()
            associate (real_kin => rsub%real_kinematics)
                if (emitter > rsub%reg_data%n_in) then
                    k_perp = real_subtraction_compute_k_perp_fsr ( &
                        real_kin%p_born_lab%get_momentum(1, emitter), &
                        rsub%real_kinematics%phi)
                else
                    k_perp = real_subtraction_compute_k_perp_isr ( &
                        real_kin%p_born_lab%get_momentum(1, emitter), &
                        rsub%real_kinematics%phi)
                end if
            end associate
        end if
    end function

```

```

        end associate
        mom_times_sqme = zero
        do mu = 1, 3
            do nu = 1, 3
                mom_times_sqme = mom_times_sqme + &
                    k_perp(mu) * k_perp(nu) * rsub%sqme_born_spin_c (mu, nu, emitter, i_born)
            end do
        end do
    else
        mom_times_sqme = zero
    end if
contains
    subroutine check_me_consistency ()
        real(default) :: sqme_sum
        if (debug_on) call msg_debug2 (D_SUBTRACTION, "Spin-correlation: Consistency check")
        sqme_sum = &
            - rsub%sqme_born_spin_c(1,1,emitter,i_born) &
            - rsub%sqme_born_spin_c(2,2,emitter,i_born) &
            - rsub%sqme_born_spin_c(3,3,emitter,i_born)
        if (.not. nearly_equal (sqme_sum, -rsub%sqme_born(i_born))) then
            print *, 'Spin-correlated matrix elements are not consistent: '
            print *, 'emitter: ', emitter
            print *, 'g^{mu,nu} B_{mu,nu}: ', -sqme_sum
            print *, 'all Born matrix elements: ', rsub%sqme_born
            call msg_fatal ("FAIL")
        else
            call msg_print_color ("Success", COL_GREEN)
        end if
    end subroutine check_me_consistency
end function real_subtraction_get_spin_correlation_term

```

Construct a normalised momentum perpendicular to momentum p and rotate by an arbitrary angle ϕ . The angular conventions we use here are equivalent to those used by POWHEG.

```

<real subtraction: public>+≡
    public :: real_subtraction_compute_k_perp_fsr, &
        real_subtraction_compute_k_perp_isr

<real subtraction: procedures>+≡
    function real_subtraction_compute_k_perp_fsr (p, phi) result (k_perp_fsr)
        real(default), dimension(0:3) :: k_perp_fsr
        type(vector4_t), intent(in) :: p
        real(default), intent(in) :: phi
        type(vector4_t) :: k
        type(vector3_t) :: vec
        type(lorentz_transformation_t) :: rot
        vec = p%p(1:3) / p%p(0)
        k%p(0) = zero
        k%p(1) = p%p(1); k%p(2) = p%p(2)
        k%p(3) = - (p%p(1)**2 + p%p(2)**2) / p%p(3)
        rot = rotation (cos(phi), sin(phi), vec)
        k = rot * k
        k%p(1:3) = k%p(1:3) / space_part_norm (k)
        k_perp_fsr = k%p
    end function

```

```

end function real_subtraction_compute_k_perp_fsr

function real_subtraction_compute_k_perp_isr (p, phi) result (k_perp_isr)
  real(default), dimension(0:3) :: k_perp_isr
  type(vector4_t), intent(in) :: p
  real(default), intent(in) :: phi
  k_perp_isr(0) = zero
  k_perp_isr(1) = sin(phi)
  k_perp_isr(2) = cos(phi)
  k_perp_isr(3) = zero
end function real_subtraction_compute_k_perp_isr

<real subtraction: real subtraction: TBP>+≡
  procedure :: compute_sub_coll => real_subtraction_compute_sub_coll

<real subtraction: procedures>+≡
  function real_subtraction_compute_sub_coll (rsub, alr, em, i_phs, alpha_coupling) &
    result (sqme_coll)
    real(default) :: sqme_coll
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, em, i_phs
    real(default), intent(in) :: alpha_coupling
    real(default) :: xi, xi_max
    real(default) :: mom_times_sqme_spin_c, sqme_born_coll
    real(default) :: N_col
    integer :: i_con, i
    real(default) :: pfr
    associate (sregion => rsub%reg_data%regions(alr))
      sqme_coll = zero
      sqme_born_coll = zero
      N_col = 1
      if (sregion%has_collinear_divergence ()) then
        xi = rsub%real_kinematics%xi_tilde * rsub%real_kinematics%xi_max(i_phs)
        if (rsub%sub_coll%use_resonance_mappings) then
          i_con = rsub%reg_data%alr_to_i_contributor (alr)
        else
          i_con = 1
        end if
        mom_times_sqme_spin_c = rsub%get_spin_correlation_term (alr, sregion%uborn_index, em)
        if (rsub%reg_data%nlo_correction_type == "EW" .and. &
          sregion%nlo_correction_type == "QCD" .and. &
          qcd_ew_interferences (sregion%flst_uborn%flst)) then
          do i = 1, size (sregion%flst_uborn%flst)
            if (is_quark (sregion%flst_uborn%flst (i))) then
              sqme_born_coll = -rsub%sqme_born_color_c (i, i, sregion%uborn_index)/CF
              exit
            end if
          end do
        else
          sqme_born_coll = rsub%sqme_born(sregion%uborn_index)
        end if
        if (em <= rsub%sub_coll%n_in) then
          select case (rsub%isr_kinematics%isr_mode)
            case (SQRTS_FIXED)

```

```

        xi_max = rsub%real_kinematics%xi_max(i_phs)
    case (SQRTS_VAR)
        xi_max = one - rsub%isr_kinematics%x(em)
    end select
    xi = rsub%real_kinematics%xi_tilde * xi_max
    if (sregion%nlo_correction_type == "QCD") then
        call rsub%sub_coll%set_parameters (CA = CA, CF = CF, TR = TR)
    else if (sregion%nlo_correction_type == "EW") then
        if (is_quark (sregion%flst_real%flst(size(sregion%flst_real%flst)))) N_col = 3
        call rsub%sub_coll%set_parameters (CA = zero, &
            CF = sregion%flst_real%charge(em)**2, &
            TR = N_col*sregion%flst_real%charge(size(sregion%flst_real%flst))**2)
    end if
    sqme_coll = rsub%sub_coll%compute_isr (em, sregion%flst_real%flst, &
        rsub%real_kinematics%p_born_lab%phs_point(1)%get (), &
        sqme_born_coll * rsub%sf_factors(alr, em), &
        mom_times_sqme_spin_c * rsub%sf_factors(alr, em), &
        xi, alpha_coupling, rsub%isr_kinematics%isr_mode)
else
    if (sregion%nlo_correction_type == "QCD") then
        call rsub%sub_coll%set_parameters (CA = CA, CF = CF, TR = TR)
    else if (sregion%nlo_correction_type == "EW") then
        if (is_quark (sregion%flst_real%flst(sregion%emitter))) N_col = 3
        call rsub%sub_coll%set_parameters (CA = zero, &
            CF = sregion%flst_real%charge(sregion%emitter)**2, &
            TR = N_col*sregion%flst_real%charge(sregion%emitter)**2)
    end if
    sqme_coll = rsub%sub_coll%compute_fsr (sregion%emitter, sregion%flst_real%flst, &
        rsub%real_kinematics%xi_ref_momenta (i_con), &
        rsub%real_kinematics%p_born_lab%get_momenta(1), &
        sqme_born_coll, &
        mom_times_sqme_spin_c, &
        xi, alpha_coupling, sregion%double_fsr)
    if (rsub%sub_coll%use_resonance_mappings) then
        select type (fks_mapping => rsub%reg_data%fks_mapping)
        type is (fks_mapping_resonances_t)
            pfr = fks_mapping%get_resonance_weight (alr, &
                rsub%real_kinematics%p_born_cms%get_momenta(1))
        end select
        sqme_coll = sqme_coll * pfr
    end if
end if
end if
end if
end associate
end function real_subtraction_compute_sub_coll

```

Computes the soft-collinear subtraction term. For alpha regions with emitter 0, this routine is called with `em == 1` and `em == 2` separately. To still be able to use the unrescaled pdf factors stored in `sf_factors(alr, 0)` in this case, we need to differentiate between `em` and `em_pdf = 0`.

(real subtraction: real subtraction: TBP)+≡

`procedure :: compute_sub_coll_soft => real_subtraction_compute_sub_coll_soft`

(real subtraction: procedures)+≡

```

function real_subtraction_compute_sub_coll_soft (rsub, alr, em, i_phs, alpha_coupling) &
    result (sqme_cs)
    real(default) :: sqme_cs
    class(real_subtraction_t), intent(inout) :: rsub
    integer, intent(in) :: alr, em, i_phs
    real(default), intent(in) :: alpha_coupling
    real(default) :: mom_times_sqme_spin_c, sqme_born_coll
    real(default) :: N_col
    integer :: i_con, em_pdf, i
    associate (sregion => rsub%reg_data%regions(alr))
        sqme_cs = zero
        sqme_born_coll = zero
        N_col = 1
        if (sregion%has_collinear_divergence ()) then
            if (rsub%sub_coll%use_resonance_mappings) then
                i_con = rsub%reg_data%alr_to_i_contributor (alr)
            else
                i_con = 1
            end if
            mom_times_sqme_spin_c = rsub%get_spin_correlation_term (alr, sregion%uborn_index, em)
            if (rsub%reg_data%nlo_correction_type == "EW" .and. &
                sregion%nlo_correction_type == "QCD" .and. &
                qcd_ew_interferences (sregion%flst_uborn%flst)) then
                do i = 1, size (sregion%flst_uborn%flst)
                    if (is_quark (sregion%flst_uborn%flst (i))) then
                        sqme_born_coll = -rsub%sqme_born_color_c (i, i, sregion%uborn_index)/CF
                        exit
                    end if
                end do
            else
                sqme_born_coll = rsub%sqme_born(sregion%uborn_index)
            end if
            if (em <= rsub%sub_coll%n_in) then
                em_pdf = 0
                if (sregion%nlo_correction_type == "QCD") then
                    call rsub%sub_coll%set_parameters (CA = CA, CF = CF, TR = TR)
                else if (sregion%nlo_correction_type == "EW") then
                    if (is_quark (sregion%flst_real%flst(size(sregion%flst_real%flst)))) N_col = 3
                    call rsub%sub_coll%set_parameters (CA = zero, &
                        CF = sregion%flst_real%charge(em)**2, &
                        TR = N_col*sregion%flst_real%charge(size(sregion%flst_real%flst))**2)
                end if
                sqme_cs = rsub%sub_coll%compute_isr (em, sregion%flst_real%flst, &
                    rsub%real_kinematics%p_born_lab%phs_point(1)%get (), &
                    sqme_born_coll * rsub%sf_factors(alr, em_pdf), &
                    mom_times_sqme_spin_c * rsub%sf_factors(alr, em_pdf), &
                    zero, alpha_coupling, rsub%isr_kinematics%isr_mode)
            else
                if (sregion%nlo_correction_type == "QCD") then
                    call rsub%sub_coll%set_parameters (CA = CA, CF = CF, TR = TR)
                else if (sregion%nlo_correction_type == "EW") then
                    if (is_quark (sregion%flst_real%flst(sregion%emitter))) N_col = 3
                    call rsub%sub_coll%set_parameters (CA = zero, &
                        CF = sregion%flst_real%charge(sregion%emitter)**2, &

```

```

        TR = N_col*sregion%flst_real%charge(sregion%emitter)**2)
    end if
    sqme_cs = rsub%sub_coll%compute_fsr (sregion%emitter, sregion%flst_real%flst, &
        rsub%real_kinematics%xi_ref_momenta(i_con), &
        rsub%real_kinematics%p_born_lab%phs_point(1)%get (), &
        sqme_born_coll, &
        mom_times_sqme_spin_c, &
        zero, alpha_coupling, sregion%double_fsr)
    end if
end if
end associate
end function real_subtraction_compute_sub_coll_soft

<real subtraction: real subtraction: TBP>+=
procedure :: requires_spin_correlations => &
    real_subtraction_requires_spin_correlations

<real subtraction: procedures>+=
function real_subtraction_requires_spin_correlations (rsub) result (val)
    logical :: val
    class(real_subtraction_t), intent(in) :: rsub
    val = any (rsub%sc_required)
end function real_subtraction_requires_spin_correlations

<real subtraction: real subtraction: TBP>+=
procedure :: final => real_subtraction_final

<real subtraction: procedures>+=
subroutine real_subtraction_final (rsub)
    class(real_subtraction_t), intent(inout) :: rsub
    call rsub%sub_soft%final ()
    call rsub%sub_coll%final ()
    !!! Finalization of region data is done in pcm_nlo_final
    if (associated (rsub%reg_data)) nullify (rsub%reg_data)
    !!! Finalization of real kinematics is done in pcm_instance_nlo_final
    if (associated (rsub%real_kinematics)) nullify (rsub%real_kinematics)
    if (associated (rsub%isr_kinematics)) nullify (rsub%isr_kinematics)
    if (allocated (rsub%sqme_real_non_sub)) deallocate (rsub%sqme_real_non_sub)
    if (allocated (rsub%sqme_born)) deallocate (rsub%sqme_born)
    if (allocated (rsub%sf_factors)) deallocate (rsub%sf_factors)
    if (allocated (rsub%sqme_born_color_c)) deallocate (rsub%sqme_born_color_c)
    if (allocated (rsub%sqme_born_charge_c)) deallocate (rsub%sqme_born_charge_c)
    if (allocated (rsub%sc_required)) deallocate (rsub%sc_required)
    if (allocated (rsub%selected_alr)) deallocate (rsub%selected_alr)
end subroutine real_subtraction_final

```

Partitions of the real matrix element and Powheg damping

```

<real subtraction: public>+=
public :: real_partition_t

<real subtraction: types>+=
type, abstract :: real_partition_t

```

```

contains
  <real subtraction: real partition: TBP>
end type real_partition_t

<real subtraction: real partition: TBP>≡
  procedure (real_partition_init), deferred :: init
<real subtraction: interfaces>≡
  abstract interface
    subroutine real_partition_init (partition, scale, reg_data)
      import
      class(real_partition_t), intent(out) :: partition
      real(default), intent(in) :: scale
      type(region_data_t), intent(in) :: reg_data
    end subroutine real_partition_init
  end interface

  <real subtraction: real partition: TBP>+≡
    procedure (real_partition_write), deferred :: write
  <real subtraction: interfaces>+≡
    abstract interface
      subroutine real_partition_write (partition, unit)
        import
        class(real_partition_t), intent(in) :: partition
        integer, intent(in), optional :: unit
      end subroutine real_partition_write
    end interface

    To allow really arbitrary damping functions, get_f should get the full real phase
    space as argument and not just some pt2 that is extracted higher up.

    <real subtraction: real partition: TBP>+≡
      procedure (real_partition_get_f), deferred :: get_f
    <real subtraction: interfaces>+≡
      abstract interface
        function real_partition_get_f (partition, p) result (f)
          import
          real(default) :: f
          class(real_partition_t), intent(in) :: partition
          type(vector4_t), intent(in), dimension(:) :: p
        end function real_partition_get_f
      end interface

      <real subtraction: public>+≡
        public :: powheg_damping_simple_t
      <real subtraction: types>+≡
        type, extends (real_partition_t) :: powheg_damping_simple_t
          real(default) :: h2 = 5._default
          integer :: emitter
        contains
          <real subtraction: powheg damping simple: TBP>
        end type powheg_damping_simple_t

```

```

<real subtraction: powheg damping simple: TBP>≡
  procedure :: get_f => powheg_damping_simple_get_f

<real subtraction: procedures>+≡
  function powheg_damping_simple_get_f (partition, p) result (f)
    real(default) :: f
    class(powheg_damping_simple_t), intent(in) :: partition
    type(vector4_t), intent(in), dimension(:) :: p
    !!! real(default) :: pt2
    f = 1
    call msg_bug ("Simple damping currently not available")
    !!! TODO (cw-2017-03-01) Compute pt2 from emitter
    !!! f = partition%h2 / (pt2 + partition%h2)
  end function powheg_damping_simple_get_f

<real subtraction: powheg damping simple: TBP>+≡
  procedure :: init => powheg_damping_simple_init

<real subtraction: procedures>+≡
  subroutine powheg_damping_simple_init (partition, scale, reg_data)
    class(powheg_damping_simple_t), intent(out) :: partition
    real(default), intent(in) :: scale
    type(region_data_t), intent(in) :: reg_data
    partition%h2 = scale**2
  end subroutine powheg_damping_simple_init

<real subtraction: powheg damping simple: TBP>+≡
  procedure :: write => powheg_damping_simple_write

<real subtraction: procedures>+≡
  subroutine powheg_damping_simple_write (partition, unit)
    class(powheg_damping_simple_t), intent(in) :: partition
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "Powheg damping simple: "
    write (u, "(1x,A, "// FMT_15 // ")") "scale h2: ", partition%h2
  end subroutine powheg_damping_simple_write

<real subtraction: public>+≡
  public :: real_partition_fixed_order_t

<real subtraction: types>+≡
  type, extends (real_partition_t) :: real_partition_fixed_order_t
    real(default) :: scale
    type(ftuple_t), dimension(:), allocatable :: fks_pairs
  contains
    <real subtraction: real partition fixed order: TBP>
  end type real_partition_fixed_order_t

<real subtraction: real partition fixed order: TBP>≡
  procedure :: init => real_partition_fixed_order_init

```



```

<real subtraction: procedures>+≡
  subroutine real_partition_fixed_order_init (partition, scale, reg_data)
    class(real_partition_fixed_order_t), intent(out) :: partition
    real(default), intent(in) :: scale
    type(region_data_t), intent(in) :: reg_data
  end subroutine real_partition_fixed_order_init

```

```

<real subtraction: real partition fixed order: TBP>+≡
  procedure :: write => real_partition_fixed_order_write

```

```

<real subtraction: procedures>+≡
  subroutine real_partition_fixed_order_write (partition, unit)
    class(real_partition_fixed_order_t), intent(in) :: partition
    integer, intent(in), optional :: unit
  end subroutine real_partition_fixed_order_write

```

Implements the suppression factor

$$F(\Phi_{n+1}) = 1 - \prod_{(i,j) \in P_{FKS}} \theta \left[m_i + m_j + h - \sqrt{(p_j + p_j)^2} \right] \quad (27.43)$$

to split the real matrix element into singular and finite part.

```

<real subtraction: real partition fixed order: TBP>+≡
  procedure :: get_f => real_partition_fixed_order_get_f

<real subtraction: procedures>+≡
  function real_partition_fixed_order_get_f (partition, p) result (f)
    real(default) :: f
    class(real_partition_fixed_order_t), intent(in) :: partition
    type(vector4_t), intent(in), dimension(:) :: p
    integer :: i, em
    f = zero
    PAIRS: do i = 1, size (partition%fks_pairs)
      associate (ii => partition%fks_pairs(i)%ireg)
        if (ii(1) == 0) then
          IS: do em = 1, 2
            if ((p(em) + p(ii(2)))**1 < p(em)**1 + p(ii(2))**1 + partition%scale) then
              f = one
              exit PAIRS
            end if
          end do IS
        else
          if ((p(ii(1)) + p(ii(2)))**1 < p(ii(1))**1 + p(ii(2))**1 + partition%scale) then
            f = one
            exit PAIRS
          end if
        end if
      end associate
    end do PAIRS
  end function real_partition_fixed_order_get_f

```

27.5.5 Unit tests

Test module, followed by the corresponding implementation module.

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

```
  module real_subtraction_ut  
    use unit_tests  
    use real_subtraction_util
```

```
  <Standard module head>
```

```
  <Real subtraction: public test>
```

```
  contains
```

```
  <Real subtraction: test driver>
```

```
  end module real_subtraction_ut
```

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

```
  module real_subtraction_util  
    <Use kinds>
```

```
    use physics_defs  
    use lorentz  
    use numeric_utils  
    use real_subtraction
```

```
  <Standard module head>
```

```
  <Real subtraction: test declarations>
```

```
  contains
```

```
  <Real subtraction: tests>
```

```
  end module real_subtraction_util
```

API: driver for the unit tests below.

```
<Real subtraction: public test>≡  
  public :: real_subtraction_test
```

```
<Real subtraction: test driver>≡  
  subroutine real_subtraction_test (u, results)  
    integer, intent(in) :: u  
    type(test_results_t), intent(inout) :: results  
    <Real subtraction: execute tests>  
  end subroutine real_subtraction_test
```

Test the final-state collinear subtraction.

```
<Real subtraction: execute tests>≡  
  call test (real_subtraction_1, "real_subtraction_1", &
```

```

        "final-state collinear subtraction", &
        u, results)

<Real subtraction: test declarations>≡
    public :: real_subtraction_1

<Real subtraction: tests>≡
    subroutine real_subtraction_1 (u)
        integer, intent(in) :: u

        type(coll_subtraction_t) :: coll_sub
        real(default) :: sqme_coll
        type(vector4_t) :: p_res
        type(vector4_t), dimension(5) :: p_born
        real(default), dimension(4) :: k_perp
        real(default), dimension(4,4) :: b_munu
        integer :: mu, nu
        real(default) :: born, born_c
        integer, dimension(6) :: flst

        p_born(1)%p = [500, 0, 0, 500]
        p_born(2)%p = [500, 0, 0, -500]
        p_born(3)%p = [3.7755E+02, 2.2716E+02, -95.4172, 2.8608E+02]
        p_born(4)%p = [4.9529E+02, -2.739E+02, 84.8535, -4.0385E+02]
        p_born(5)%p = [1.2715E+02, 46.7375, 10.5637, 1.1778E+02]
        p_res = p_born(1) + p_born(2)
        flst = [11, -11, -2, 2, -2, 2]

        b_munu(1, :) = [0., 0., 0., 0.]
        b_munu(2, :) = [0., 1., 1., 1.]
        b_munu(3, :) = [0., 1., 1., 1.]
        b_munu(4, :) = [0., 1., 1., 1.]

        k_perp = real_subtraction_compute_k_perp_fsr (p = p_born(5), phi = 0.5_default)
        born = - b_munu(1, 1) + b_munu(2, 2) + b_munu(3, 3) + b_munu(4, 4)
        born_c = 0.
        do mu = 1, 4
            do nu = 1, 4
                born_c = born_c + k_perp(mu) * k_perp(nu) * b_munu(mu, nu)
            end do
        end do

        write (u, "(A)") "* Test output: real_subtraction_1"
        write (u, "(A)") "* Purpose: final-state collinear subtraction"
        write (u, "(A)")

        write (u, "(A, L1)") "* vanishing scalar-product of 3-momenta k_perp and p_born(emitter): ", &
            nearly_equal (dot_product (p_born(5)%p(1:3), k_perp(2:4)), 0._default)

        call coll_sub%init (n_alr = 1, n_in = 2)
        call coll_sub%set_parameters (CA, CF, TR)

        write (u, "(A)")
        write (u, "(A)") "* g -> qq splitting"
        write (u, "(A)")

```

```

sqme_coll = coll_sub%compute_fsr(5, flst, p_res, p_born, &
    born, born_c, 0.5_default, 0.25_default, .false.)

write (u, "(A,F15.12)") "ME: ", sqme_coll

write (u, "(A)")
write (u, "(A)") "* g -> gg splitting"
write (u, "(A)")

b_munu(1, :) = [0., 0., 0., 0.]
b_munu(2, :) = [0., 0., 0., 1.]
b_munu(3, :) = [0., 0., 1., 1.]
b_munu(4, :) = [0., 0., 1., 1.]

k_perp = real_subtraction_compute_k_perp_fsr (p = p_born(5), phi = 0.5_default)
born = - b_munu(1, 1) + b_munu(2, 2) + b_munu(3, 3) + b_munu(4, 4)
born_c = 0.
do mu = 1, 4
    do nu = 1, 4
        born_c = born_c + k_perp(mu) * k_perp(nu) * b_munu(mu, nu)
    end do
end do

flst = [11, -11, 2, -2, 21, 21]
sqme_coll = coll_sub%compute_fsr(5, flst, p_res, p_born, &
    born, born_c, 0.5_default, 0.25_default, .true.)

write (u, "(A,F15.12)") "ME: ", sqme_coll

write (u, "(A)")
write (u, "(A)") "* Test output end: real_subtraction_1"
write (u, "(A)")
end subroutine real_subtraction_1

```

27.6 Combining the FKS Pieces

```

<nlo_data.f90>≡
  <File header>

  module nlo_data

    <Use kinds>
    <Use strings>
    use diagnostics
    use constants, only: zero
    use string_utils, only: split_string, read_ival, string_contains_word
    use io_units
    use lorentz
    use variables, only: var_list_t
    use format_defs, only: FMT_15
    use physics_defs, only: THR_POS_WP, THR_POS_WM
    use physics_defs, only: THR_POS_B, THR_POS_BBAR
    use physics_defs, only: NO_FACTORIZATION, FACTORIZATION_THRESHOLD

    <Standard module head>

    <nlo data: public>

    <nlo data: parameters>

    <nlo data: types>
    <nlo data: interfaces>

    contains

    <nlo data: procedures>

  end module nlo_data

<nlo data: parameters>≡
  integer, parameter, public :: FKS_DEFAULT = 1
  integer, parameter, public :: FKS_RESONANCES = 2

  integer, dimension(2), parameter, public :: ASSOCIATED_LEG_PAIR = [1, 3]

<nlo data: public>≡
  public :: fks_template_t

<nlo data: types>≡
  type :: fks_template_t
    logical :: subtraction_disabled = .false.
    integer :: mapping_type = FKS_DEFAULT
    logical :: count_kinematics = .false.
    real(default) :: fks_dij_exp1
    real(default) :: fks_dij_exp2
    real(default) :: xi_min
    real(default) :: y_max
    real(default) :: xi_cut, delta_o, delta_i

```

```

        type(string_t), dimension(:), allocatable :: excluded_resonances
        integer :: n_f
contains
<nlo data: fks template: TBP>
end type fks_template_t

```

```

<nlo data: fks template: TBP>≡
    procedure :: write => fks_template_write

<nlo data: procedures>≡
    subroutine fks_template_write (template, unit)
        class(fks_template_t), intent(in) :: template
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u,'(1x,A)') 'FKS Template: '
        write (u,'(1x,A)', advance = 'no') 'Mapping Type: '
        select case (template%mapping_type)
        case (FKS_DEFAULT)
            write (u,'(A)') 'Default'
        case (FKS_RESONANCES)
            write (u,'(A)') 'Resonances'
        case default
            write (u,'(A)') 'Unkown'
        end select
        write (u,'(1x,A,ES4.3,ES4.3)') 'd_ij exponentials: ', &
            template%fks_dij_exp1, template%fks_dij_exp2
        write (u, '(1x,A,ES4.3,ES4.3)') 'xi_cut: ', &
            template%xi_cut
        write (u, '(1x,A,ES4.3,ES4.3)') 'delta_o: ', &
            template%delta_o
        write (u, '(1x,A,ES4.3,ES4.3)') 'delta_i: ', &
            template%delta_i
    end subroutine fks_template_write

```

Set FKS parameters. ξ_{cut} , δ_o and δ_i steer the ratio of the integrated and real subtraction.

```

<nlo data: fks template: TBP>+≡
    procedure :: set_parameters => fks_template_set_parameters

<nlo data: procedures>+≡
    subroutine fks_template_set_parameters (template, exp1, exp2, xi_min, &
        y_max, xi_cut, delta_o, delta_i)
        class(fks_template_t), intent(inout) :: template
        real(default), intent(in) :: exp1, exp2
        real(default), intent(in) :: xi_min, y_max, &
            xi_cut, delta_o, delta_i
        template%fks_dij_exp1 = exp1
        template%fks_dij_exp2 = exp2
        template%xi_min = xi_min
        template%y_max = y_max
        template%xi_cut = xi_cut
        template%delta_o = delta_o
        template%delta_i = delta_i
    end subroutine fks_template_set_parameters

```

```

        end subroutine fks_template_set_parameters

<nlo data: fks template: TBP>+≡
    procedure :: set_mapping_type => fks_template_set_mapping_type

<nlo data: procedures>+≡
    subroutine fks_template_set_mapping_type (template, val)
        class(fks_template_t), intent(inout) :: template
        integer, intent(in) :: val
        template%mapping_type = val
    end subroutine fks_template_set_mapping_type

<nlo data: fks template: TBP>+≡
    procedure :: set_counter => fks_template_set_counter

<nlo data: procedures>+≡
    subroutine fks_template_set_counter (template)
        class(fks_template_t), intent(inout) :: template
        template%count_kinematics = .true.
    end subroutine fks_template_set_counter

<nlo data: public>+≡
    public :: real_scales_t

<nlo data: types>+≡
    type :: real_scales_t
        real(default) :: scale
        real(default) :: ren_scale
        real(default) :: fac_scale
        real(default) :: scale_born
        real(default) :: fac_scale_born
        real(default) :: ren_scale_born
    end type real_scales_t

<nlo data: public>+≡
    public :: get_threshold_momenta

<nlo data: procedures>+≡
    function get_threshold_momenta (p) result (p_thr)
        type(vector4_t), dimension(4) :: p_thr
        type(vector4_t), intent(in), dimension(:) :: p
        p_thr(1) = p(THR_POS_WP) + p(THR_POS_B)
        p_thr(2) = p(THR_POS_B)
        p_thr(3) = p(THR_POS_WM) + p(THR_POS_BBAR)
        p_thr(4) = p(THR_POS_BBAR)
    end function get_threshold_momenta

```

27.6.1 Putting it together

```

<nlo data: public>+≡
    public :: nlo_settings_t

```

```

<nlo data: types>+≡
type :: nlo_settings_t
  logical :: use_internal_color_correlations = .true.
  logical :: use_internal_spin_correlations = .false.
  logical :: use_resonance_mappings = .false.
  logical :: combined_integration = .false.
  logical :: fixed_order_nlo = .false.
  logical :: test_soft_limit = .false.
  logical :: test_coll_limit = .false.
  logical :: test_anti_coll_limit = .false.
  integer, dimension(:), allocatable :: selected_alr
  integer :: factorization_mode = NO_FACTORIZATION
  !!! Probably not the right place for this. Revisit after refactoring
  real(default) :: powheg_damping_scale = zero
  type(fks_template_t) :: fks_template
  type(string_t) :: virtual_selection
  logical :: virtual_resonance_aware_collinear = .true.
  logical :: use_born_scale = .false.
  logical :: cut_all_real_sqmes = .false.
  type(string_t) :: nlo_correction_type
  logical :: reuse_amplitudes_fks = .false.
contains
<nlo data: nlo settings: TBP>
end type nlo_settings_t

```

```

<nlo data: nlo settings: TBP>≡
procedure :: init => nlo_settings_init

```

```

<nlo data: procedures>+≡
subroutine nlo_settings_init (nlo_settings, var_list, fks_template)
  class(nlo_settings_t), intent(inout) :: nlo_settings
  type(var_list_t), intent(in) :: var_list
  type(fks_template_t), intent(in), optional :: fks_template
  type(string_t) :: color_method
  if (present (fks_template)) nlo_settings%fks_template = fks_template
  color_method = var_list%get_sval (var_str ('$correlation_method'))
  if (color_method == "") color_method = var_list%get_sval (var_str ('$method'))
  nlo_settings%use_internal_color_correlations = color_method == 'omega' &
    .or. color_method == 'threshold'
  nlo_settings%combined_integration = var_list%get_lval &
    (var_str ("?combined_nlo_integration"))
  nlo_settings%fixed_order_nlo = var_list%get_lval &
    (var_str ("?fixed_order_nlo_events"))
  nlo_settings%test_soft_limit = var_list%get_lval (var_str ('?test_soft_limit'))
  nlo_settings%test_coll_limit = var_list%get_lval (var_str ('?test_coll_limit'))
  nlo_settings%test_anti_coll_limit = var_list%get_lval (var_str ('?test_anti_coll_limit'))
  call setup_alr_selection ()
  nlo_settings%virtual_selection = var_list%get_sval (var_str ('$virtual_selection'))
  nlo_settings%virtual_resonance_aware_collinear = &
    var_list%get_lval (var_str ('?virtual_collinear_resonance_aware'))
  nlo_settings%powheg_damping_scale = &
    var_list%get_rval (var_str ('powheg_damping_scale'))
  nlo_settings%use_born_scale = &
    var_list%get_lval (var_str ("?nlo_use_born_scale"))

```



```

nlo_settings%cut_all_real_sqmes = &
    var_list%get_lval (var_str ("?nlo_cut_all_real_sqmes"))
nlo_settings%nlo_correction_type = var_list%get_sval (var_str ('$nlo_correction_type'))
nlo_settings%reuse_amplitudes_fks = var_list%get_lval (var_str ('?nlo_reuse_amplitudes_fks'))
contains
subroutine setup_alr_selection ()
    type(string_t) :: alr_selection
    type(string_t), dimension(:), allocatable :: alr_split
    integer :: i, i1, i2
    alr_selection = var_list%get_sval (var_str ('$select_alpha_regions'))
    if (string_contains_word (alr_selection, var_str (","))) then
        call split_string (alr_selection, var_str (","), alr_split)
        allocate (nlo_settings%selected_alr (size (alr_split)))
        do i = 1, size (alr_split)
            nlo_settings%selected_alr(i) = read_ival(alr_split(i))
        end do
    else if (string_contains_word (alr_selection, var_str (":"))) then
        call split_string (alr_selection, var_str (":"), alr_split)
        if (size (alr_split) == 2) then
            i1 = read_ival (alr_split(1))
            i2 = read_ival (alr_split(2))
            allocate (nlo_settings%selected_alr (i2 - i1 + 1))
            do i = 1, i2 - i1 + 1
                nlo_settings%selected_alr(i) = read_ival (alr_split(i))
            end do
        else
            call msg_fatal ("select_alpha_regions: ':' specifies a range!")
        end if
    else if (len(alr_selection) == 1) then
        allocate (nlo_settings%selected_alr (1))
        nlo_settings%selected_alr(1) = read_ival (alr_selection)
    end if
    if (allocated (alr_split)) deallocate (alr_split)
end subroutine setup_alr_selection
end subroutine nlo_settings_init

```

<nlo data: nlo settings: TBP>+≡

```

procedure :: write => nlo_settings_write

```

<nlo data: procedures>+≡

```

subroutine nlo_settings_write (nlo_settings, unit)
    class(nlo_settings_t), intent(in) :: nlo_settings
    integer, intent(in), optional :: unit
    integer :: i, u
    u = given_output_unit (unit); if (u < 0) return
    write (u, '(A)') 'nlo_settings:'
    write (u, '(3X,A,L1)') 'internal_color_correlations = ', &
        nlo_settings%use_internal_color_correlations
    write (u, '(3X,A,L1)') 'internal_spin_correlations = ', &
        nlo_settings%use_internal_spin_correlations
    write (u, '(3X,A,L1)') 'use_resonance_mappings = ', &
        nlo_settings%use_resonance_mappings
    write (u, '(3X,A,L1)') 'combined_integration = ', &
        nlo_settings%combined_integration

```

```

write (u, '(3X,A,L1)') 'test_soft_limit = ', &
    nlo_settings%test_soft_limit
write (u, '(3X,A,L1)') 'test_coll_limit = ', &
    nlo_settings%test_coll_limit
write (u, '(3X,A,L1)') 'test_anti_coll_limit = ', &
    nlo_settings%test_anti_coll_limit
if (allocated (nlo_settings%selected_alr)) then
    write (u, '(3x,A)', advance = "no") 'selected alpha regions = ['
    do i = 1, size (nlo_settings%selected_alr)
        write (u, '(A,I0)', advance = "no") ", ", nlo_settings%selected_alr(i)
    end do
    write (u, '(A)') "]"
end if
write (u, '(3X,A,' // FMT_15 // ')') 'powheg_damping_scale = ', &
    nlo_settings%powheg_damping_scale
write (u, '(3X,A,A)') 'virtual_selection = ', &
    char (nlo_settings%virtual_selection)
write (u, '(3X,A,A)') 'Real factorization mode = ', &
    char (factorization_mode (nlo_settings%factorization_mode))
contains
function factorization_mode (fm)
    type(string_t) :: factorization_mode
    integer, intent(in) :: fm
    select case (fm)
    case (NO_FACTORIZATION)
        factorization_mode = var_str ("None")
    case (FACTORIZATION_THRESHOLD)
        factorization_mode = var_str ("Threshold")
    case default
        factorization_mode = var_str ("Undefined!")
    end select
end function factorization_mode
end subroutine nlo_settings_write

```

27.7 Contribution of divergencies due to PDF Evolution

References:

- arXiv:hep-ph/9512328, (2.1)-(2.5), (4.29)-(4.53)
- arXiv:0709.2092, (2.102)-(2.106)

The parton distribution densities have to be evaluated at NLO, too. The NLO PDF evolution is given by

$$f(\bar{x}) = \int_0^1 \int_0^1 dx dz f(x) \Gamma(z) \delta(\bar{x} - xz), \quad (27.44)$$

where Γ are the DGLAP evolution kernels for an $a \rightarrow d$ splitting,

$$\Gamma_a^{(d)} = \delta_{ad} \delta(1-x) - \frac{\alpha_s}{2\pi} \left(\frac{1}{\epsilon} P_{ad}(x, 0) - K_{ad}(x) \right) + \mathcal{O}(\alpha_s^2). \quad (27.45)$$

K_{ad} is a renormalization scheme matching factor, which is exactly zero in $\overline{\text{MS}}$. Let the leading-order hadronic cross section be given by

$$d\sigma^{(0)}(s) = \int dx_{\oplus} dx_{\ominus} f_{\oplus}(x_{\oplus}) f_{\ominus}(x_{\ominus}) d\tilde{\sigma}^{(0)}(x_{\oplus} x_{\ominus} s), \quad (27.46)$$

then the NLO hadronic cross section is

$$d\sigma^{(1)}(s) = \int dx_{\oplus} dx_{\ominus} dz_{\oplus} dz_{\ominus} f_{\oplus}(x_{\oplus}) f_{\ominus}(x_{\ominus}) \underbrace{\Gamma_{\oplus}(z_{\oplus}) \Gamma_{\ominus}(z_{\ominus}) d\tilde{\sigma}^{(1)}(z_{\oplus} z_{\ominus} s)}_{d\hat{\sigma}^{(1)}}. \quad (27.47)$$

$d\hat{\sigma}$ is called the subtracted partonic cross section. Expanding in α_s we find

$$d\hat{\sigma}_{ab}^{(0)}(k_1, k_2) = d\tilde{\sigma}_{ab}^{(0)}(k_1, k_2), \quad (27.48)$$

$$d\hat{\sigma}_{ab}^{(1)}(k_1, k_2) = d\tilde{\sigma}_{ab}^{(1)}(k_1, k_2) \quad (27.49)$$

$$+ \frac{\alpha_s}{2\pi} \sum_d \int dx \left(\frac{1}{\epsilon} P_{da}(x, 0) - K_{da}(x) \right) d\tilde{\sigma}_{db}^{(0)}(xk_1, k_2) \quad (27.50)$$

$$+ \frac{\alpha_s}{2\pi} \sum_d \int \left(\frac{1}{\epsilon} P_{db}(x, 0) - K_{db}(x) \right) d\tilde{\sigma}_{ad}^{(0)}(k_1, xk_2). \quad (27.51)$$

$$= d\tilde{\sigma}_{ab}^{(1)} + d\tilde{\sigma}_{ab}^{(cnt,+)} + d\tilde{\sigma}_{ab}^{(cnt,-)} \quad (27.52)$$

Let us now turn to the soft-subtracted real part of the cross section. For ease of notation, it is constrained to one singular region,

$$d\sigma_{\alpha}^{(in)} = \left[\left(\frac{1}{\xi} \right)_c - 2\epsilon \left(\frac{\log \xi}{\xi} \right)_c \right] (1-y^2) \xi^2 \mathcal{R}_{\alpha} \mathcal{S}_{\alpha} \\ \times \frac{1}{2(2\pi)^{3-2\epsilon}} \left(\frac{\sqrt{s}}{2} \right)^{2-2\epsilon} (1-y^2)^{-1-\epsilon} d\phi d\xi dy d\Omega^{2-2\epsilon},$$

where we regularize collinear divergencies using the identity

$$(1 - y^2)^{-1-\epsilon} = -\frac{2^{-\epsilon}}{2\epsilon} (\delta(1 - y) + \delta(1 + y)) + \underbrace{\frac{1}{2} \left[\left(\frac{1}{1 - y} \right)_c + \left(\frac{1}{1 + y} \right)_c \right]}_{\mathcal{P}(y)}.$$

This enables us to split the cross section into a finite and a singular part. The latter can further be separated into a contribution of the incoming and of the outgoing particles,

$$d\sigma_\alpha^{(in)} = d\sigma_\alpha^{(in,+)} + d\sigma_\alpha^{(in,-)} + d\sigma_\alpha^{(in,f)}.$$

They are given by

$$d\sigma_\alpha^{(in,f)} = \mathcal{P}(y) \left[\left(\frac{1}{\xi} \right)_c - 2\epsilon \left(\frac{\log \xi}{\xi} \right)_c \right] \frac{1}{2(2\pi)^{3-2\epsilon}} \left(\frac{\sqrt{s}}{2} \right)^{2-2\epsilon} \times (1 - y^2) \xi^2 \mathcal{R}_\alpha \mathcal{S}_\alpha d\phi d\xi dy d\Omega^{2-2\epsilon} \quad (27.53)$$

and

$$d\sigma_\alpha^{(in,\pm)} = -\frac{2^{-\epsilon}}{2\epsilon} \delta(1 \mp y) \left[\left(\frac{1}{\xi} \right)_c - 2\epsilon \left(\frac{\log \xi}{\xi} \right)_c \right] \times \frac{1}{2(2\pi)^{3-2\epsilon}} \left(\frac{\sqrt{s}}{2} \right)^{2-2\epsilon} (1 - y^2) \xi^2 \mathcal{R}_\alpha \mathcal{S}_\alpha d\phi d\xi dy d\Omega^{2-2\epsilon}. \quad (27.54)$$

Equation 27.53 is the contribution to the real cross section which is computed in `evaluate_region_isr`. It is regularized both in the soft and collinear limit via the plus distributions. Equation 27.54 is a different contribution. It is only present exactly in the collinear limit, due to the delta function. The divergences present in this term do not completely cancel out divergences in the virtual matrix element, because the beam axis is distinguished. Thus, the conditions in which the KLN theorem applies are not met. To see this, we carry out the collinear limit, obtaining

$$\lim_{y \rightarrow 1} (1 - y^2) \xi^2 \mathcal{R}_\alpha = 8\pi\alpha_s \mu^{2\epsilon} \left(\frac{2}{\sqrt{s}} \right)^2 \xi P^<(1 - \xi, \epsilon) \mathcal{R}_\alpha,$$

with the Altarelli-Parisi splitting kernel for $z < 1$, $P^<(z, \epsilon)$. Moreover, $\lim_{\vec{k}_1 \parallel \vec{k}_1} d\phi = d\phi_3$ violates spatial averaging. The integration over the spherical angle $d\Omega$ can be carried out easily, yielding a factor of $2\pi^{1-\epsilon}/\Gamma(1 - \epsilon)$. This allows us to redefine ϵ ,

$$\frac{1}{\epsilon} - \gamma_E + \log(4\pi) \rightarrow \frac{1}{\epsilon}. \quad (27.55)$$

Coming back to $d\tilde{\sigma}_{ab}^{(cnt,+)}$ in order to make a connection to $d\sigma_\alpha^{(in,+)}$, we relate $P_{ab}(z, 0)$ to $P_{ab}^<(z, 0)$ via the equation

$$P_{ab}(z, 0) = (1 - z) P_{ab}^<(z, 0) \left(\frac{1}{1 - z} \right)_+ + \gamma(a) \delta_{ab} \delta(1 - z),$$

which yields

$$d\tilde{\sigma}_\alpha^{(cnt,+)} = \frac{\alpha_s}{2\pi} \sum_d \left\{ -K_{da}(1 - \xi) + \frac{1}{\epsilon} \left[\left(\frac{1}{\xi} \right)_+ \xi P_{da}^<(1 - \xi, 0) + \delta_{da} \delta(\xi) \gamma(d) \right] \right\} \mathcal{R}_\alpha \mathcal{S}_\alpha d\phi d\xi dy. \quad (27.56)$$

This term has the same pole structure as eqn. 27.54. This makes clear that the quantity

$$d\hat{\sigma}^{(in,+)} = d\tilde{\sigma}^{(in,+)} + d\tilde{\sigma}^{(cnt,+)} \quad (27.57)$$

has no collinear poles. Therefore, our task is to add up eqns. 27.54 and 27.56 in order to compute the finite remainder. This is the integrand which is evaluated in the `dglap_remnant` component.

So, we have to perform an expansion of $d\hat{\sigma}^{(in,+)}$ in ϵ . Hereby, we must not neglect the implicit ϵ -dependence of $P^<$, which leads to additional terms involving the first derivative,

$$P_{ab}^<(z, \epsilon) = P_{ab}^<(z, 0) + \epsilon \frac{\partial P_{ab}^<(z, \epsilon)}{\partial \epsilon} \Big|_{\epsilon=0} + \mathcal{O}(\alpha_s^2).$$

This finally gives us the equation for the collinear remnant. Note that there is still one soft $1/\epsilon$ -pole, which cancels out with the corresponding expression in the soft-virtual terms.

$$\begin{aligned} d\hat{\sigma}^{(in,+)} &= \frac{\alpha_s}{2\pi} \frac{1}{\epsilon} \gamma(a) \mathcal{R}_\alpha \mathcal{S}_\alpha \\ &+ \frac{\alpha_s}{2\pi} \sum_d \left\{ (1-z) P_{da}^<(z, 0) \left[\left(\frac{1}{1-z} \right)_c \log \frac{s\delta_1}{2\mu^2} + 2 \left(\frac{\log(1-z)}{1-z} \right)_c \right] \right. \\ &\quad \left. - (1-z) \frac{\partial P_{da}^<(z, \epsilon)}{\partial \epsilon} \left(\frac{1}{1-z} \right)_c - K_{da}(z) \right\} \mathcal{R}_\alpha \mathcal{S}_\alpha d\phi d\xi dy \end{aligned} \quad (27.58)$$

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

```

module dglap_remnant

  <Use kinds with double>
  <Use strings>
  use numeric_utils
  use diagnostics
  use constants
  use physics_defs
  use pdg_arrays
  use phs_fks, only: isr_kinematics_t
  use fks_regions, only: region_data_t

  use nlo_data

  <Standard module head>

  <dglap remnant: public>

  <dglap remnant: types>

contains

  <dglap remnant: procedures>

end module dglap_remnant

```

```

⟨dglap remnant: public⟩≡
  public :: dglap_remnant_t

⟨dglap remnant: types⟩≡
  type :: dglap_remnant_t
    type(nlo_settings_t), pointer :: settings => null ()
    type(region_data_t), pointer :: reg_data => null ()
    type(isr_kinematics_t), pointer :: isr_kinematics => null ()
    real(default) :: CA = 0, CF = 0, TR = 0
    real(default), dimension(:), allocatable :: sqme_born
    real(default), dimension(:,:), allocatable :: sf_factors
    real(default), dimension(:,:,:), allocatable :: sqme_color_c_extra
  contains
    ⟨dglap remnant: dglap remnant: TBP⟩
  end type dglap_remnant_t

⟨dglap remnant: dglap remnant: TBP⟩≡
  procedure :: init => dglap_remnant_init

⟨dglap remnant: procedures⟩≡
  subroutine dglap_remnant_init (dglap, settings, reg_data, isr_kinematics)
    class(dglap_remnant_t), intent(inout) :: dglap
    type(nlo_settings_t), intent(in), target :: settings
    type(region_data_t), intent(in), target :: reg_data
    integer :: n_flv_born
    type(isr_kinematics_t), intent(in), target :: isr_kinematics
    dglap%reg_data => reg_data
    n_flv_born = reg_data%get_n_flv_born ()
    allocate (dglap%sf_factors (reg_data%n_regions, 0:reg_data%n_in))
    dglap%sf_factors = zero
    dglap%settings => settings
    allocate (dglap%sqme_born(n_flv_born))
    dglap%sqme_born = zero
    allocate (dglap%sqme_color_c_extra (reg_data%n_legs_born, reg_data%n_legs_born, &
      reg_data%n_flv_born))
    dglap%sqme_color_c_extra = zero
    dglap%isr_kinematics => isr_kinematics
  end subroutine dglap_remnant_init

⟨dglap remnant: dglap remnant: TBP⟩+≡
  procedure :: set_parameters => dglap_remnant_set_parameters

⟨dglap remnant: procedures⟩+≡
  subroutine dglap_remnant_set_parameters (dglap, CA, CF, TR)
    class(dglap_remnant_t), intent(inout) :: dglap
    real(default), intent(in) :: CA, CF, TR
    dglap%CA = CA
    dglap%CF = CF
    dglap%TR = TR
  end subroutine dglap_remnant_set_parameters

```

Evaluates formula 27.58. Note that, as also in the case for the real subtraction, we have to take into account an additional term, occuring because the integral

the plus distribution is evaluated over is not constrained on the interval $[0, 1]$. Explicitly, this means (see JHEP 06(2010)043, (4.11)-(4.12))

$$\int_{\bar{x}_{\oplus}}^1 dz \left(\frac{1}{1-z} \right)_{\xi_{\text{cut}}} = \log \frac{1-\bar{x}_{\oplus}}{\xi_{\text{cut}}} f(1) + \int_{\bar{x}_{\oplus}}^1 \frac{f(z) - f(1)}{1-z}, \quad (27.59)$$

$$\int_{\bar{x}_{\oplus}}^1 dz \left(\frac{\log(1-z)}{1-z} \right)_{\xi_{\text{cut}}} f(z) = \frac{1}{2} (\log^2(1-\bar{x}_{\oplus}) - \log^2(\xi_{\text{cut}})) f(1) + \int_{\bar{x}_{\oplus}}^1 \frac{\log(1-z)[f(z) - f(1)]}{1-z}, \quad (27.60)$$

and the same of course for \bar{x}_{\ominus} . These two terms are stored in the `plus_dist_remnant` variable below.

The option `separate_uborns` allows to compute the contribution of the DGLAP remnant separately for each underlying Born flavor structure. We need this option during event generation to generate counter events with a specific Born flavor structure.

```

<dglap remnant: dglap remnant: TBP>+≡
  procedure :: evaluate => dglap_remnant_evaluate

<dglap remnant: procedures>+≡
  subroutine dglap_remnant_evaluate (dglap, alpha_coupling, separate_uborns, sqme_dglap)
    class(dglap_remnant_t), intent(inout) :: dglap
    real(default), dimension(2), intent(in) :: alpha_coupling
    logical, intent(in) :: separate_uborns
    real(default), intent(inout), dimension(:) :: sqme_dglap
    integer :: alr, emitter, i_corr
    real(default) :: sqme_alr
    logical, dimension(:, :, :), allocatable :: evaluated
    real(default) :: sb, fac_scale2
    sb = dglap%isr_kinematics%sqrts_born**2
    fac_scale2 = dglap%isr_kinematics%fac_scale**2
    allocate (evaluated(dglap%reg_data%get_n_flv_born (), dglap%reg_data%get_n_flv_real (), &
      dglap%reg_data%n_in))
    evaluated = .false.
    do alr = 1, dglap%reg_data%n_regions
      i_corr = 0
      if (dglap%reg_data%regions(alr)%nlo_correction_type == "QCD") then
        i_corr = 1
      else if (dglap%reg_data%regions(alr)%nlo_correction_type == "EW") then
        i_corr = 2
      end if
      if (allocated (dglap%settings%selected_alr)) then
        if (.not. any (dglap%settings%selected_alr == alr)) cycle
      end if
      sqme_alr = zero
      emitter = dglap%reg_data%regions(alr)%emitter
      if (emitter > dglap%reg_data%n_in .or. i_corr == 0) cycle
      associate (i_flv_born => dglap%reg_data%regions(alr)%uborn_index, &
        i_flv_real => dglap%reg_data%regions(alr)%real_index)
        if (emitter == 0) then
          do emitter = 1, 2
            if (evaluated(i_flv_born, i_flv_real, emitter)) cycle
            call evaluate_alr (alr, emitter, i_flv_born, i_flv_real, sqme_alr, evaluated)
          end do
        end if
      end associate
    end do
  end subroutine

```

```

else if (emitter > 0) then
  if (evaluated(i_flv_born, i_flv_real, emitter)) cycle
  call evaluate_alr (alr, emitter, i_flv_born, i_flv_real, sqme_alr, evaluated)
end if
if (separate_uborns) then
  sqme_dglap(i_flv_born) = sqme_dglap(i_flv_born) &
                          + alpha_coupling (i_corr)/ twopi * sqme_alr
else
  sqme_dglap(1) = sqme_dglap(1) + alpha_coupling (i_corr)/ twopi * sqme_alr
end if
end associate
end do

contains
<dglap remnant: dglap remnant evaluate: procedures>
end subroutine dglap_remnant_evaluate

```

We introduce $\hat{P}(z, \epsilon) = (1 - z)P(z, \epsilon)$ and have

$$\hat{P}_{g \rightarrow gg}(z) = 2C_A \left[z + \frac{(1-z)^2}{z} + z(1-z)^2 \right], \quad (27.61)$$

$$\hat{P}_{g \rightarrow qq}(z) = C_F(1-z) \frac{1 + (1-z)^2}{z}, \quad (27.62)$$

$$\hat{P}_{q \rightarrow gg}(z) = T_F(1-z-2z(1-z)^2), \quad (27.63)$$

$$\hat{P}_{q \rightarrow qq}(z) = C_F(1+z^2). \quad (27.64)$$

<dglap remnant: dglap remnant evaluate: procedures>≡

```

function p_hat_gtogg (z)
  real(default) :: p_hat_gtogg
  <p variables>
  p_hat_gtogg = two * dglap%CA * (z + onemz**2 / z + z * onemz**2)
end function p_hat_gtogg

function p_hat_gtoqq (z)
  real(default) :: p_hat_gtoqq
  <p variables>
  p_hat_gtoqq = dglap%CF * onemz / z * (one + onemz**2)
end function p_hat_gtoqq

function p_hat_qtogq (z)
  real(default) :: p_hat_qtogq
  <p variables>
  p_hat_qtogq = dglap%TR * (onemz - two * z * onemz**2)
end function p_hat_qtogq

function p_hat_qtoqg (z)
  real(default) :: p_hat_qtoqg
  real(default), intent(in) :: z
  p_hat_qtoqg = dglap%CF * (one + z**2)
end function p_hat_qtoqg

```


$$\left. \frac{\partial P_{g \rightarrow gg}(z, \epsilon)}{\partial \epsilon} \right|_{\epsilon=0} = 0, \quad (27.65)$$

$$\left. \frac{\partial P_{g \rightarrow qq}(z, \epsilon)}{\partial \epsilon} \right|_{\epsilon=0} = -C_F z, \quad (27.66)$$

$$\left. \frac{\partial P_{q \rightarrow gg}(z, \epsilon)}{\partial \epsilon} \right|_{\epsilon=0} = -2T_F z(1-z), \quad (27.67)$$

$$\left. \frac{\partial P_{q \rightarrow qq}(z, \epsilon)}{\partial \epsilon} \right|_{\epsilon=0} = -C_F(1-z). \quad (27.68)$$

$$(27.69)$$

(dglap remnant: dglap remnant evaluate: procedures)+≡

```
function p_derived_gtogg (z)
  real(default) :: p_derived_gtogg
  real(default), intent(in) :: z
  p_derived_gtogg = zero
end function p_derived_gtogg

function p_derived_gtoqq (z)
  real(default) :: p_derived_gtoqq
  real(default), intent(in) :: z
  p_derived_gtoqq = -dglap%CF * z
end function p_derived_gtoqq

function p_derived_qtogq (z)
  real(default) :: p_derived_qtogq
  <p variables>
  p_derived_qtogq = -two * dglap%TR * z * onemz
end function p_derived_qtogq

function p_derived_qtoqg (z)
  real(default) :: p_derived_qtoqg
  <p variables>
  p_derived_qtoqg = -dglap%CF * onemz
end function p_derived_qtoqg
```

(dglap remnant: dglap remnant evaluate: procedures)+≡

```
subroutine evaluate_alr (alr, emitter, i_flv_born, i_flv_real, sqme_alr, evaluated)
  integer, intent(in) :: alr, emitter, i_flv_born, i_flv_real
  real(default), intent(inout) :: sqme_alr
  logical, intent(inout), dimension(:, :, :) :: evaluated
  real(default) :: z, jac
  real(default) :: factor, factor_soft, plus_dist_remnant
  real(default) :: xb, onemz
  real(default) :: sqme_scaled, sqme_born_dglap
  real(default) :: charge_rad2, charge_em2
  integer :: flv_em, flv_rad, N_col, i
  N_col = 1
  sqme_born_dglap = zero
  associate (template => dglap%settings%fks_template)
    z = dglap%isr_kinematics%z(emitter)
    flv_rad = dglap%reg_data%regions(alr)%flst_real%flst(dglap%reg_data%n_legs_real)
    flv_em = dglap%reg_data%regions(alr)%flst_real%flst(emitter)
    charge_rad2 = dglap%reg_data%regions(alr)%flst_real%charge(dglap%reg_data%n_legs_real)**2
```

```

charge_em2 = dglap%reg_data%regions(alr)%flst_real%charge(emitter)**2
if (dglap%reg_data%regions(alr)%nlo_correction_type == "QCD") then
  call dglap%set_parameters (CA = CA, CF = CF, TR = TR)
else if (dglap%reg_data%regions(alr)%nlo_correction_type == "EW") then
  if (is_quark(flv_rad)) N_col = NC
  call dglap%set_parameters (CA = zero, CF = charge_em2, TR = N_col*charge_rad2)
end if
jac = dglap%isr_kinematics%jacobian(emitter)
onemz = one - z
factor = log (sb * template%delta_i / two / z / fac_scale2) / &
  onemz + two * log (onemz) / onemz
factor_soft = log (sb * template%delta_i / two / fac_scale2) / &
  onemz + two * log (onemz) / onemz
xb = dglap%isr_kinematics%x(emitter)
plus_dist_remnant = log ((one - xb) / template%xi_cut) * log (sb * template%delta_i / &
  two / fac_scale2) + (log (one - xb)**2 - log (template%xi_cut)**2)
end associate
if (dglap%reg_data%nlo_correction_type == "EW" .and. &
  dglap%reg_data%regions(alr)%nlo_correction_type == "QCD" .and. &
  qcd_ew_interferences (dglap%reg_data%regions(alr)%flst_uborn%flst)) then
  do i = 1, size (dglap%reg_data%regions(alr)%flst_uborn%flst)
    if (is_quark (dglap%reg_data%regions(alr)%flst_uborn%flst (i))) then
      sqme_born_dglap = -dglap%sqme_color_c_extra (i, i, i_flv_born)/CF
      exit
    end if
  end do
else
  sqme_born_dglap = dglap%sqme_born(i_flv_born)
end if
sqme_scaled = sqme_born_dglap * dglap%sf_factors(alr, emitter)
if (is_massless_vector (flv_em) .and. is_massless_vector (flv_rad)) then
  sqme_alr = sqme_alr + p_hat_gtogg(z) * factor / z * sqme_scaled * jac &
    - p_hat_gtogg(one) * factor_soft * sqme_born_dglap * jac &
    + p_hat_gtogg(one) * plus_dist_remnant * sqme_born_dglap
else if (is_fermion (flv_em) .and. is_massless_vector (flv_rad)) then
  sqme_alr = sqme_alr + p_hat_qtoqg(z) * factor / z * sqme_scaled * jac &
    - p_derived_qtoqg(z) / z * sqme_scaled * jac &
    - p_hat_qtoqg(one) * factor_soft * sqme_born_dglap * jac &
    + p_hat_qtoqg(one) * plus_dist_remnant * sqme_born_dglap
else if (is_fermion (flv_em) .and. is_fermion (flv_rad)) then
  sqme_alr = sqme_alr + (p_hat_gtoqg(z) * factor - p_derived_gtoqg(z)) / z * jac * &
    sqme_scaled
else if (is_massless_vector (flv_em) .and. is_fermion (flv_rad)) then
  sqme_alr = sqme_alr + (p_hat_qtogq(z) * factor - p_derived_qtogq(z)) / z * sqme_scaled * jac
else
  sqme_alr = sqme_alr + zero
end if
evaluated(i_flv_born, i_flv_real, emitter) = .true.
end subroutine evaluate_alr

<p variables>≡
real(default), intent(in) :: z
real(default) :: onemz
onemz = one - z

```

```

⟨dglap remnant: dglap remnant: TBP⟩+≡
  procedure :: final => dglap_remnant_final

⟨dglap remnant: procedures⟩+≡
  subroutine dglap_remnant_final (dglap)
    class(dglap_remnant_t), intent(inout) :: dglap
    if (associated (dglap%isr_kinematics)) nullify (dglap%isr_kinematics)
    if (associated (dglap%reg_data)) nullify (dglap%reg_data)
    if (associated (dglap%settings)) nullify (dglap%settings)
    if (allocated (dglap%sqme_born)) deallocate (dglap%sqme_born)
    if (allocated (dglap%sf_factors)) deallocate (dglap%sf_factors)
  end subroutine dglap_remnant_final

```

27.8 Dispatch

```

⟨dispatch fks.f90⟩≡
  ⟨File header⟩

  module dispatch_fks

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use string_utils, only: split_string
    use variables, only: var_list_t
    use nlo_data, only: fks_template_t, FKS_DEFAULT, FKS_RESONANCES

    ⟨Standard module head⟩

    ⟨Dispatch fks: public⟩

    contains

    ⟨Dispatch fks: procedures⟩

  end module dispatch_fks

```

Initialize parameters used to optimize FKS calculations.

```

⟨Dispatch fks: public⟩≡
  public :: dispatch_fks_s

⟨Dispatch fks: procedures⟩≡
  subroutine dispatch_fks_s (fks_template, var_list)
    type(fks_template_t), intent(inout) :: fks_template
    type(var_list_t), intent(in) :: var_list
    real(default) :: fks_dij_exp1, fks_dij_exp2
    type(string_t) :: fks_mapping_type
    logical :: subtraction_disabled
    type(string_t) :: exclude_from_resonance
    fks_dij_exp1 = &
      var_list%get_rval (var_str ("fks_dij_exp1"))
    fks_dij_exp2 = &
      var_list%get_rval (var_str ("fks_dij_exp2"))
    fks_mapping_type = &

```

```

        var_list%get_sval (var_str ("fks_mapping_type"))
subtraction_disabled = &
        var_list%get_lval (var_str ("?disable_subtraction"))
exclude_from_resonance = &
        var_list%get_sval (var_str ("resonances_exclude_particles"))
if (exclude_from_resonance /= var_str ("default")) &
        call split_string (exclude_from_resonance, var_str (":"), &
        fks_template%excluded_resonances)
call fks_template%set_parameters ( &
        exp1 = fks_dij_exp1, exp2 = fks_dij_exp2, &
        xi_min = var_list%get_rval (var_str ("fks_xi_min")), &
        y_max = var_list%get_rval (var_str ("fks_y_max")), &
        xi_cut = var_list%get_rval (var_str ("fks_xi_cut")), &
        delta_o = var_list%get_rval (var_str ("fks_delta_o")), &
        delta_i = var_list%get_rval (var_str ("fks_delta_i")))
select case (char (fks_mapping_type))
case ("default")
        call fks_template%set_mapping_type (FKS_DEFAULT)
case ("resonances")
        call fks_template%set_mapping_type (FKS_RESONANCES)
end select
fks_template%subtraction_disabled = subtraction_disabled
fks_template%n_f = var_list%get_ival (var_str ("alphas_nf"))
end subroutine dispatch_fks_s

```

Chapter 28

Model Handling and Features

These modules deal with process definitions and physics models.

These modules use the `model_data` methods to automatically generate process definitions.

auto_components Generic process-definition generator. We can specify a basic process or initial particle(s) and some rules to extend this process, given a model definition with particle names and vertex structures.

radiation_generator Applies the generic generator to the specific problem of generating NLO corrections in a restricted setup.

Model construction:

eval_trees Implementation of the generic `expr_t` type for the concrete evaluation of expressions that access user variables.

This module is actually part of the Sindarin language implementation, and should be moved elsewhere. Currently, the `models` module relies on it.

models Extends the `model_data.t` structure by user-variable objects for easy access, and provides the means to read a model definition from file.

slha_interface Read/write a SUSY model in the standardized SLHA format. The format defines fields and parameters, but no vertices.

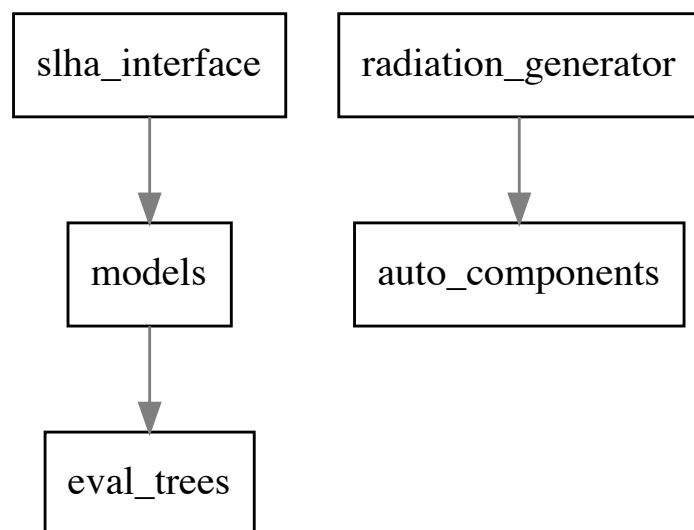


Figure 28.1: Module dependencies in `src/model_features`.

28.1 Automatic generation of process components

This module provides the functionality for automatically generating radiation corrections or decays, provided as lists of PDG codes.

```
<auto_components.f90>≡  
  <File header>  
  
  module auto_components  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use diagnostics  
    use model_data  
    use pdg_arrays  
    use physics_defs, only: PHOTON, GLUON, Z_BOSON, W_BOSON  
    use numeric_utils, only: extend_integer_array  
  
    <Standard module head>  
  
    <Auto components: public>  
  
    <Auto components: parameters>  
  
    <Auto components: types>  
  
    <Auto components: interfaces>  
  
    contains  
  
    <Auto components: procedures>  
  
  end module auto_components
```

28.1.1 Constraints: Abstract types

An abstract type that denotes a constraint on the automatically generated states. The concrete objects are applied as visitor objects at certain hooks during the splitting algorithm.

```
<Auto components: types>≡  
  type, abstract :: split_constraint_t  
  contains  
    <Auto components: split constraint: TBP>  
  end type split_constraint_t
```

By default, all checks return true.

```
<Auto components: split constraint: TBP>≡  
  procedure :: check_before_split => split_constraint_check_before_split  
  procedure :: check_before_insert => split_constraint_check_before_insert  
  procedure :: check_before_record => split_constraint_check_before_record
```

```

<Auto components: procedures>≡
  subroutine split_constraint_check_before_split (c, table, pl, k, passed)
    class(split_constraint_t), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: k
    logical, intent(out) :: passed
    passed = .true.
  end subroutine split_constraint_check_before_split

  subroutine split_constraint_check_before_insert (c, table, pa, pl, passed)
    class(split_constraint_t), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_array_t), intent(in) :: pa
    type(pdg_list_t), intent(inout) :: pl
    logical, intent(out) :: passed
    passed = .true.
  end subroutine split_constraint_check_before_insert

  subroutine split_constraint_check_before_record (c, table, pl, n_loop, passed)
    class(split_constraint_t), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    passed = .true.
  end subroutine split_constraint_check_before_record

```

A transparent wrapper, so we can collect constraints of different type.

```

<Auto components: types>+≡
  type :: split_constraint_wrap_t
    class(split_constraint_t), allocatable :: c
  end type split_constraint_wrap_t

```

A collection of constraints.

```

<Auto components: public>≡
  public :: split_constraints_t

<Auto components: types>+≡
  type :: split_constraints_t
    class(split_constraint_wrap_t), dimension(:), allocatable :: cc
    contains
    <Auto components: split constraints: TBP>
  end type split_constraints_t

```

Initialize the constraints set with a specific number of elements.

```

<Auto components: split constraints: TBP>≡
  procedure :: init => split_constraints_init

<Auto components: procedures>+≡
  subroutine split_constraints_init (constraints, n)
    class(split_constraints_t), intent(out) :: constraints
    integer, intent(in) :: n

```



```

        allocate (constraints%cc (n))
    end subroutine split_constraints_init

```

Set a constraint.

```

<Auto components: split constraints: TBP>+≡
    procedure :: set => split_constraints_set

```

```

<Auto components: procedures>+≡
    subroutine split_constraints_set (constraints, i, c)
        class(split_constraints_t), intent(inout) :: constraints
        integer, intent(in) :: i
        class(split_constraint_t), intent(in) :: c
        allocate (constraints%cc(i)%c, source = c)
    end subroutine split_constraints_set

```

Apply checks.

`check_before_split` is applied to the particle list that we want to split.

`check_before_insert` is applied to the particle list `pl` that is to replace the particle `pa` that is split. This check may transform the particle list.

`check_before_record` is applied to the complete new particle list that results from splitting before it is recorded.

```

<Auto components: split constraints: TBP>+≡
    procedure :: check_before_split => split_constraints_check_before_split
    procedure :: check_before_insert => split_constraints_check_before_insert
    procedure :: check_before_record => split_constraints_check_before_record

```

```

<Auto components: procedures>+≡
    subroutine split_constraints_check_before_split &
        (constraints, table, pl, k, passed)
        class(split_constraints_t), intent(in) :: constraints
        class(ps_table_t), intent(in) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: k
        logical, intent(out) :: passed
        integer :: i
        passed = .true.
        do i = 1, size (constraints%cc)
            call constraints%cc(i)%c%check_before_split (table, pl, k, passed)
            if (.not. passed) return
        end do
    end subroutine split_constraints_check_before_split

    subroutine split_constraints_check_before_insert &
        (constraints, table, pa, pl, passed)
        class(split_constraints_t), intent(in) :: constraints
        class(ps_table_t), intent(in) :: table
        type(pdg_array_t), intent(in) :: pa
        type(pdg_list_t), intent(inout) :: pl
        logical, intent(out) :: passed
        integer :: i
        passed = .true.
        do i = 1, size (constraints%cc)
            call constraints%cc(i)%c%check_before_insert (table, pa, pl, passed)

```

```

        if (.not. passed) return
    end do
end subroutine split_constraints_check_before_insert

subroutine split_constraints_check_before_record &
    (constraints, table, pl, n_loop, passed)
    class(split_constraints_t), intent(in) :: constraints
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    integer :: i
    passed = .true.
    do i = 1, size (constraints%cc)
        call constraints%cc(i)%check_before_record (table, pl, n_loop, passed)
        if (.not. passed) return
    end do
end subroutine split_constraints_check_before_record

```

28.1.2 Specific constraints

Number of particles

Specific constraint: The number of particles plus the number of loops, if any, must remain less than the given limit. Note that the number of loops is defined only when we are recording the entry.

```

<Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_n_tot
    private
    integer :: n_max = 0
    contains
    procedure :: check_before_split => constraint_n_tot_check_before_split
    procedure :: check_before_record => constraint_n_tot_check_before_record
end type constraint_n_tot

<Auto components: public>+≡
    public :: constrain_n_tot

<Auto components: procedures>+≡
    function constrain_n_tot (n_max) result (c)
    integer, intent(in) :: n_max
    type(constraint_n_tot) :: c
    c%n_max = n_max
end function constrain_n_tot

subroutine constraint_n_tot_check_before_split (c, table, pl, k, passed)
    class(constraint_n_tot), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: k
    logical, intent(out) :: passed
    passed = pl%get_size () < c%n_max
end subroutine constraint_n_tot_check_before_split

```

```

subroutine constraint_n_tot_check_before_record (c, table, pl, n_loop, passed)
  class(constraint_n_tot), intent(in) :: c
  class(ps_table_t), intent(in) :: table
  type(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: n_loop
  logical, intent(out) :: passed
  passed = pl%get_size () + n_loop <= c%n_max
end subroutine constraint_n_tot_check_before_record

```

Number of loops

Specific constraint: The number of loops is limited, independent of the total number of particles.

```

<Auto components: types>+≡
  type, extends (split_constraint_t) :: constraint_n_loop
  private
  integer :: n_loop_max = 0
  contains
  procedure :: check_before_record => constraint_n_loop_check_before_record
end type constraint_n_loop

<Auto components: public>+≡
  public :: constrain_n_loop

<Auto components: procedures>+≡
  function constrain_n_loop (n_loop_max) result (c)
    integer, intent(in) :: n_loop_max
    type(constraint_n_loop) :: c
    c%n_loop_max = n_loop_max
  end function constrain_n_loop

  subroutine constraint_n_loop_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_n_loop), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    passed = n_loop <= c%n_loop_max
  end subroutine constraint_n_loop_check_before_record

```

Particles allowed in splitting

Specific constraint: The entries in the particle list ready for insertion are matched to a given list of particle patterns. If a match occurs, the entry is replaced by the corresponding pattern. If there is no match, the check fails. If a massless gauge boson splitting is detected, the splitting partners are checked against a list of excluded particles. If a match occurs, the check fails.

```

<Auto components: types>+≡

```

```

type, extends (split_constraint_t) :: constraintSplittings
private
  type(pdg_list_t) :: pl_match, pl_excluded_gaugeSplittings
contains
  procedure :: check_before_insert => constraintSplittings_check_before_insert
end type constraintSplittings

<Auto components: public>+≡
  public :: constrainSplittings

<Auto components: procedures>+≡
  function constrainSplittings (pl_match, pl_excluded_gaugeSplittings) result (c)
    type(pdg_list_t), intent(in) :: pl_match
    type(pdg_list_t), intent(in) :: pl_excluded_gaugeSplittings
    type(constraintSplittings) :: c
    c%pl_match = pl_match
    c%pl_excluded_gaugeSplittings = pl_excluded_gaugeSplittings
  end function constrainSplittings

  subroutine constraintSplittings_check_before_insert (c, table, pa, pl, passed)
    class(constraintSplittings), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_array_t), intent(in) :: pa
    type(pdg_list_t), intent(inout) :: pl
    logical, intent(out) :: passed
    logical :: has_massless_vector
    integer :: i
    has_massless_vector = .false.
    do i = 1, pa%get_length ()
      if (is_massless_vector(pa%get(i))) then
        has_massless_vector = .true.
        exit
      end if
    end do
    passed = .false.
    if (has_massless_vector .and. count (is_fermion(pl%a%get ())) == 2) then
      do i = 1, c%pl_excluded_gaugeSplittings%get_size ()
        if (pl .match. c%pl_excluded_gaugeSplittings%a(i)) return
      end do
      call pl%match_replace (c%pl_match, passed)
      passed = .true.
    else
      call pl%match_replace (c%pl_match, passed)
    end if
  end subroutine constraintSplittings_check_before_insert

```

Specific constraint: The entries in the particle list ready for insertion are matched to a given list of particle patterns. If a match occurs, the entry is replaced by the corresponding pattern. If there is no match, the check fails.

```

<Auto components: types>+≡
  type, extends (split_constraint_t) :: constraintInsert
  private
    type(pdg_list_t) :: pl_match

```

```

contains
  procedure :: check_before_insert => constraint_insert_check_before_insert
end type constraint_insert

<Auto components: public>+≡
  public :: constrain_insert

<Auto components: procedures>+≡
  function constrain_insert (pl_match) result (c)
    type(pdg_list_t), intent(in) :: pl_match
    type(constraint_insert) :: c
    c%pl_match = pl_match
  end function constrain_insert

  subroutine constraint_insert_check_before_insert (c, table, pa, pl, passed)
    class(constraint_insert), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_array_t), intent(in) :: pa
    type(pdg_list_t), intent(inout) :: pl
    logical, intent(out) :: passed
    call pl%match_replace (c%pl_match, passed)
  end subroutine constraint_insert_check_before_insert

```

Particles required in final state

Specific constraint: The entries in the recorded state must be a superset of the entries in the given list (for instance, the lowest-order state).

```

<Auto components: types>+≡
  type, extends (split_constraint_t) :: constraint_require
  private
  type(pdg_list_t) :: pl
  contains
  procedure :: check_before_record => constraint_require_check_before_record
end type constraint_require

```

We check the current state by matching all particle entries against the stored particle list, and crossing out the particles in the latter list when a match is found. The constraint passed if all entries have been crossed out.

For an `if_table` in particular, we check the final state only.

```

<Auto components: public>+≡
  public :: constrain_require

<Auto components: procedures>+≡
  function constrain_require (pl) result (c)
    type(pdg_list_t), intent(in) :: pl
    type(constraint_require) :: c
    c%pl = pl
  end function constrain_require

  subroutine constraint_require_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_require), intent(in) :: c

```

```

class(ps_table_t), intent(in) :: table
type(pdg_list_t), intent(in) :: pl
integer, intent(in) :: n_loop
logical, intent(out) :: passed
logical, dimension(:), allocatable :: mask
integer :: i, k, n_in
select type (table)
type is (if_table_t)
    if (table%proc_type > 0) then
        select case (table%proc_type)
        case (PROC_DECAY)
            n_in = 1
        case (PROC_SCATTER)
            n_in = 2
        end select
    else
        call msg_fatal ("Neither a decay nor a scattering process")
    end if
class default
    n_in = 0
end select
allocate (mask (c%pl%get_size ()), source = .true.)
do i = n_in + 1, pl%get_size ()
    k = c%pl%find_match (pl%get (i), mask)
    if (k /= 0) mask(k) = .false.
end do
passed = .not. any (mask)
end subroutine constraint_require_check_before_record

```

Radiation

Specific constraint: We have radiation pattern if the original particle matches an entry in the list of particles that should replace it. The constraint prohibits this situation.

```

<Auto components: public>+≡
    public :: constrain_radiation

```

```

<Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_radiation
    private
    contains
    procedure :: check_before_insert => &
        constraint_radiation_check_before_insert
    end type constraint_radiation

```

```

<Auto components: procedures>+≡
    function constrain_radiation () result (c)
        type(constraint_radiation) :: c
    end function constrain_radiation

```

```

subroutine constraint_radiation_check_before_insert (c, table, pa, pl, passed)
    class(constraint_radiation), intent(in) :: c

```

```

class(ps_table_t), intent(in) :: table
type(pdg_array_t), intent(in) :: pa
type(pdg_list_t), intent(inout) :: pl
logical, intent(out) :: passed
passed = .not. (pl .match. pa)
end subroutine constraint_radiation_check_before_insert

```

Mass sum

Specific constraint: The sum of masses within the particle list must be smaller than a given limit. For in/out state combinations, we check initial and final state separately.

If we specify `margin` in the initialization, the sum must be strictly less than the limit minus the given margin (which may be zero). If not, equality is allowed.

```

<Auto components: public>+≡
  public :: constrain_mass_sum

<Auto components: types>+≡
  type, extends (split_constraint_t) :: constraint_mass_sum
  private
    real(default) :: mass_limit = 0
    logical :: strictly_less = .false.
    real(default) :: margin = 0
  contains
    procedure :: check_before_record => constraint_mass_sum_check_before_record
  end type constraint_mass_sum

<Auto components: procedures>+≡
  function constrain_mass_sum (mass_limit, margin) result (c)
    real(default), intent(in) :: mass_limit
    real(default), intent(in), optional :: margin
    type(constraint_mass_sum) :: c
    c%mass_limit = mass_limit
    if (present (margin)) then
      c%strictly_less = .true.
      c%margin = margin
    end if
  end function constrain_mass_sum

  subroutine constraint_mass_sum_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_mass_sum), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    real(default) :: limit
    if (c%strictly_less) then
      limit = c%mass_limit - c%margin
      select type (table)
        type is (if_table_t)
          passed = mass_sum (pl, 1, 2, table%model) < limit &

```

```

        .and. mass_sum (pl, 3, pl%get_size (), table%model) < limit
class default
    passed = mass_sum (pl, 1, pl%get_size (), table%model) < limit
end select
else
    limit = c%mass_limit
    select type (table)
    type is (if_table_t)
        passed = mass_sum (pl, 1, 2, table%model) <= limit &
        .and. mass_sum (pl, 3, pl%get_size (), table%model) <= limit
    class default
        passed = mass_sum (pl, 1, pl%get_size (), table%model) <= limit
    end select
end if
end subroutine constraint_mass_sum_check_before_record

```

Initial state particles

Specific constraint: The two incoming particles must both match the given particle list. This is checked for the generated particle list, just before it is recorded.

```

<Auto components: public>+≡
    public :: constrain_in_state

<Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_in_state
    private
    type(pdg_list_t) :: pl
    contains
    procedure :: check_before_record => constraint_in_state_check_before_record
end type constraint_in_state

<Auto components: procedures>+≡
    function constrain_in_state (pl) result (c)
        type(pdg_list_t), intent(in) :: pl
        type(constraint_in_state) :: c
        c%pl = pl
    end function constrain_in_state

subroutine constraint_in_state_check_before_record &
    (c, table, pl, n_loop, passed)
    class(constraint_in_state), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    integer :: i
    select type (table)
    type is (if_table_t)
        passed = .false.
        do i = 1, 2
            if (.not. (c%pl .match. pl%get (i))) return

```



```

        end do
    end select
    passed = .true.
end subroutine constraint_in_state_check_before_record

```

Photon induced processes

If set, filter out photon induced processes.

```

<Auto components: public>+≡
    public :: constrain_photon_induced_processes

<Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_photon_induced_processes
    private
    integer :: n_in
    contains
    procedure :: check_before_record => &
        constraint_photon_induced_processes_check_before_record
    end type constraint_photon_induced_processes

<Auto components: procedures>+≡
    function constrain_photon_induced_processes (n_in) result (c)
    integer, intent(in) :: n_in
    type(constraint_photon_induced_processes) :: c
    c%n_in = n_in
    end function constrain_photon_induced_processes

    subroutine constraint_photon_induced_processes_check_before_record &
        (c, table, pl, n_loop, passed)
    class(constraint_photon_induced_processes), intent(in) :: c
    class(ps_table_t), intent(in) :: table
    type(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_loop
    logical, intent(out) :: passed
    integer :: i
    select type (table)
    type is (if_table_t)
        passed = .false.
        do i = 1, c%n_in
            if (pl%a(i)%get () == 22) return
        end do
    end select
    passed = .true.
end subroutine constraint_photon_induced_processes_check_before_record

```

Coupling constraint

Filters vertices which do not match the desired NLO pattern.

```

<Auto components: types>+≡
    type, extends (split_constraint_t) :: constraint_coupling_t
    private

```

```

    logical :: qed = .false.
    logical :: qcd = .true.
    logical :: ew = .false.
    integer :: n_nlo_correction_types
contains
  <Auto components: constraint coupling: TBP>
end type constraint_coupling_t

<Auto components: public>+≡
  public :: constrain_couplings

<Auto components: procedures>+≡
  function constrain_couplings (qcd, qed, n_nlo_correction_types) result (c)
    type(constraint_coupling_t) :: c
    logical, intent(in) :: qcd, qed
    integer, intent(in) :: n_nlo_correction_types
    c%qcd = qcd; c%qed = qed
    c%n_nlo_correction_types = n_nlo_correction_types
  end function constrain_couplings

  <Auto components: constraint coupling: TBP>≡
    procedure :: check_before_insert => constraint_coupling_check_before_insert

  <Auto components: procedures>+≡
    subroutine constraint_coupling_check_before_insert (c, table, pa, pl, passed)
      class(constraint_coupling_t), intent(in) :: c
      class(ps_table_t), intent(in) :: table
      type(pdg_array_t), intent(in) :: pa
      type(pdg_list_t), intent(inout) :: pl
      logical, intent(out) :: passed
      type(pdg_list_t) :: pl_vertex
      type(pdg_array_t) :: pdg_gluon, pdg_photon, pdg_W_Z, pdg_gauge_bosons
      integer :: i, j
      pdg_gluon = GLUON; pdg_photon = PHOTON
      pdg_W_Z = [W_BOSON, -W_BOSON, Z_BOSON]
      if (c%qcd) pdg_gauge_bosons = pdg_gauge_bosons // pdg_gluon
      if (c%qed) pdg_gauge_bosons = pdg_gauge_bosons // pdg_photon
      if (c%ew) pdg_gauge_bosons = pdg_gauge_bosons // pdg_W_Z
      do j = 1, pa%get_length ()
        call pl_vertex%init (pl%get_size () + 1)
        call pl_vertex%set (1, pa%get(j))
        do i = 1, pl%get_size ()
          call pl_vertex%set (i + 1, pl%get(i))
        end do
        if (pl_vertex%get_size () > 3) then
          passed = .false.
          cycle
        end if
        if (is_massless_vector(pa%get(j))) then
          if (.not. table%model%check_vertex &
              (pl_vertex%a(1)%get (), pl_vertex%a(2)%get (), pl_vertex%a(3)%get ())) then
            passed = .false.
            cycle
          end if
        end if
      end do
    end subroutine
  end if

```

```

else if (.not. table%model%check_vertex &
  (- pl_vertex%a(1)%get (), pl_vertex%a(2)%get (), pl_vertex%a(3)%get ())) then
  passed = .false.
  cycle
end if
if (.not. (pl_vertex .match. pdg_gauge_bosons)) then
  passed = .false.
  cycle
end if
passed = .true.
exit
end do
end subroutine constraint_coupling_check_before_insert

```

28.1.3 Tables of states

Automatically generate a list of possible process components for a given initial set (a single massive particle or a preset list of states).

The set of process components are generated by recursive splitting, applying constraints on the fly that control and limit the process. The generated states are accumulated in a table that we can read out after completion.

```

<Auto components: types>+≡
type, extends (pdg_list_t) :: ps_entry_t
  integer :: n_loop = 0
  integer :: n_rad = 0
  type(ps_entry_t), pointer :: previous => null ()
  type(ps_entry_t), pointer :: next => null ()
end type ps_entry_t

```

```

<Auto components: parameters>≡
integer, parameter :: PROC_UNDEFINED = 0
integer, parameter :: PROC_DECAY = 1
integer, parameter :: PROC_SCATTER = 2

```

This is the wrapper type for the decay tree for the list of final states and the final array. First, an abstract base type:

```

<Auto components: public>+≡
public :: ps_table_t

<Auto components: types>+≡
type, abstract :: ps_table_t
  private
  class(model_data_t), pointer :: model => null ()
  logical :: loops = .false.
  type(ps_entry_t), pointer :: first => null ()
  type(ps_entry_t), pointer :: last => null ()
  integer :: proc_type
contains
  <Auto components: ps table: TBP>
end type ps_table_t

```

The extensions: one for decay, one for generic final states. The decay-state table stores the initial particle. The final-state table is indifferent, and the initial/final state table treats the first two particles in its list as incoming antiparticles.

```

<Auto components: public>+≡
  public :: ds_table_t
  public :: fs_table_t
  public :: if_table_t

<Auto components: types>+≡
  type, extends (ps_table_t) :: ds_table_t
    private
      integer :: pdg_in = 0
    contains
      <Auto components: ds table: TBP>
    end type ds_table_t

  type, extends (ps_table_t) :: fs_table_t
    contains
      <Auto components: fs table: TBP>
    end type fs_table_t

  type, extends (fs_table_t) :: if_table_t
    contains
      <Auto components: if table: TBP>
    end type if_table_t

```

Finalizer: we must deallocate the embedded list.

```

<Auto components: ps table: TBP>≡
  procedure :: final => ps_table_final

<Auto components: procedures>+≡
  subroutine ps_table_final (object)
    class(ps_table_t), intent(inout) :: object
    type(ps_entry_t), pointer :: current
    do while (associated (object%first))
      current => object%first
      object%first => current%next
      deallocate (current)
    end do
    nullify (object%last)
  end subroutine ps_table_final

```

Write the table. A base writer for the body and specific writers for the headers.

```

<Auto components: ps table: TBP>+≡
  procedure :: base_write => ps_table_base_write
  procedure (ps_table_write), deferred :: write

<Auto components: interfaces>≡
  interface
    subroutine ps_table_write (object, unit)
      import
      class(ps_table_t), intent(in) :: object
      integer, intent(in), optional :: unit
    end subroutine ps_table_write
  end interface

```

```

<Auto components: ds table: TBP>≡
  procedure :: write => ds_table_write

```

```

<Auto components: fs table: TBP>≡
  procedure :: write => fs_table_write

```

```

<Auto components: if table: TBP>≡
  procedure :: write => if_table_write

```

The first `n_in` particles will be replaced by antiparticles in the output, and we write an arrow if `n_in` is present.

```

<Auto components: procedures>+≡
  subroutine ps_table_base_write (object, unit, n_in)
    class(ps_table_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: n_in
    integer, dimension(:), allocatable :: pdg
    type(ps_entry_t), pointer :: entry
    type(field_data_t), pointer :: prt
    integer :: u, i, j, n0
    u = given_output_unit (unit)
    entry => object%first
    do while (associated (entry))
      write (u, "(2x)", advance = "no")
      if (present (n_in)) then
        do i = 1, n_in
          write (u, "(1x)", advance = "no")
          pdg = entry%get (i)
          do j = 1, size (pdg)
            prt => object%model%get_field_ptr (pdg(j))
            if (j > 1) write (u, "(::)", advance = "no")
            write (u, "(A)", advance = "no") &
              char (prt%get_name (pdg(j) >= 0))
          end do
        end do
        write (u, "(1x,A)", advance = "no")  "=>"
        n0 = n_in + 1
      else
        n0 = 1
      end if
      do i = n0, entry%get_size ()
        write (u, "(1x)", advance = "no")
        pdg = entry%get (i)
        do j = 1, size (pdg)
          prt => object%model%get_field_ptr (pdg(j))
          if (j > 1) write (u, "(::)", advance = "no")
          write (u, "(A)", advance = "no") &
            char (prt%get_name (pdg(j) < 0))
        end do
      end do
      if (object%loops) then
        write (u, "(2x,['I0','I0','I0'])" entry%n_loop, entry%n_rad
      else
        write (u, "(A)")
      end if
      entry => entry%next
    end do
  end subroutine

```

```

        end do
    end subroutine ps_table_base_write

    subroutine ds_table_write (object, unit)
        class(ds_table_t), intent(in) :: object
        integer, intent(in), optional :: unit
        type(field_data_t), pointer :: prt
        integer :: u
        u = given_output_unit (unit)
        prt => object%model%get_field_ptr (object%pdg_in)
        write (u, "(1x,A,1x,A)") "Decays for particle:", &
            char (prt%get_name (object%pdg_in < 0))
        call object%base_write (u)
    end subroutine ds_table_write

    subroutine fs_table_write (object, unit)
        class(fs_table_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Table of final states:"
        call object%base_write (u)
    end subroutine fs_table_write

    subroutine if_table_write (object, unit)
        class(if_table_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Table of in/out states:"
        select case (object%proc_type)
        case (PROC_DECAY)
            call object%base_write (u, n_in = 1)
        case (PROC_SCATTER)
            call object%base_write (u, n_in = 2)
        end select
    end subroutine if_table_write

```

Obtain a particle string for a given index in the pdg list

<Auto components: ps table: TBP>+≡

```
procedure :: get_particle_string => ps_table_get_particle_string
```

<Auto components: procedures>+≡

```

subroutine ps_table_get_particle_string (object, index, prt_in, prt_out)
    class(ps_table_t), intent(in) :: object
    integer, intent(in) :: index
    type(string_t), intent(out), dimension(:), allocatable :: prt_in, prt_out
    integer :: n_in
    type(field_data_t), pointer :: prt
    type(ps_entry_t), pointer :: entry
    integer, dimension(:), allocatable :: pdg
    integer :: n0
    integer :: i, j
    entry => object%first

```

```

i = 1
do while (i < index)
  if (associated (entry%next)) then
    entry => entry%next
    i = i + 1
  else
    call msg_fatal ("ps_table: entry with requested index does not exist!")
  end if
end do

if (object%proc_type > 0) then
  select case (object%proc_type)
  case (PROC_DECAY)
    n_in = 1
  case (PROC_SCATTER)
    n_in = 2
  end select
else
  call msg_fatal ("Neither decay nor scattering process")
end if

n0 = n_in + 1
allocate (prt_in (n_in), prt_out (entry%get_size () - n_in))
do i = 1, n_in
  prt_in(i) = ""
  pdg = entry%get(i)
  do j = 1, size (pdg)
    prt => object%model%get_field_ptr (pdg(j))
    prt_in(i) = prt_in(i) // prt%get_name (pdg(j) >= 0)
    if (j /= size (pdg)) prt_in(i) = prt_in(i) // ":"
  end do
end do
do i = n0, entry%get_size ()
  prt_out(i-n_in) = ""
  pdg = entry%get(i)
  do j = 1, size (pdg)
    prt => object%model%get_field_ptr (pdg(j))
    prt_out(i-n_in) = prt_out(i-n_in) // prt%get_name (pdg(j) < 0)
    if (j /= size (pdg)) prt_out(i-n_in) = prt_out(i-n_in) // ":"
  end do
end do
end subroutine ps_table_get_particle_string

```

Initialize with a predefined set of final states, or in/out state lists.

```

<Auto components: ps table: TBP>+≡
  generic :: init => ps_table_init
  procedure, private :: ps_table_init

<Auto components: if table: TBP>+≡
  generic :: init => if_table_init
  procedure, private :: if_table_init

<Auto components: procedures>+≡
  subroutine ps_table_init (table, model, pl, constraints, n_in, do_not_check_regular)
    class(ps_table_t), intent(out) :: table

```

```

class(model_data_t), intent(in), target :: model
type(pdg_list_t), dimension(:), intent(in) :: pl
type(split_constraints_t), intent(in) :: constraints
integer, intent(in), optional :: n_in
logical, intent(in), optional :: do_not_check_regular
logical :: passed
integer :: i
table%model => model

if (present (n_in)) then
  select case (n_in)
  case (1)
    table%proc_type = PROC_DECAY
  case (2)
    table%proc_type = PROC_SCATTER
  case default
    table%proc_type = PROC_UNDEFINED
  end select
else
  table%proc_type = PROC_UNDEFINED
end if

do i = 1, size (pl)
  call table%record (pl(i), 0, 0, constraints, &
    do_not_check_regular, passed)
  if (.not. passed) then
    call msg_fatal ("ps_table: Registering process components failed")
  end if
end do
end subroutine ps_table_init

subroutine if_table_init (table, model, pl_in, pl_out, constraints)
class(if_table_t), intent(out) :: table
class(model_data_t), intent(in), target :: model
type(pdg_list_t), dimension(:), intent(in) :: pl_in, pl_out
type(split_constraints_t), intent(in) :: constraints
integer :: i, j, k, p, n_in, n_out
type(pdg_array_t), dimension(:), allocatable :: pa_in
type(pdg_list_t), dimension(:), allocatable :: pl
allocate (pl (size (pl_in) * size (pl_out)))
k = 0
do i = 1, size (pl_in)
  n_in = pl_in(i)%get_size ()
  allocate (pa_in (n_in))
  do p = 1, n_in
    pa_in(p) = pl_in(i)%get (p)
  end do
  do j = 1, size (pl_out)
    n_out = pl_out(j)%get_size ()
    k = k + 1
    call pl(k)%init (n_in + n_out)
    do p = 1, n_in
      call pl(k)%set (p, invert_pdg_array (pa_in(p), model))
    end do
  end do
end do

```



```

        do p = 1, n_out
            call pl(k)%set (n_in + p, pl_out(j)%get (p))
        end do
    end do
    deallocate (pa_in)
end do
n_in = size (pl_in(1)%a)
call table%init (model, pl, constraints, n_in, do_not_check_regular = .true.)
end subroutine if_table_init

```

Enable loops for the table. This affects both splitting and output.

```

<Auto components: ps table: TBP>+≡
    procedure :: enable_loops => ps_table_enable_loops

<Auto components: procedures>+≡
    subroutine ps_table_enable_loops (table)
        class(ps_table_t), intent(inout) :: table
        table%loops = .true.
    end subroutine ps_table_enable_loops

```

28.1.4 Top-level methods

Create a table for a single-particle decay. Construct all possible final states from a single particle with PDG code `pdg_in`. The construction is limited by the given `constraints`.

```

<Auto components: ds table: TBP>+≡
    procedure :: make => ds_table_make

<Auto components: procedures>+≡
    subroutine ds_table_make (table, model, pdg_in, constraints)
        class(ds_table_t), intent(out) :: table
        class(model_data_t), intent(in), target :: model
        integer, intent(in) :: pdg_in
        type(split_constraints_t), intent(in) :: constraints
        type(pdg_list_t) :: pl_in
        type(pdg_list_t), dimension(0) :: pl
        call table%init (model, pl, constraints)
        table%pdg_in = pdg_in
        call pl_in%init (1)
        call pl_in%set (1, [pdg_in])
        call table%split (pl_in, 0, constraints)
    end subroutine ds_table_make

```

Split all entries in a growing table, starting from a table that may already contain states. Add and record split states on the fly.

```

<Auto components: fs table: TBP>+≡
    procedure :: radiate => fs_table_radiate

<Auto components: procedures>+≡
    subroutine fs_table_radiate (table, constraints, do_not_check_regular)
        class(fs_table_t), intent(inout) :: table
        type(split_constraints_t) :: constraints

```

```

logical, intent(in), optional :: do_not_check_regular
type(ps_entry_t), pointer :: current
current => table%first
do while (associated (current))
    call table%split (current, 0, constraints, record = .true., &
        do_not_check_regular = do_not_check_regular)
    current => current%next
end do
end subroutine fs_table_radiate

```

28.1.5 Splitting algorithm

Recursive splitting. First of all, we record the current `pdg_list` in the table, subject to `constraints`, if requested. We also record copies of the list marked as loop corrections.

When we record a particle list, we sort it first.

If there is room for splitting, We take a PDG array list and the index of an element, and split this element in all possible ways. The split entry is inserted into the list, which we split further.

The recursion terminates whenever the split array would have a length greater than n_{\max} .

(Auto components: ps table: TBP)+≡

```

procedure :: split => ps_table_split

```

(Auto components: procedures)+≡

```

recursive subroutine ps_table_split (table, pl, n_rad, constraints, &
    record, do_not_check_regular)
    class(ps_table_t), intent(inout) :: table
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_rad
    type(split_constraints_t), intent(in) :: constraints
    logical, intent(in), optional :: record, do_not_check_regular
    integer :: n_loop, i
    logical :: passed, save_pdg_index
    type(vertex_iterator_t) :: vit
    integer, dimension(:), allocatable :: pdg1
    integer, dimension(:), allocatable :: pdg2
    if (present (record)) then
        if (record) then
            n_loop = 0
            INCR_LOOPS: do
                call table%record_sorted (pl, n_loop, n_rad, constraints, &
                    do_not_check_regular, passed)
                if (.not. passed) exit INCR_LOOPS
                if (.not. table%loops) exit INCR_LOOPS
                n_loop = n_loop + 1
            end do INCR_LOOPS
        end if
    end if
    select type (table)
    type is (if_table_t)
        save_pdg_index = .true.

```

```

class default
  save_pdg_index = .false.
end select
do i = 1, pl%get_size ()
  call constraints%check_before_split (table, pl, i, passed)
  if (passed) then
    pdg1 = pl%get (i)
    call vit%init (table%model, pdg1, save_pdg_index)
    SCAN_VERTICES: do
      call vit%get_next_match (pdg2)
      if (allocated (pdg2)) then
        call table%insert (pl, n_rad, i, pdg2, constraints, &
          do_not_check_regular = do_not_check_regular)
      else
        exit SCAN_VERTICES
      end if
    end do SCAN_VERTICES
  end if
end do
end subroutine ps_table_split

```

The worker part: insert the list of particles found by vertex matching in place of entry *i* in the PDG list. Then split/record further.

The *n_in* parameter tells the replacement routine to insert the new particles after entry *n_in*. Otherwise, they follow index *i*.

(Auto components: ps table: TBP)+≡

```

procedure :: insert => ps_table_insert

```

(Auto components: procedures)+≡

```

recursive subroutine ps_table_insert &
  (table, pl, n_rad, i, pdg, constraints, n_in, do_not_check_regular)
class(ps_table_t), intent(inout) :: table
class(pdg_list_t), intent(in) :: pl
integer, intent(in) :: n_rad, i
integer, dimension(:), intent(in) :: pdg
type(split_constraints_t), intent(in) :: constraints
integer, intent(in), optional :: n_in
logical, intent(in), optional :: do_not_check_regular
type(pdg_list_t) :: pl_insert
logical :: passed
integer :: k, s
s = size (pdg)
call pl_insert%init (s)
do k = 1, s
  call pl_insert%set (k, pdg(k))
end do
call constraints%check_before_insert (table, pl%get (i), pl_insert, passed)
if (passed) then
  if (.not. is_colored_isr ()) return
  call table%split (pl%replace (i, pl_insert, n_in), n_rad + s - 1, &
    constraints, record = .true., do_not_check_regular = .true.)
end if
contains
  logical function is_colored_isr () result (ok)

```

```

type(pdg_list_t) :: pl_replaced
ok = .true.
if (present (n_in)) then
  if (i <= n_in) then
    ok = pl_insert%contains_colored_particles ()
    if (.not. ok) then
      pl_replaced = pl%replace (i, pl_insert, n_in)
      associate (size_replaced => pl_replaced%get_pdg_sizes (), &
        size => pl%get_pdg_sizes ())
        ok = all (size_replaced(:n_in) == size(:n_in))
      end associate
    end if
  end if
end if
end function is_colored_isr
end subroutine ps_table_insert

```

Special case: If we are splitting an initial particle, there is slightly more to do. We loop over the particles from the vertex match and replace the initial particle by each of them in turn. The remaining particles must be appended after the second initial particle, so they will end up in the out state. This is done by providing the `n_in` argument to the base method as an optional argument.

Note that we must call the base-method procedure explicitly, so the `table` argument keeps its dynamic type as `if_table` inside this procedure.

```

<Auto components: if table: TBP>+≡
  procedure :: insert => if_table_insert

<Auto components: procedures>+≡
  recursive subroutine if_table_insert &
    (table, pl, n_rad, i, pdg, constraints, n_in, do_not_check_regular)
    class(if_table_t), intent(inout) :: table
    class(pdg_list_t), intent(in) :: pl
    integer, intent(in) :: n_rad, i
    integer, dimension(:), intent(in) :: pdg
    type(split_constraints_t), intent(in) :: constraints
    integer, intent(in), optional :: n_in
    logical, intent(in), optional :: do_not_check_regular
    integer, dimension(:), allocatable :: pdg_work
    integer :: p
    if (i > 2) then
      call ps_table_insert (table, pl, n_rad, i, pdg, constraints, &
        do_not_check_regular = do_not_check_regular)
    else
      allocate (pdg_work (size (pdg)))
      do p = 1, size (pdg)
        pdg_work(1) = pdg(p)
        pdg_work(2:p) = pdg(1:p-1)
        pdg_work(p+1:) = pdg(p+1:)
        select case (table%proc_type)
          case (PROC_DECAY)
            call ps_table_insert (table, &
              pl, n_rad, i, pdg_work, constraints, n_in = 1, &
              do_not_check_regular = do_not_check_regular)

```

```

        case (PROC_SCATTER)
            call ps_table_insert (table, &
                pl, n_rad, i, pdg_work, constraints, n_in = 2, &
                do_not_check_regular = do_not_check_regular)
        end select
    end do
end if
end subroutine if_table_insert

```

Sort before recording. In the case of the `if_table`, we do not sort the first `n_in` particle entries. Instead, we check whether they are allowed in the `pl_beam` PDG list, if that is provided.

```

<Auto components: ps table: TBP>+≡
    procedure :: record_sorted => ps_table_record_sorted

<Auto components: if table: TBP>+≡
    procedure :: record_sorted => if_table_record_sorted

<Auto components: procedures>+≡
    subroutine ps_table_record_sorted &
        (table, pl, n_loop, n_rad, constraints, do_not_check_regular, passed)
        class(ps_table_t), intent(inout) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop, n_rad
        type(split_constraints_t), intent(in) :: constraints
        logical, intent(in), optional :: do_not_check_regular
        logical, intent(out) :: passed
        call table%record (pl%sort_abs (), n_loop, n_rad, constraints, &
            do_not_check_regular, passed)
    end subroutine ps_table_record_sorted

    subroutine if_table_record_sorted &
        (table, pl, n_loop, n_rad, constraints, do_not_check_regular, passed)
        class(if_table_t), intent(inout) :: table
        type(pdg_list_t), intent(in) :: pl
        integer, intent(in) :: n_loop, n_rad
        type(split_constraints_t), intent(in) :: constraints
        logical, intent(in), optional :: do_not_check_regular
        logical, intent(out) :: passed
        call table%record (pl%sort_abs (2), n_loop, n_rad, constraints, &
            do_not_check_regular, passed)
    end subroutine if_table_record_sorted

```

Record an entry: insert into the list. Check the ordering and insert it at the correct place, unless it is already there.

We record an array only if its mass sum is less than the total available energy. This restriction is removed by setting `constrained` to false.

```

<Auto components: ps table: TBP>+≡
    procedure :: record => ps_table_record

<Auto components: procedures>+≡
    subroutine ps_table_record (table, pl, n_loop, n_rad, constraints, &
        do_not_check_regular, passed)
        class(ps_table_t), intent(inout) :: table

```

```

type(pdg_list_t), intent(in) :: pl
integer, intent(in) :: n_loop, n_rad
type(split_constraints_t), intent(in) :: constraints
logical, intent(in), optional :: do_not_check_regular
logical, intent(out) :: passed
type(ps_entry_t), pointer :: current
logical :: needs_check
passed = .false.
needs_check = .true.
if (present (do_not_check_regular)) needs_check = .not. do_not_check_regular
if (needs_check .and. .not. pl%is_regular ()) then
    call msg_warning ("Record ps_table entry: Irregular pdg-list encountered!")
    return
end if
call constraints%check_before_record (table, pl, n_loop, passed)
if (.not. passed) then
    return
end if
current => table%first
do while (associated (current))
    if (pl == current) then
        if (n_loop == current%n_loop) return
    else if (pl < current) then
        call insert
        return
    end if
    current => current%next
end do
call insert
contains
subroutine insert ()
    type(ps_entry_t), pointer :: entry
    allocate (entry)
    entry%pdg_list_t = pl
    entry%n_loop = n_loop
    entry%n_rad = n_rad
    if (associated (current)) then
        if (associated (current%previous)) then
            current%previous%next => entry
            entry%previous => current%previous
        else
            table%first => entry
        end if
        entry%next => current
        current%previous => entry
    else
        if (associated (table%last)) then
            table%last%next => entry
            entry%previous => table%last
        else
            table%first => entry
        end if
        table%last => entry
    end if
end if

```

```

    end subroutine insert
end subroutine ps_table_record

```

28.1.6 Tools

Compute the mass sum for a PDG list object, counting the entries with indices between (including) `n1` and `n2`. Rely on the requirement that if an entry is a PDG array, this array must be degenerate in mass.

```

⟨Auto components: procedures⟩+≡
function mass_sum (pl, n1, n2, model) result (m)
  type(pdg_list_t), intent(in) :: pl
  integer, intent(in) :: n1, n2
  class(model_data_t), intent(in), target :: model
  integer, dimension(:), allocatable :: pdg
  real(default) :: m
  type(field_data_t), pointer :: prt
  integer :: i
  m = 0
  do i = n1, n2
    pdg = pl%get (i)
    prt => model%get_field_ptr (pdg(1))
    m = m + prt%get_mass ()
  end do
end function mass_sum

```

Invert a PDG array, replacing particles by antiparticles. This depends on the model.

```

⟨Auto components: procedures⟩+≡
function invert_pdg_array (pa, model) result (pa_inv)
  type(pdg_array_t), intent(in) :: pa
  class(model_data_t), intent(in), target :: model
  type(pdg_array_t) :: pa_inv
  type(field_data_t), pointer :: prt
  integer :: i, pdg
  pa_inv = pa
  do i = 1, pa_inv%get_length ()
    pdg = pa_inv%get (i)
    prt => model%get_field_ptr (pdg)
    if (prt%has_antiparticle ()) call pa_inv%set (i, -pdg)
  end do
end function invert_pdg_array

```

28.1.7 Access results

Return the number of generated decays.

```

⟨Auto components: ps table: TBP⟩+≡
procedure :: get_length => ps_table_get_length

```

```

<Auto components: procedures>+≡
function ps_table_get_length (ps_table) result (n)
  class(ps_table_t), intent(in) :: ps_table
  integer :: n
  type(ps_entry_t), pointer :: entry
  n = 0
  entry => ps_table%first
  do while (associated (entry))
    n = n + 1
    entry => entry%next
  end do
end function ps_table_get_length

<Auto components: ps table: TBP>+≡
procedure :: get_emitters => ps_table_get_emitters

<Auto components: procedures>+≡
subroutine ps_table_get_emitters (table, constraints, emitters)
  class(ps_table_t), intent(in) :: table
  type(split_constraints_t), intent(in) :: constraints
  integer, dimension(:), allocatable, intent(out) :: emitters
  class(pdg_list_t), pointer :: pl
  integer :: i
  logical :: passed
  type(vertex_iterator_t) :: vit
  integer, dimension(:), allocatable :: pdg1, pdg2
  integer :: n_emitters
  integer, dimension(:), allocatable :: emitters_tmp
  integer, parameter :: buf0 = 6
  n_emitters = 0
  pl => table%first
  allocate (emitters_tmp (buf0))
  do i = 1, pl%get_size ()
    call constraints%check_before_split (table, pl, i, passed)
    if (passed) then
      pdg1 = pl%get(i)
      call vit%init (table%model, pdg1, .false.)
      do
        call vit%get_next_match(pdg2)
        if (allocated (pdg2)) then
          if (n_emitters + 1 > size (emitters_tmp)) &
            call extend_integer_array (emitters_tmp, 10)
          emitters_tmp (n_emitters + 1) = pdg1(1)
          n_emitters = n_emitters + 1
        else
          exit
        end if
      end do
    end if
  end do
  allocate (emitters (n_emitters))
  emitters = emitters_tmp (1:n_emitters)
  deallocate (emitters_tmp)
end subroutine ps_table_get_emitters

```


Return an allocated array of decay products (PDG codes). If requested, return also the loop and radiation order count.

<Auto components: ps table: TBP>+≡

```
procedure :: get_pdg_out => ps_table_get_pdg_out
```

<Auto components: procedures>+≡

```
subroutine ps_table_get_pdg_out (ps_table, i, pa_out, n_loop, n_rad)
  class(ps_table_t), intent(in) :: ps_table
  integer, intent(in) :: i
  type(pdg_array_t), dimension(:), allocatable, intent(out) :: pa_out
  integer, intent(out), optional :: n_loop, n_rad
  type(ps_entry_t), pointer :: entry
  integer :: n, j
  n = 0
  entry => ps_table%first
  FIND_ENTRY: do while (associated (entry))
    n = n + 1
    if (n == i) then
      allocate (pa_out (entry%get_size ()))
      do j = 1, entry%get_size ()
        pa_out(j) = entry%get (j)
        if (present (n_loop)) n_loop = entry%n_loop
        if (present (n_rad)) n_rad = entry%n_rad
      end do
      exit FIND_ENTRY
    end if
    entry => entry%next
  end do FIND_ENTRY
end subroutine ps_table_get_pdg_out
```

28.1.8 Unit tests

Test module, followed by the corresponding implementation module.

<auto_components_ut.f90>≡

<File header>

```
module auto_components_ut
  use unit_tests
  use auto_components_ut1
```

<Standard module head>

<Auto components: public test>

```
contains
```

<Auto components: test driver>

```
end module auto_components_ut
```

```

<auto_components_util.f90>≡
  <File header>

  module auto_components_util

    <Use kinds>
    <Use strings>
    use pdg_arrays
    use model_data
    use model_testbed, only: prepare_model, cleanup_model

    use auto_components

    <Standard module head>

    <Auto components: test declarations>

    contains

    <Auto components: tests>

  end module auto_components_util
API: driver for the unit tests below.
<Auto components: public test>≡
  public :: auto_components_test
<Auto components: test driver>≡
  subroutine auto_components_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Auto components: execute tests>
  end subroutine auto_components_test

```

Generate Decay Table

Determine all kinematically allowed decay channels for a Higgs boson, using default parameter values.

```

<Auto components: execute tests>≡
  call test (auto_components_1, "auto_components_1", &
    "generate decay table", &
    u, results)
<Auto components: test declarations>≡
  public :: auto_components_1
<Auto components: tests>≡
  subroutine auto_components_1 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: model
    type(field_data_t), pointer :: prt
    type(ds_table_t) :: ds_table
    type(split_constraints_t) :: constraints

```

```

write (u, "(A)")  "* Test output: auto_components_1"
write (u, "(A)")  "* Purpose: determine Higgs decay table"
write (u, *)

write (u, "(A)")  "* Read Standard Model"

model => null ()
call prepare_model (model, var_str ("SM"))

prt => model%get_field_ptr (25)

write (u, *)
write (u, "(A)")  "* Higgs decays n = 2"
write (u, *)

call constraints%init (2)
call constraints%set (1, constrain_n_tot (2))
call constraints%set (2, constrain_mass_sum (prt%get_mass ()))

call ds_table%make (model, 25, constraints)
call ds_table%write (u)
call ds_table%final ()

write (u, *)
write (u, "(A)")  "* Higgs decays n = 3 (w/o radiative)"
write (u, *)

call constraints%init (3)
call constraints%set (1, constrain_n_tot (3))
call constraints%set (2, constrain_mass_sum (prt%get_mass ()))
call constraints%set (3, constrain_radiation ())

call ds_table%make (model, 25, constraints)
call ds_table%write (u)
call ds_table%final ()

write (u, *)
write (u, "(A)")  "* Higgs decays n = 3 (w/ radiative)"
write (u, *)

call constraints%init (2)
call constraints%set (1, constrain_n_tot (3))
call constraints%set (2, constrain_mass_sum (prt%get_mass ()))

call ds_table%make (model, 25, constraints)
call ds_table%write (u)
call ds_table%final ()

write (u, *)
write (u, "(A)")  "* Cleanup"

call cleanup_model (model)
deallocate (model)

```

```

write (u, *)
write (u, "(A)")  "* Test output end: auto_components_1"

end subroutine auto_components_1

```

Generate radiation

Given a final state, add radiation (NLO and NNLO). We provide a list of particles that is allowed to occur in the generated final states.

```

<Auto components: execute tests>+≡
  call test (auto_components_2, "auto_components_2", &
    "generate NLO corrections, final state", &
    u, results)

<Auto components: test declarations>+≡
  public :: auto_components_2

<Auto components: tests>+≡
  subroutine auto_components_2 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: model
    type(pdg_list_t), dimension(:), allocatable :: pl, pl_zzh
    type(pdg_list_t) :: pl_match
    type(fs_table_t) :: fs_table
    type(split_constraints_t) :: constraints
    real(default) :: sqrts
    integer :: i

    write (u, "(A)")  "* Test output: auto_components_2"
    write (u, "(A)")  "* Purpose: generate radiation (NLO)"
    write (u, *)

    write (u, "(A)")  "* Read Standard Model"

    model => null ()
    call prepare_model (model, var_str ("SM"))

    write (u, *)
    write (u, "(A)")  "* LO final state"
    write (u, *)

    allocate (pl (2))
    call pl(1)%init (2)
    call pl(1)%set (1, 1)
    call pl(1)%set (2, -1)
    call pl(2)%init (2)
    call pl(2)%set (1, 21)
    call pl(2)%set (2, 21)
    do i = 1, 2
      call pl(i)%write (u); write (u, *)
    end do

```

```

write (u, *)
write (u, "(A)")  "* Initialize FS table"
write (u, *)

call constraints%init (1)
call constraints%set (1, constrain_n_tot (3))

call fs_table%init (model, pl, constraints)
call fs_table%write (u)

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, unconstrained"
write (u, *)

call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, &
                  &complete but mass-constrained"
write (u, *)

sqrts = 50

call constraints%init (2)
call constraints%set (1, constrain_n_tot (3))
call constraints%set (2, constrain_mass_sum (sqrts))

call fs_table%init (model, pl, constraints)
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, restricted"
write (u, *)

call pl_match%init ([1, -1, 21])

call constraints%init (2)
call constraints%set (1, constrain_n_tot (3))
call constraints%set (2, constrain_insert (pl_match))

call fs_table%init (model, pl, constraints)
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NNLO corrections, restricted, with one loop"
write (u, *)

call pl_match%init ([1, -1, 21])

```

```

call constraints%init (3)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_n_loop (1))
call constraints%set (3, constrain_insert (pl_match))

call fs_table%init (model, pl, constraints)
call fs_table%enable_loops ()
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "** Generate NNLO corrections, restricted, with loops"
write (u, *)

call constraints%init (2)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_insert (pl_match))

call fs_table%init (model, pl, constraints)
call fs_table%enable_loops ()
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

write (u, *)
write (u, "(A)")  "** Generate NNLO corrections, restricted, to Z Z H, &
                  &no loops"
write (u, *)

allocate (pl_zzh (1))
call pl_zzh(1)%init (3)
call pl_zzh(1)%set (1, 23)
call pl_zzh(1)%set (2, 23)
call pl_zzh(1)%set (3, 25)

call constraints%init (3)
call constraints%set (1, constrain_n_tot (5))
call constraints%set (2, constrain_mass_sum (500._default))
call constraints%set (3, constrain_require (pl_zzh(1)))

call fs_table%init (model, pl_zzh, constraints)
call fs_table%radiate (constraints)
call fs_table%write (u)
call fs_table%final ()

call cleanup_model (model)
deallocate (model)

write (u, *)
write (u, "(A)")  "** Test output end: auto_components_2"

end subroutine auto_components_2

```

Generate radiation from initial and final state

Given a process, add radiation (NLO and NNLO). We provide a list of particles that is allowed to occur in the generated final states.

```
<Auto components: execute tests>+≡
  call test (auto_components_3, "auto_components_3", &
    "generate NLO corrections, in and out", &
    u, results)

<Auto components: test declarations>+≡
  public :: auto_components_3

<Auto components: tests>+≡
  subroutine auto_components_3 (u)
    integer, intent(in) :: u
    class(model_data_t), pointer :: model
    type(pdg_list_t), dimension(:), allocatable :: pl_in, pl_out
    type(pdg_list_t) :: pl_match, pl_beam
    type(if_table_t) :: if_table
    type(split_constraints_t) :: constraints
    real(default) :: sqrts
    integer :: i

    write (u, "(A)")  "* Test output: auto_components_3"
    write (u, "(A)")  "*   Purpose: generate radiation (NLO)"
    write (u, *)

    write (u, "(A)")  "* Read Standard Model"

    model => null ()
    call prepare_model (model, var_str ("SM"))

    write (u, *)
    write (u, "(A)")  "* LO initial state"
    write (u, *)

    allocate (pl_in (2))
    call pl_in(1)%init (2)
    call pl_in(1)%set (1, 1)
    call pl_in(1)%set (2, -1)
    call pl_in(2)%init (2)
    call pl_in(2)%set (1, -1)
    call pl_in(2)%set (2, 1)
    do i = 1, 2
      call pl_in(i)%write (u); write (u, *)
    end do

    write (u, *)
    write (u, "(A)")  "* LO final state"
    write (u, *)

    allocate (pl_out (1))
```

```

call pl_out(1)%init (1)
call pl_out(1)%set (1, 23)
call pl_out(1)%write (u); write (u, *)

write (u, *)
write (u, "(A)")  "* Initialize FS table"
write (u, *)

call constraints%init (1)
call constraints%set (1, constrain_n_tot (4))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%write (u)

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, unconstrained"
write (u, *)

call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, &
                  &complete but mass-constrained"
write (u, *)

sqrts = 100
call constraints%init (2)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_mass_sum (sqrts))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

write (u, *)
write (u, "(A)")  "* Generate NLO corrections, &
                  &mass-constrained, restricted beams"
write (u, *)

call pl_beam%init (3)
call pl_beam%set (1, 1)
call pl_beam%set (2, -1)
call pl_beam%set (3, 21)

call constraints%init (3)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_in_state (pl_beam))
call constraints%set (3, constrain_mass_sum (sqrts))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%radiate (constraints)

```



```

call if_table%write (u)
call if_table%final ()

write (u, *)
write (u, "(A)")  "** Generate NLO corrections, restricted"
write (u, *)

call pl_match%init ([1, -1, 21])

call constraints%init (4)
call constraints%set (1, constrain_n_tot (4))
call constraints%set (2, constrain_in_state (pl_beam))
call constraints%set (3, constrain_mass_sum (sqrts))
call constraints%set (4, constrain_insert (pl_match))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

write (u, *)
write (u, "(A)")  "** Generate NNLO corrections, restricted, Z preserved, &
                  &with loops"
write (u, *)

call constraints%init (5)
call constraints%set (1, constrain_n_tot (5))
call constraints%set (2, constrain_in_state (pl_beam))
call constraints%set (3, constrain_mass_sum (sqrts))
call constraints%set (4, constrain_insert (pl_match))
call constraints%set (5, constrain_require (pl_out(1)))

call if_table%init (model, pl_in, pl_out, constraints)
call if_table%enable_loops ()
call if_table%radiate (constraints)
call if_table%write (u)
call if_table%final ()

call cleanup_model (model)
deallocate (model)

write (u, *)
write (u, "(A)")  "** Test output end: auto_components_3"

end subroutine auto_components_3

```

28.2 Creating the real flavor structure

```

<radiation_generator.f90>≡
  <File header>

  module radiation_generator

```

```

    <Use kinds>
    <Use strings>
    use diagnostics
    use io_units
    use physics_defs, only: PHOTON, GLUON
    use pdg_arrays
    use flavors
    use model_data
    use auto_components
    use string_utils, only: split_string, string_contains_word

    implicit none
    private

    <radiation generator: public>

    <radiation generator: types>

    contains

    <radiation generator: procedures>

    end module radiation_generator

    <radiation generator: types>≡
    type :: pdg_sorter_t
        integer :: pdg
        logical :: checked = .false.
        integer :: associated_born = 0
    end type pdg_sorter_t

    <radiation generator: types>+≡
    type :: pdg_states_t
        type(pdg_array_t), dimension(:), allocatable :: pdg
        type(pdg_states_t), pointer :: next
        integer :: n_particles
    contains
    <radiation generator: pdg states: TBP>
    end type pdg_states_t

    <radiation generator: pdg states: TBP>≡
    procedure :: init => pdg_states_init

    <radiation generator: procedures>≡
    subroutine pdg_states_init (states)
        class(pdg_states_t), intent(inout) :: states
        nullify (states%next)
    end subroutine pdg_states_init

    <radiation generator: pdg states: TBP>+≡
    procedure :: add => pdg_states_add

```

```

<radiation generator: procedures>+≡
subroutine pdg_states_add (states, pdg)
  class(pdg_states_t), intent(inout), target :: states
  type(pdg_array_t), dimension(:), intent(in) :: pdg
  type(pdg_states_t), pointer :: current_state
  select type (states)
  type is (pdg_states_t)
    current_state => states
  do
    if (associated (current_state%next)) then
      current_state => current_state%next
    else
      allocate (current_state%next)
      nullify(current_state%next%next)
      current_state%pdg = pdg
      exit
    end if
  end do
end select
end subroutine pdg_states_add

<radiation generator: pdg states: TBP>+≡
procedure :: get_n_states => pdg_states_get_n_states

<radiation generator: procedures>+≡
function pdg_states_get_n_states (states) result (n)
  class(pdg_states_t), intent(in), target :: states
  integer :: n
  type(pdg_states_t), pointer :: current_state
  n = 0
  select type(states)
  type is (pdg_states_t)
    current_state => states
  do
    if (associated (current_state%next)) then
      n = n+1
      current_state => current_state%next
    else
      exit
    end if
  end do
end select
end function pdg_states_get_n_states

<radiation generator: types>+≡
type :: prt_queue_t
  type(string_t), dimension(:), allocatable :: prt_string
  type(prt_queue_t), pointer :: next => null ()
  type(prt_queue_t), pointer :: previous => null ()
  type(prt_queue_t), pointer :: front => null ()
  type(prt_queue_t), pointer :: current_prt => null ()
  type(prt_queue_t), pointer :: back => null ()
  integer :: n_lists = 0

```

```

contains
  <radiation generator: prt queue: TBP>
end type prt_queue_t

<radiation generator: prt queue: TBP>≡
  procedure :: null => prt_queue_null

<radiation generator: procedures>+≡
  subroutine prt_queue_null (queue)
    class(prt_queue_t), intent(out) :: queue
    queue%next => null ()
    queue%previous => null ()
    queue%front => null ()
    queue%current_prt => null ()
    queue%back => null ()
    queue%n_lists = 0
    if (allocated (queue%prt_string)) deallocate (queue%prt_string)
  end subroutine prt_queue_null

<radiation generator: prt queue: TBP>+≡
  procedure :: append => prt_queue_append

<radiation generator: procedures>+≡
  subroutine prt_queue_append (queue, prt_string)
    class(prt_queue_t), intent(inout) :: queue
    type(string_t), intent(in), dimension(:) :: prt_string
    type(prt_queue_t), pointer :: new_element => null ()
    type(prt_queue_t), pointer :: current_back => null ()
    allocate (new_element)
    allocate (new_element%prt_string(size (prt_string)))
    new_element%prt_string = prt_string
    if (associated (queue%back)) then
      current_back => queue%back
      current_back%next => new_element
      new_element%previous => current_back
      queue%back => new_element
    else
      !!! Initial entry
      queue%front => new_element
      queue%back => queue%front
      queue%current_prt => queue%front
    end if
    queue%n_lists = queue%n_lists + 1
  end subroutine prt_queue_append

<radiation generator: prt queue: TBP>+≡
  procedure :: get => prt_queue_get

<radiation generator: procedures>+≡
  subroutine prt_queue_get (queue, prt_string)
    class(prt_queue_t), intent(inout) :: queue
    type(string_t), dimension(:), allocatable, intent(out) :: prt_string
    if (associated (queue%current_prt)) then
      prt_string = queue%current_prt%prt_string

```

```

        if (associated (queue%current_prt%next)) &
            queue%current_prt => queue%current_prt%next
        else
            prt_string = " "
        end if
    end subroutine prt_queue_get

```

As above.

```

<radiation generator: prt queue: TBP>+≡
    procedure :: get_last => prt_queue_get_last

```

```

<radiation generator: procedures>+≡
    subroutine prt_queue_get_last (queue, prt_string)
        class(prt_queue_t), intent(in) :: queue
        type(string_t), dimension(:), allocatable, intent(out) :: prt_string
        if (associated (queue%back)) then
            allocate (prt_string(size (queue%back%prt_string)))
            prt_string = queue%back%prt_string
        else
            prt_string = " "
        end if
    end subroutine prt_queue_get_last

```

```

<radiation generator: prt queue: TBP>+≡
    procedure :: reset => prt_queue_reset

```

```

<radiation generator: procedures>+≡
    subroutine prt_queue_reset (queue)
        class(prt_queue_t), intent(inout) :: queue
        queue%current_prt => queue%front
    end subroutine prt_queue_reset

```

```

<radiation generator: prt queue: TBP>+≡
    procedure :: check_for_same_prt_strings => prt_queue_check_for_same_prt_strings

```

```

<radiation generator: procedures>+≡
    function prt_queue_check_for_same_prt_strings (queue) result (val)
        class(prt_queue_t), intent(inout) :: queue
        logical :: val
        type(string_t), dimension(:), allocatable :: prt_string
        integer, dimension(:,:), allocatable :: i_particle
        integer :: n_d, n_dbar, n_u, n_ubar, n_s, n_sbar, n_gl, n_e, n_ep, n_mu, n_mup, n_A
        integer :: i, j
        call queue%reset ()
        allocate (i_particle (queue%n_lists, 12))
        do i = 1, queue%n_lists
            call queue%get (prt_string)
            n_d = count_particle (prt_string, 1)
            n_dbar = count_particle (prt_string, -1)
            n_u = count_particle (prt_string, 2)
            n_ubar = count_particle (prt_string, -2)
            n_s = count_particle (prt_string, 3)
            n_sbar = count_particle (prt_string, -3)
            n_gl = count_particle (prt_string, 21)

```

```

n_e = count_particle (prt_string, 11)
n_ep = count_particle (prt_string, -11)
n_mu = count_particle (prt_string, 13)
n_mup = count_particle (prt_string, -13)
n_A = count_particle (prt_string, 22)
i_particle (i, 1) = n_d
i_particle (i, 2) = n_dbar
i_particle (i, 3) = n_u
i_particle (i, 4) = n_ubar
i_particle (i, 5) = n_s
i_particle (i, 6) = n_sbar
i_particle (i, 7) = n_gl
i_particle (i, 8) = n_e
i_particle (i, 9) = n_ep
i_particle (i, 10) = n_mu
i_particle (i, 11) = n_mup
i_particle (i, 12) = n_A
end do
val = .false.
do i = 1, queue%n_lists
  do j = 1, queue%n_lists
    if (i == j) cycle
    val = val .or. all (i_particle (i,:) == i_particle(j,:))
  end do
end do
contains
function count_particle (prt_string, pdg) result (n)
  type(string_t), dimension(:), intent(in) :: prt_string
  integer, intent(in) :: pdg
  integer :: n
  integer :: i
  type(string_t) :: prt_ref
  n = 0
  select case (pdg)
  case (1)
    prt_ref = "d"
  case (-1)
    prt_ref = "dbar"
  case (2)
    prt_ref = "u"
  case (-2)
    prt_ref = "ubar"
  case (3)
    prt_ref = "s"
  case (-3)
    prt_ref = "sbar"
  case (21)
    prt_ref = "gl"
  case (11)
    prt_ref = "e-"
  case (-11)
    prt_ref = "e+"
  case (13)
    prt_ref = "mu-"

```

```

        case (-13)
            prt_ref = "mu+"
        case (22)
            prt_ref = "A"
        end select
        do i = 1, size (prt_string)
            if (prt_string(i) == prt_ref) n = n+1
        end do
    end function count_particle

end function prt_queue_check_for_same_prt_strings

<radiation generator: prt queue: TBP>+≡
    procedure :: contains => prt_queue_contains

<radiation generator: procedures>+≡
    function prt_queue_contains (queue, prt_string) result (val)
        class(prt_queue_t), intent(in) :: queue
        type(string_t), intent(in), dimension(:) :: prt_string
        logical :: val
        type(prt_queue_t), pointer :: current => null()
        if (associated (queue%front)) then
            current => queue%front
        else
            call msg_fatal ("Trying to access empty particle queue")
        end if
        val = .false.
        do
            if (size (current%prt_string) == size (prt_string)) then
                if (all (current%prt_string == prt_string)) then
                    val = .true.
                    exit
                end if
            end if
            if (associated (current%next)) then
                current => current%next
            else
                exit
            end if
        end do
    end function prt_queue_contains

<radiation generator: prt queue: TBP>+≡
    procedure :: write => prt_queue_write

<radiation generator: procedures>+≡
    subroutine prt_queue_write (queue, unit)
        class(prt_queue_t), intent(in) :: queue
        integer, optional :: unit
        type(prt_queue_t), pointer :: current => null ()
        integer :: i, j, u
        u = given_output_unit (unit)
        if (associated (queue%front)) then
            current => queue%front

```

```

else
  write (u, "(A)") "[Particle queue is empty]"
  return
end if
j = 1
do
  write (u, "(I2,A,1X)", advance = 'no') j , ":"
  do i = 1, size (current%prt_string)
    write (u, "(A,1X)", advance = 'no') char (current%prt_string(i))
  end do
  write (u, "(A)")
  if (associated (current%next)) then
    current => current%next
    j = j+1
  else
    exit
  end if
end do
end subroutine prt_queue_write

```

(radiation generator: procedures)+≡

```

subroutine sort_prt (prt, model)
  type(string_t), dimension(:), intent(inout) :: prt
  class(model_data_t), intent(in), target :: model
  type(pdg_array_t), dimension(:), allocatable :: pdg
  type(flavor_t) :: flv
  integer :: i
  call create_pdg_array (prt, model, pdg)
  call sort_pdg (pdg)
  do i = 1, size (pdg)
    call flv%init (pdg(i)%get(), model)
    prt(i) = flv%get_name ()
  end do
end subroutine sort_prt

subroutine sort_pdg (pdg)
  type(pdg_array_t), dimension(:), intent(inout) :: pdg
  integer, dimension(:), allocatable :: i_pdg
  integer :: i
  allocate (i_pdg (size (pdg)))
  do i = 1, size (pdg)
    i_pdg(i) = pdg(i)%get ()
  end do
  i_pdg = sort_abs (i_pdg)
  do i = 1, size (pdg)
    call pdg(i)%set (1, i_pdg(i))
  end do
end subroutine sort_pdg

subroutine create_pdg_array (prt, model, pdg)
  type (string_t), dimension(:), intent(in) :: prt
  class (model_data_t), intent(in), target :: model
  type(pdg_array_t), dimension(:), allocatable, intent(out) :: pdg
  type(flavor_t) :: flv

```



```

integer :: i
allocate (pdg (size (prt)))
do i = 1, size (prt)
    call flv%init (prt(i), model)
    pdg(i) = flv%get_pdg ()
end do
end subroutine create_pdg_array

```

This is used in unit tests:

```

<radiation generator: test auxiliary>≡
subroutine write_pdg_array (pdg, u)
    use pdg_arrays
    type(pdg_array_t), dimension(:), intent(in) :: pdg
    integer, intent(in) :: u
    integer :: i
    do i = 1, size (pdg)
        call pdg(i)%write (u)
    end do
    write (u, "(A)")
end subroutine write_pdg_array

subroutine write_particle_string (prt, u)
    <Use strings>
    type(string_t), dimension(:), intent(in) :: prt
    integer, intent(in) :: u
    integer :: i
    do i = 1, size (prt)
        write (u, "(A,1X)", advance = "no") char (prt(i))
    end do
    write (u, "(A)")
end subroutine write_particle_string

<radiation generator: types>+≡
type :: reshuffle_list_t
    integer, dimension(:), allocatable :: ii
    type(reshuffle_list_t), pointer :: next => null ()
contains
    <radiation generator: reshuffle list: TBP>
end type reshuffle_list_t

```

```

<radiation generator: reshuffle list: TBP>≡
procedure :: write => reshuffle_list_write

<radiation generator: procedures>+≡
subroutine reshuffle_list_write (rlist)
    class(reshuffle_list_t), intent(in) :: rlist
    type(reshuffle_list_t), pointer :: current => null ()
    integer :: i
    print *, 'Content of reshuffling list: '
    if (associated (rlist%next)) then
        current => rlist%next
        i = 1
        do

```

```

        print *, 'i: ', i, 'list: ', current%ii
        i = i + 1
        if (associated (current%next)) then
            current => current%next
        else
            exit
        end if
    end do
else
    print *, '[EMPTY]'
end if
end subroutine reshuffle_list_write

```

<radiation generator: reshuffle list: TBP>+≡

```

    procedure :: append => reshuffle_list_append

```

<radiation generator: procedures>+≡

```

    subroutine reshuffle_list_append (rlist, ii)
        class(reshuffle_list_t), intent(inout) :: rlist
        integer, dimension(:), allocatable, intent(in) :: ii
        type(reshuffle_list_t), pointer :: current
        if (associated (rlist%next)) then
            current => rlist%next
        do
            if (associated (current%next)) then
                current => current%next
            else
                allocate (current%next)
                allocate (current%next%ii (size (ii)))
                current%next%ii = ii
                exit
            end if
        end do
    else
        allocate (rlist%next)
        allocate (rlist%next%ii (size (ii)))
        rlist%next%ii = ii
    end if
end subroutine reshuffle_list_append

```

<radiation generator: reshuffle list: TBP>+≡

```

    procedure :: is_empty => reshuffle_list_is_empty

```

<radiation generator: procedures>+≡

```

    elemental function reshuffle_list_is_empty (rlist) result (is_empty)
        logical :: is_empty
        class(reshuffle_list_t), intent(in) :: rlist
        is_empty = .not. associated (rlist%next)
    end function reshuffle_list_is_empty

```

<radiation generator: reshuffle list: TBP>+≡

```

    procedure :: get => reshuffle_list_get

```

```

<radiation generator: procedures>+≡
function reshuffle_list_get (rlist, index) result (ii)
  integer, dimension(:), allocatable :: ii
  class(reshuffle_list_t), intent(inout) :: rlist
  integer, intent(in) :: index
  type(reshuffle_list_t), pointer :: current => null ()
  integer :: i
  current => rlist%next
  do i = 1, index - 1
    if (associated (current%next)) then
      current => current%next
    else
      call msg_fatal ("Index exceeds size of reshuffling list")
    end if
  end do
  allocate (ii (size (current%ii)))
  ii = current%ii
end function reshuffle_list_get

```

We need to reset the `reshuffle_list` in order to deal with subsequent usages of the `radiation_generator`. Below is obviously the lazy and dirty solution. Otherwise, we would have to equip this auxiliary type with additional information about `last` and `previous` pointers. Considering that at most n_{legs} integers are saved in the lists, and that the subroutine is only called during the initialization phase (more precisely: at the moment only in the `radiation_generator` unit tests), I think this quick fix is justified.

```

<radiation generator: reshuffle list: TBP>+≡
procedure :: reset => reshuffle_list_reset

<radiation generator: procedures>+≡
subroutine reshuffle_list_reset (rlist)
  class(reshuffle_list_t), intent(inout) :: rlist
  rlist%next => null ()
end subroutine reshuffle_list_reset

<radiation generator: public>≡
public :: radiation_generator_t

<radiation generator: types>+≡
type :: radiation_generator_t
  logical :: qcd_enabled = .false.
  logical :: qed_enabled = .false.
  logical :: is_gluon = .false.
  logical :: fs_gluon = .false.
  logical :: is_photon = .false.
  logical :: fs_photon = .false.
  logical :: only_final_state = .true.
  type(pdg_list_t) :: pl_in, pl_out
  type(pdg_list_t) :: pl_excluded_gauge_splittings
  type(split_constraints_t) :: constraints
  integer :: n_tot
  integer :: n_in, n_out
  integer :: n_loops

```

```

integer :: n_light_quarks
real(default) :: mass_sum
type(prt_queue_t) :: prt_queue
type(pdg_states_t) :: pdg_raw
type(pdg_array_t), dimension(:), allocatable :: pdg_in_born, pdg_out_born
type(if_table_t) :: if_table
type(reshuffle_list_t) :: reshuffle_list
contains
<radiation generator: radiation generator: TBP>
end type radiation_generator_t

```

<radiation generator: radiation generator: TBP>≡

```

generic :: init => init_pdg_list, init_pdg_array
procedure :: init_pdg_list => radiation_generator_init_pdg_list
procedure :: init_pdg_array => radiation_generator_init_pdg_array

```

<radiation generator: procedures>+≡

```

subroutine radiation_generator_init_pdg_list &
  (generator, pl_in, pl_out, pl_excluded_gaugeSplittings, qcd, qed)
class(radiation_generator_t), intent(inout) :: generator
type(pdg_list_t), intent(in) :: pl_in, pl_out
type(pdg_list_t), intent(in) :: pl_excluded_gaugeSplittings
logical, intent(in), optional :: qcd, qed
if (present (qcd)) generator%qcd_enabled = qcd
if (present (qed)) generator%qed_enabled = qed
generator%pl_in = pl_in
generator%pl_out = pl_out
generator%pl_excluded_gaugeSplittings = pl_excluded_gaugeSplittings
generator%is_gluon = pl_in%search_for_particle (GLUON)
generator%fs_gluon = pl_out%search_for_particle (GLUON)
generator%is_photon = pl_in%search_for_particle (PHOTON)
generator%fs_photon = pl_out%search_for_particle (PHOTON)
generator%mass_sum = 0._default
call generator%pdg_raw%init ()
end subroutine radiation_generator_init_pdg_list

subroutine radiation_generator_init_pdg_array &
  (generator, pdg_in, pdg_out, pdg_excluded_gaugeSplittings, qcd, qed)
class(radiation_generator_t), intent(inout) :: generator
type(pdg_array_t), intent(in), dimension(:) :: pdg_in, pdg_out
type(pdg_array_t), intent(in), dimension(:) :: pdg_excluded_gaugeSplittings
logical, intent(in), optional :: qcd, qed
type(pdg_list_t) :: pl_in, pl_out
type(pdg_list_t) :: pl_excluded_gaugeSplittings
integer :: i
call pl_in%init(size (pdg_in))
call pl_out%init(size (pdg_out))
do i = 1, size (pdg_in)
  call pl_in%set (i, pdg_in(i))
end do
do i = 1, size (pdg_out)
  call pl_out%set (i, pdg_out(i))
end do
call pl_excluded_gaugeSplittings%init(size (pdg_excluded_gaugeSplittings))

```

```

do i = 1, size (pdg_excluded_gaugeSplittings)
  call pl_excluded_gaugeSplittings%set &
    (i, pdg_excluded_gaugeSplittings(i))
end do
call generator%init (pl_in, pl_out, pl_excluded_gaugeSplittings, qcd, qed)
end subroutine radiation_generator_init_pdg_array

<radiation generator: radiation generator: TBP>+≡
  procedure :: set_initial_state_emissions => &
    radiation_generator_set_initial_state_emissions

<radiation generator: procedures>+≡
  subroutine radiation_generator_set_initial_state_emissions (generator)
    class(radiation_generator_t), intent(inout) :: generator
    generator%only_final_state = .false.
  end subroutine radiation_generator_set_initial_state_emissions

<radiation generator: radiation generator: TBP>+≡
  procedure :: setup_if_table => radiation_generator_setup_if_table

<radiation generator: procedures>+≡
  subroutine radiation_generator_setup_if_table (generator, model)
    class(radiation_generator_t), intent(inout) :: generator
    class(model_data_t), intent(in), target :: model
    type(pdg_list_t), dimension(:), allocatable :: pl_in, pl_out

    allocate (pl_in(1), pl_out(1))

    pl_in(1) = generator%pl_in
    pl_out(1) = generator%pl_out

    call generator%if_table%init &
      (model, pl_in, pl_out, generator%constraints)
  end subroutine radiation_generator_setup_if_table

<radiation generator: radiation generator: TBP>+≡
  generic :: reset_particle_content => reset_particle_content_pdg_array, &
    reset_particle_content_pdg_list

  procedure :: reset_particle_content_pdg_list => &
    radiation_generator_reset_particle_content_pdg_list
  procedure :: reset_particle_content_pdg_array => &
    radiation_generator_reset_particle_content_pdg_array

<radiation generator: procedures>+≡
  subroutine radiation_generator_reset_particle_content_pdg_list (generator, pl)
    class(radiation_generator_t), intent(inout) :: generator
    type(pdg_list_t), intent(in) :: pl
    generator%pl_out = pl
    generator%fs_gluon = pl%search_for_particle (GLUON)
    generator%fs_photon = pl%search_for_particle (PHOTON)
  end subroutine radiation_generator_reset_particle_content_pdg_list

  subroutine radiation_generator_reset_particle_content_pdg_array (generator, pdg)
    class(radiation_generator_t), intent(inout) :: generator

```

```

type(pdg_array_t), intent(in), dimension(:) :: pdg
type(pdg_list_t) :: pl
integer :: i
call pl%init (size (pdg))
do i = 1, size (pdg)
    call pl%set (i, pdg(i))
end do
call generator%reset_particle_content (pl)
end subroutine radiation_generator_reset_particle_content_pdg_array

<radiation generator: radiation generator: TBP>+≡
    procedure :: reset_resuffle_list=> radiation_generator_reset_resuffle_list

<radiation generator: procedures>+≡
    subroutine radiation_generator_reset_resuffle_list (generator)
        class(radiation_generator_t), intent(inout) :: generator
        call generator%reshuffle_list%reset ()
    end subroutine radiation_generator_reset_resuffle_list

<radiation generator: radiation generator: TBP>+≡
    procedure :: set_n => radiation_generator_set_n

<radiation generator: procedures>+≡
    subroutine radiation_generator_set_n (generator, n_in, n_out, n_loops)
        class(radiation_generator_t), intent(inout) :: generator
        integer, intent(in) :: n_in, n_out, n_loops
        generator%n_tot = n_in + n_out + 1
        generator%n_in = n_in
        generator%n_out = n_out
        generator%n_loops = n_loops
    end subroutine radiation_generator_set_n

<radiation generator: radiation generator: TBP>+≡
    procedure :: set_constraints => radiation_generator_set_constraints

<radiation generator: procedures>+≡
    subroutine radiation_generator_set_constraints &
        (generator, set_n_loop, set_mass_sum, &
        set_selected_particles, set_required_particles)
        class(radiation_generator_t), intent(inout), target :: generator
        logical, intent(in) :: set_n_loop
        logical, intent(in) :: set_mass_sum
        logical, intent(in) :: set_selected_particles
        logical, intent(in) :: set_required_particles
        logical :: set_no_photon_induced = .true.
        integer :: i, j, n, n_constraints
        type(pdg_list_t) :: pl_req, pl_insert
        type(pdg_list_t) :: pl_antiparticles
        type(pdg_array_t) :: pdg_gluon, pdg_photon
        type(pdg_array_t) :: pdg_add, pdg_tmp
        integer :: last_index
        integer :: n_new_particles, n_skip
        integer, dimension(:), allocatable :: i_skip
        integer :: n_nlo_correction_types

```

```

n_nlo_correction_types = count ([generator%qcd_enabled, generator%qed_enabled])
if (generator%is_photon) set_no_photon_induced = .false.

allocate (i_skip (generator%n_tot))
i_skip = -1

n_constraints = 2 + count([set_n_loop, set_mass_sum, &
    set_selected_particles, set_required_particles, set_no_photon_induced])
associate (constraints => generator%constraints)
  n = 1
  call constraints%init (n_constraints)
  call constraints%set (n, constrain_n_tot (generator%n_tot))
  n = 2
  call constraints%set (n, constrain_couplings (generator%qcd_enabled, &
    generator%qed_enabled, n_nlo_correction_types))
  n = n + 1
  if (set_no_photon_induced) then
    call constraints%set (n, constrain_photon_induced_processes (generator%n_in))
    n = n + 1
  end if
  if (set_n_loop) then
    call constraints%set (n, constrain_n_loop(generator%n_loops))
    n = n + 1
  end if
  if (set_mass_sum) then
    call constraints%set (n, constrain_mass_sum(generator%mass_sum))
    n = n + 1
  end if
  if (set_required_particles) then
    if (generator%fs_gluon .or. generator%fs_photon) then
      do i = 1, generator%n_out
        pdg_tmp = generator%pl_out%get(i)
        if (pdg_tmp%search_for_particle (GLUON) &
            .or. pdg_tmp%search_for_particle (PHOTON)) then
          i_skip(i) = i
        end if
      end do

      n_skip = count (i_skip > 0)
      call pl_req%init (generator%n_out-n_skip)
    else
      call pl_req%init (generator%n_out)
    end if
    j = 1
    do i = 1, generator%n_out
      if (any (i == i_skip)) cycle
      call pl_req%set (j, generator%pl_out%get(i))
      j = j + 1
    end do
    call constraints%set (n, constrain_require (pl_req))
    n = n + 1
  end if
  if (set_selected_particles) then

```

```

if (generator%only_final_state ) then
  call pl_insert%init (generator%n_out + n_nlo_correction_types)
  do i = 1, generator%n_out
    call pl_insert%set(i, generator%pl_out%get(i))
  end do
  last_index = generator%n_out + 1
else
  call generator%pl_in%create_antiparticles (pl_antiparticles, n_new_particles)
  call pl_insert%init (generator%n_tot + n_new_particles &
    + n_nlo_correction_types)
  do i = 1, generator%n_in
    call pl_insert%set(i, generator%pl_in%get(i))
  end do
  do i = 1, generator%n_out
    j = i + generator%n_in
    call pl_insert%set(j, generator%pl_out%get(i))
  end do
  do i = 1, n_new_particles
    j = i + generator%n_in + generator%n_out
    call pl_insert%set(j, pl_antiparticles%get(i))
  end do
  last_index = generator%n_tot + n_new_particles + 1
end if
pdg_gluon = GLUON; pdg_photon = PHOTON
if (generator%qcd_enabled) then
  pdg_add = pdg_gluon
  call pl_insert%set (last_index, pdg_add)
  last_index = last_index + 1
end if
if (generator%qed_enabled) then
  pdg_add = pdg_photon
  call pl_insert%set (last_index, pdg_add)
end if
call constraints%set (n, constrainSplittings (pl_insert, &
  generator%pl_excluded_gaugeSplittings))
end if
end associate
end subroutine radiation_generator_set_constraints

```

(radiation generator: radiation generator: TBP)+≡

```

procedure :: findSplittings => radiation_generator_findSplittings

```

(radiation generator: procedures)+≡

```

subroutine radiation_generator_findSplittings (generator)
  class(radiation_generator_t), intent(inout) :: generator
  integer :: i
  type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out, pdg_tmp
  integer, dimension(:), allocatable :: reshuffle_list

  call generator%pl_in%create_pdg_array (pdg_in)
  call generator%pl_out%create_pdg_array (pdg_out)

  associate (if_table => generator%if_table)
    call if_table%radiate (generator%constraints, do_not_check_regular = .true.)
  end associate

```



```

do i = 1, if_table%get_length ()
  call if_table%get_pdg_out (i, pdg_tmp)
  if (size (pdg_tmp) == generator%n_tot) then
    call pdg_reshuffle (pdg_out, pdg_tmp, reshuffle_list)
    call generator%reshuffle_list%append (reshuffle_list)
  end if
end do
end associate

```

contains

```

subroutine pdg_reshuffle (pdg_born, pdg_real, list)
  type(pdg_array_t), intent(in), dimension(:) :: pdg_born, pdg_real
  integer, intent(out), dimension(:), allocatable :: list
  type(pdg_sorter_t), dimension(:), allocatable :: sort_born
  type(pdg_sorter_t), dimension(:), allocatable :: sort_real
  integer :: i_min, n_in, n_born, n_real
  integer :: ib, ir

  n_in = generator%n_in
  n_born = size (pdg_born)
  n_real = size (pdg_real)
  allocate (list (n_real - n_in))
  allocate (sort_born (n_born))
  allocate (sort_real (n_real - n_in))
  sort_born%pdg = pdg_born%get ()
  sort_real%pdg = pdg_real(n_in + 1 : n_real)%get()
  do ib = 1, n_born
    if (any (sort_born(ib)%pdg == sort_real%pdg)) &
      call associate_born_indices (sort_born(ib), sort_real, ib, n_real)
  end do
  i_min = maxval (sort_real%associated_born) + 1
  do ir = 1, n_real - n_in
    if (sort_real(ir)%associated_born == 0) then
      sort_real(ir)%associated_born = i_min
      i_min = i_min + 1
    end if
  end do
  list = sort_real%associated_born
end subroutine pdg_reshuffle

```

```

subroutine associate_born_indices (sort_born, sort_real, ib, n_real)
  type(pdg_sorter_t), intent(in) :: sort_born
  type(pdg_sorter_t), intent(inout), dimension(:) :: sort_real
  integer, intent(in) :: ib, n_real
  integer :: ir
  do ir = 1, n_real - generator%n_in
    if (sort_born%pdg == sort_real(ir)%pdg &
      .and..not. sort_real(ir)%checked) then
      sort_real(ir)%associated_born = ib
      sort_real(ir)%checked = .true.
    exit
  end if

```

```

        end do
    end subroutine associate_born_indices
end subroutine radiation_generator_findSplittings

```

(radiation generator: radiation generator: TBP)+≡

```

    procedure :: generate_real_particle_strings &
        => radiation_generator_generate_real_particle_strings

```

(radiation generator: procedures)+≡

```

    subroutine radiation_generator_generate_real_particle_strings &
        (generator, prt_tot_in, prt_tot_out)
    type :: prt_array_t
        type(string_t), dimension(:), allocatable :: prt
    end type
    class(radiation_generator_t), intent(inout) :: generator
    type(string_t), intent(out), dimension(:), allocatable :: prt_tot_in, prt_tot_out
    type(prt_array_t), dimension(:), allocatable :: prt_in, prt_out
    type(prt_array_t), dimension(:), allocatable :: prt_out0, prt_in0
    type(pdg_array_t), dimension(:), allocatable :: pdg_tmp, pdg_out, pdg_in
    type(pdg_list_t), dimension(:), allocatable :: pl_in, pl_out
    type(prt_array_t) :: prt_out0_tmp, prt_in0_tmp
    integer :: i, j
    integer, dimension(:), allocatable :: reshuffle_list_local
    type(reshuffle_list_t) :: reshuffle_list
    integer :: flv
    type(string_t), dimension(:), allocatable :: buf
    integer :: i_buf

    flv = 0
    allocate (prt_in0(0), prt_out0(0))
    associate (if_table => generator%if_table)
        do i = 1, if_table%get_length ()
            call if_table%get_pdg_out (i, pdg_tmp)
            if (size (pdg_tmp) == generator%n_tot) then
                call if_table%get_particle_string (i, &
                    prt_in0_tmp%prt, prt_out0_tmp%prt)
                prt_in0 = [prt_in0, prt_in0_tmp]
                prt_out0 = [prt_out0, prt_out0_tmp]
                flv = flv + 1
            end if
        end do
    end associate

    allocate (prt_in(size (prt_in0)), prt_out(size (prt_out0)))
    do i = 1, flv
        allocate (prt_in(i)%prt (generator%n_in))
        allocate (prt_out(i)%prt (generator%n_tot - generator%n_in))
    end do
    allocate (prt_tot_in (generator%n_in))
    allocate (prt_tot_out (generator%n_tot - generator%n_in))
    allocate (buf (generator%n_tot))
    buf = ""

    do j = 1, flv

```

```

do i = 1, generator%n_in
  prt_in(j)%prt(i) = prt_in0(j)%prt(i)
  call fill_buffer (buf(i), prt_in0(j)%prt(i))
end do
end do
prt_tot_in = buf(1 : generator%n_in)

do j = 1, flv
  allocate (reshuffle_list_local (size (generator%reshuffle_list%get(j))))
  reshuffle_list_local = generator%reshuffle_list%get(j)
  do i = 1, size (reshuffle_list_local)
    prt_out(j)%prt(reshuffle_list_local(i)) = prt_out0(j)%prt(i)
    i_buf = reshuffle_list_local(i) + generator%n_in
    call fill_buffer (buf(i_buf), &
      prt_out(j)%prt(reshuffle_list_local(i)))
  end do
  !!! Need to deallocate here because in the next iteration the reshuffling
  !!! list can have a different size
  deallocate (reshuffle_list_local)
end do
prt_tot_out = buf(generator%n_in + 1 : generator%n_tot)
if (debug2_active (D_CORE)) then
  print *, 'Generated initial state: '
  do i = 1, size (prt_tot_in)
    print *, char (prt_tot_in(i))
  end do
  print *, 'Generated final state: '
  do i = 1, size (prt_tot_out)
    print *, char (prt_tot_out(i))
  end do
end if
end if

```

contains

```

subroutine fill_buffer (buffer, particle)
  type(string_t), intent(inout) :: buffer
  type(string_t), intent(in) :: particle
  logical :: particle_present
  if (len (buffer) > 0) then
    particle_present = check_for_substring (char(buffer), particle)
    if (.not. particle_present) buffer = buffer // ":" // particle
  else
    buffer = buffer // particle
  end if
end subroutine fill_buffer

function check_for_substring (buffer, substring) result (exist)
  character(len=*), intent(in) :: buffer
  type(string_t), intent(in) :: substring
  character(len=50) :: buffer_internal
  logical :: exist
  integer :: i_first, i_last
  exist = .false.

```

```

i_first = 1; i_last = 1
do
  if (buffer(i_last:i_last) == ".") then
    buffer_internal = buffer (i_first : i_last - 1)
    if (buffer_internal == char (substring)) then
      exist = .true.
      exit
    end if
    i_first = i_last + 1; i_last = i_first + 1
    if (i_last > len(buffer)) exit
  else if (i_last == len(buffer)) then
    buffer_internal = buffer (i_first : i_last)
    exist = buffer_internal == char (substring)
    exit
  else
    i_last = i_last + 1
    if (i_last > len(buffer)) exit
  end if
end do
end function check_for_substring
end subroutine radiation_generator_generate_real_particle_strings

```

```

<radiation generator: radiation generator: TBP>+≡
  procedure :: contains_emissions => radiation_generator_contains_emissions

```

```

<radiation generator: procedures>+≡
  function radiation_generator_contains_emissions (generator) result (has_em)
    logical :: has_em
    class(radiation_generator_t), intent(in) :: generator
    has_em = .not. generator%reshuffle_list%is_empty ()
  end function radiation_generator_contains_emissions

```

```

<radiation generator: radiation generator: TBP>+≡
  procedure :: generate => radiation_generator_generate

```

```

<radiation generator: procedures>+≡
  subroutine radiation_generator_generate (generator, prt_in, prt_out)
    class(radiation_generator_t), intent(inout) :: generator
    type(string_t), intent(out), dimension(:), allocatable :: prt_in, prt_out
    call generator%findSplittings ()
    call generator%generate_real_particle_strings (prt_in, prt_out)
  end subroutine radiation_generator_generate

```

```

<radiation generator: radiation generator: TBP>+≡
  procedure :: generate_multiple => radiation_generator_generate_multiple

```

```

<radiation generator: procedures>+≡
  subroutine radiation_generator_generate_multiple (generator, max_multiplicity, model)
    class(radiation_generator_t), intent(inout) :: generator
    integer, intent(in) :: max_multiplicity
    class(model_data_t), intent(in), target :: model
    if (max_multiplicity <= generator%n_out) &
      call msg_fatal ("GKS states: Multiplicity is not large enough!")
    call generator%first_emission (model)
  end subroutine radiation_generator_generate_multiple

```

```

        call generator%reset_resuffle_list ()
        if (max_multiplicity - generator%n_out > 1) &
            call generator%append_emissions (max_multiplicity, model)
    end subroutine radiation_generator_generate_multiple

<radiation generator: radiation generator: TBP>+≡
    procedure :: first_emission => radiation_generator_first_emission

<radiation generator: procedures>+≡
    subroutine radiation_generator_first_emission (generator, model)
        class(radiation_generator_t), intent(inout) :: generator
        class(model_data_t), intent(in), target :: model
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        call generator%setup_if_table (model)
        call generator%generate (prt_in, prt_out)
        call generator%prt_queue%null ()
        call generator%prt_queue%append (prt_out)
    end subroutine radiation_generator_first_emission

<radiation generator: radiation generator: TBP>+≡
    procedure :: append_emissions => radiation_generator_append_emissions

<radiation generator: procedures>+≡
    subroutine radiation_generator_append_emissions (generator, max_multiplicity, model)
        class(radiation_generator_t), intent(inout) :: generator
        integer, intent(in) :: max_multiplicity
        class(model_data_t), intent(in), target :: model
        type(string_t), dimension(:), allocatable :: prt_fetched
        type(string_t), dimension(:), allocatable :: prt_in
        type(string_t), dimension(:), allocatable :: prt_out
        type(pdg_array_t), dimension(:), allocatable :: pdg_new_out
        integer :: current_multiplicity, i, j, n_longest_length
        type :: prt_table_t
            type(string_t), dimension(:), allocatable :: prt
        end type prt_table_t
        type(prt_table_t), dimension(:), allocatable :: prt_table_out
    do
        call generator%prt_queue%get (prt_fetched)
        current_multiplicity = size (prt_fetched)
        if (current_multiplicity == max_multiplicity) exit
        call create_pdg_array (prt_fetched, model, &
            pdg_new_out)
        call generator%reset_particle_content (pdg_new_out)
        call generator%set_n (2, current_multiplicity, 0)
        call generator%set_constraints (.false., .false., .true., .true.)
        call generator%setup_if_table (model)
        call generator%generate (prt_in, prt_out)
        n_longest_length = get_length_of_longest_tuple (prt_out)
        call separate_particles (prt_out, prt_table_out)
        do i = 1, n_longest_length
            if (.not. any (prt_table_out(i)%prt == " ")) then
                call sort_prt (prt_table_out(i)%prt, model)
                if (.not. generator%prt_queue%contains (prt_table_out(i)%prt)) then
                    call generator%prt_queue%append (prt_table_out(i)%prt)
                end if
            end if
        end do
    end do

```

```

        end if
    end if
end do
    call generator%reset_resuffle_list ()
end do

contains
subroutine separate_particles (prt, prt_table)
    type(string_t), intent(in), dimension(:) :: prt
    type(string_t), dimension(:), allocatable :: prt_tmp
    type(prt_table_t), intent(out), dimension(:), allocatable :: prt_table
    integer :: i, j
    logical, dimension(:), allocatable :: tuples_occured
    allocate (prt_table (n_longest_length))
    do i = 1, n_longest_length
        allocate (prt_table(i)%prt (size (prt)))
    end do
    allocate (tuples_occured (size (prt)))
    do j = 1, size (prt)
        call split_string (prt(j), var_str (":"), prt_tmp)
        do i = 1, n_longest_length
            if (i <= size (prt_tmp)) then
                prt_table(i)%prt(j) = prt_tmp(i)
            else
                prt_table(i)%prt(j) = " "
            end if
        end do
        if (n_longest_length > 1) &
            tuples_occured(j) = prt_table(1)%prt(j) /= " " &
            .and. prt_table(2)%prt(j) /= " "
    end do
    if (any (tuples_occured)) then
        do j = 1, size (tuples_occured)
            if (.not. tuples_occured(j)) then
                do i = 2, n_longest_length
                    prt_table(i)%prt(j) = prt_table(1)%prt(j)
                end do
            end if
        end do
    end if
end subroutine separate_particles

function get_length_of_longest_tuple (prt) result (longest_length)
    type(string_t), intent(in), dimension(:) :: prt
    integer :: longest_length, i
    type(prt_table_t), dimension(:), allocatable :: prt_table
    allocate (prt_table (size (prt)))
    longest_length = 0
    do i = 1, size (prt)
        call split_string (prt(i), var_str (":"), prt_table(i)%prt)
        if (size (prt_table(i)%prt) > longest_length) &
            longest_length = size (prt_table(i)%prt)
    end do
end function get_length_of_longest_tuple

```

```

end subroutine radiation_generator_append_emissions

<radiation generator: radiation generator: TBP>+≡
  procedure :: reset_queue => radiation_generator_reset_queue

<radiation generator: procedures>+≡
  subroutine radiation_generator_reset_queue (generator)
    class(radiation_generator_t), intent(inout) :: generator
    call generator%prt_queue%reset ()
  end subroutine radiation_generator_reset_queue

<radiation generator: radiation generator: TBP>+≡
  procedure :: get_n_gks_states => radiation_generator_get_n_gks_states

<radiation generator: procedures>+≡
  function radiation_generator_get_n_gks_states (generator) result (n)
    class(radiation_generator_t), intent(in) :: generator
    integer :: n
    n = generator%prt_queue%n_lists
  end function radiation_generator_get_n_gks_states

<radiation generator: radiation generator: TBP>+≡
  procedure :: get_next_state => radiation_generator_get_next_state

<radiation generator: procedures>+≡
  function radiation_generator_get_next_state (generator) result (prt_string)
    class(radiation_generator_t), intent(inout) :: generator
    type(string_t), dimension(:), allocatable :: prt_string
    call generator%prt_queue%get (prt_string)
  end function radiation_generator_get_next_state

<radiation generator: radiation generator: TBP>+≡
  procedure :: get_emitter_indices => radiation_generator_get_emitter_indices

<radiation generator: procedures>+≡
  subroutine radiation_generator_get_emitter_indices (generator, indices)
    class(radiation_generator_t), intent(in) :: generator
    integer, dimension(:), allocatable, intent(out) :: indices
    type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
    integer, dimension(:), allocatable :: flv_in, flv_out
    integer, dimension(:), allocatable :: emitters
    integer :: i, j
    integer :: n_in, n_out

    call generator%pl_in%create_pdg_array (pdg_in)
    call generator%pl_out%create_pdg_array (pdg_out)

    n_in = size (pdg_in); n_out = size (pdg_out)
    allocate (flv_in (n_in), flv_out (n_out))
    forall (i=1:n_in) flv_in(i) = pdg_in(i)%get()
    forall (i=1:n_out) flv_out(i) = pdg_out(i)%get()

    call generator%if_table%get_emitters (generator%constraints, emitters)
    allocate (indices (size (emitters)))

```

```

j = 1
do i = 1, n_in + n_out
  if (i <= n_in) then
    if (any (flv_in(i) == emitters)) then
      indices (j) = i
      j = j + 1
    end if
  else
    if (any (flv_out(i-n_in) == emitters)) then
      indices (j) = i
      j = j + 1
    end if
  end if
end do
end subroutine radiation_generator_get_emitter_indices

```

<radiation generator: radiation generator: TBP>+≡

```

procedure :: get_raw_states => radiation_generator_get_raw_states

```

<radiation generator: procedures>+≡

```

function radiation_generator_get_raw_states (generator) result (raw_states)
  class(radiation_generator_t), intent(in), target :: generator
  integer, dimension(:,:), allocatable :: raw_states
  type(pdg_states_t), pointer :: state
  integer :: n_states, n_particles
  integer :: i_state
  integer :: j
  state => generator%pdg_raw
  n_states = generator%pdg_raw%get_n_states ()
  n_particles = size (generator%pdg_raw%pdg)
  allocate (raw_states (n_particles, n_states))
  do i_state = 1, n_states
    do j = 1, n_particles
      raw_states (j, i_state) = state%pdg(j)%get ()
    end do
    state => state%next
  end do
end function radiation_generator_get_raw_states

```

<radiation generator: radiation generator: TBP>+≡

```

procedure :: save_born_raw => radiation_generator_save_born_raw

```

<radiation generator: procedures>+≡

```

subroutine radiation_generator_save_born_raw (generator, pdg_in, pdg_out)
  class(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), dimension(:), allocatable, intent(in) :: pdg_in, pdg_out
  generator%pdg_in_born = pdg_in
  generator%pdg_out_born = pdg_out
end subroutine radiation_generator_save_born_raw

```

<radiation generator: radiation generator: TBP>+≡

```

procedure :: get_born_raw => radiation_generator_get_born_raw

```



```

<radiation generator: procedures>+≡
function radiation_generator_get_born_raw (generator) result (flv_born)
  class(radiation_generator_t), intent(in) :: generator
  integer, dimension(:,,:), allocatable :: flv_born
  integer :: i_part, n_particles
  n_particles = size (generator%pdg_in_born) + size (generator%pdg_out_born)
  allocate (flv_born (n_particles, 1))
  flv_born(1,1) = generator%pdg_in_born(1)%get ()
  flv_born(2,1) = generator%pdg_in_born(2)%get ()
  do i_part = 3, n_particles
    flv_born(i_part, 1) = generator%pdg_out_born(i_part-2)%get ()
  end do
end function radiation_generator_get_born_raw

```

28.2.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<radiation_generator_ut.f90>≡
<File header>

module radiation_generator_ut
  use unit_tests
  use radiation_generator_util

  <Standard module head>

  <radiation generator: public test>

contains

  <radiation generator: test driver>

end module radiation_generator_ut

<radiation_generator_util.f90>≡
<File header>

module radiation_generator_util

  <Use strings>
  use format_utils, only: write_separator
  use os_interface
  use pdg_arrays
  use models
  use kinds, only: default

  use radiation_generator

  <Standard module head>

  <radiation generator: test declarations>

contains

```

<radiation generator: tests>

<radiation generator: test auxiliary>

end module radiation_generator_util

API: driver for the unit tests below.

<radiation generator: public test>≡

public :: radiation_generator_test

<radiation generator: test driver>≡

```
subroutine radiation_generator_test (u, results)
  integer, intent(in) :: u
  type(test_results_t), intent(inout) :: results
  call test(radiation_generator_1, "radiation_generator_1", &
    "Test the generator of N+1-particle flavor structures in QCD", &
    u, results)
  call test(radiation_generator_2, "radiation_generator_2", &
    "Test multiple splittings in QCD", &
    u, results)
  call test(radiation_generator_3, "radiation_generator_3", &
    "Test the generator of N+1-particle flavor structures in QED", &
    u, results)
  call test(radiation_generator_4, "radiation_generator_4", &
    "Test multiple splittings in QED", &
    u, results)
end subroutine radiation_generator_test
```

<radiation generator: test declarations>≡

public :: radiation_generator_1

<radiation generator: tests>≡

```
subroutine radiation_generator_1 (u)
  integer, intent(in) :: u
  type(radiation_generator_t) :: generator
  type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
  type(os_data_t) :: os_data
  type(model_list_t) :: model_list
  type(model_t), pointer :: model => null ()

  write (u, "(A)") "* Test output: radiation_generator_1"
  write (u, "(A)") "* Purpose: Create N+1-particle flavor structures &
    &from predefined N-particle flavor structures"
  write (u, "(A)") "* One additional strong coupling, no additional electroweak coupling"
  write (u, "(A)")
  write (u, "(A)") "* Loading radiation model: SM.mdl"

  call syntax_model_file_init ()
  call os_data%init ()
  call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
    os_data, model)
  write (u, "(A)") "* Success"
```

```

allocate (pdg_in (2))
pdg_in(1) = 11; pdg_in(2) = -11

write (u, "(A)") "* Start checking processes"
call write_separator (u)

write (u, "(A)") "* Process 1: Top pair-production with additional gluon"
allocate (pdg_out(3))
pdg_out(1) = 6; pdg_out(2) = -6; pdg_out(3) = 21
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 2: Top pair-production with additional jet"
allocate (pdg_out(3))
pdg_out(1) = 6; pdg_out(2) = -6; pdg_out(3) = [-1,1,-2,2,-3,3,-4,4,-5,5,21]
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 3: Quark-antiquark production"
allocate (pdg_out(2))
pdg_out(1) = 2; pdg_out(2) = -2
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 4: Quark-antiquark production with additional gluon"
allocate (pdg_out(3))
pdg_out(1) = 2; pdg_out(2) = -2; pdg_out(3) = 21
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 5: Z + jets"
allocate (pdg_out(3))
pdg_out(1) = 2; pdg_out(2) = -2; pdg_out(3) = 23
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 6: Top Decay"
allocate (pdg_out(4))
pdg_out(1) = 24; pdg_out(2) = -24
pdg_out(3) = 5; pdg_out(4) = -5
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 7: Production of four quarks"
allocate (pdg_out(4))
pdg_out(1) = 2; pdg_out(2) = -2;
pdg_out(3) = 2; pdg_out(4) = -2
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 8: Drell-Yan lepto-production"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = 2; pdg_in(2) = -2
pdg_out(1) = 11; pdg_out(2) = -11

```

```

call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 9: WZ production at hadron-colliders"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = 1; pdg_in(2) = -2
pdg_out(1) = -24; pdg_out(2) = 23
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

contains

subroutine test_process (generator, pdg_in, pdg_out, u, include_initial_state)
  type(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), dimension(:), intent(in) :: pdg_in, pdg_out
  integer, intent(in) :: u
  logical, intent(in), optional :: include_initial_state
  type(string_t), dimension(:), allocatable :: prt_strings_in
  type(string_t), dimension(:), allocatable :: prt_strings_out
  type(pdg_array_t), dimension(10) :: pdg_excluded
  logical :: yorn
  yorn = .false.
  pdg_excluded = [-4, 4, 5, -5, 6, -6, 13, -13, 15, -15]
  if (present (include_initial_state)) yorn = include_initial_state
  write (u, "(A)") "* Leading order: "
  write (u, "(A)", advance = 'no') '* Incoming: '
  call write_pdg_array (pdg_in, u)
  write (u, "(A)", advance = 'no') '* Outgoing: '
  call write_pdg_array (pdg_out, u)

  call generator%init (pdg_in, pdg_out, &
    pdg_excluded_gaugeSplittings = pdg_excluded, qed = .true., qed = .false.)
  call generator%set_n (2, size(pdg_out), 0)
  if (yorn) call generator%set_initial_state_emissions ()
  call generator%set_constraints (.false., .false., .true., .true.)
  call generator%setup_if_table (model)
  call generator%generate (prt_strings_in, prt_strings_out)
  write (u, "(A)") "* Additional radiation: "
  write (u, "(A)") "* Incoming: "
  call write_particle_string (prt_strings_in, u)
  write (u, "(A)") "* Outgoing: "
  call write_particle_string (prt_strings_out, u)
  call write_separator(u)
  call generator%reset_resuffle_list ()
end subroutine test_process

end subroutine radiation_generator_1

<radiation generator: test declarations>+≡
public :: radiation_generator_2

<radiation generator: tests>+≡
subroutine radiation_generator_2 (u)
  integer, intent(in) :: u
  type(radiation_generator_t) :: generator

```

```

type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
type(pdg_array_t), dimension(:), allocatable :: pdg_excluded
type(os_data_t) :: os_data
type(model_list_t) :: model_list
type(model_t), pointer :: model => null ()
integer, parameter :: max_multiplicity = 10
type(string_t), dimension(:), allocatable :: prt_last

write (u, "(A)") "* Test output: radiation_generator_2"
write (u, "(A)") "* Purpose: Test the repeated application of &
    &a radiation generator splitting in QCD"
write (u, "(A)") "* Only Final state emissions! "
write (u, "(A)")
write (u, "(A)") "* Loading radiation model: SM.mdl"

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
    os_data, model)
write (u, "(A)") "* Success"

allocate (pdg_in (2))
pdg_in(1) = 11; pdg_in(2) = -11
allocate (pdg_out(2))
pdg_out(1) = 2; pdg_out(2) = -2
allocate (pdg_excluded (10))
pdg_excluded = [-4, 4, 5, -5, 6, -6, 13, -13, 15, -15]

write (u, "(A)") "* Leading order"
write (u, "(A)", advance = 'no') "* Incoming: "
call write_pdg_array (pdg_in, u)
write (u, "(A)", advance = 'no') "* Outgoing: "
call write_pdg_array (pdg_out, u)

call generator%init (pdg_in, pdg_out, &
    pdg_excluded_gaugeSplittings = pdg_excluded, qcd = .true., qed = .false.)
call generator%set_n (2, 2, 0)
call generator%set_constraints (.false., .false., .true., .true.)

call write_separator (u)
write (u, "(A)") "Generate higher-multiplicity states"
write (u, "(A,IO)") "Desired multiplicity: ", max_multiplicity
call generator%generate_multiple (max_multiplicity, model)
call generator%prt_queue%write (u)
call write_separator (u)
write (u, "(A,IO)") "Number of higher-multiplicity states: ", generator%prt_queue%n_lists

write (u, "(A)") "Check that no particle state occurs twice or more"
if (.not. generator%prt_queue%check_for_same_prt_strings()) then
    write (u, "(A)") "SUCCESS"
else
    write (u, "(A)") "FAIL"
end if

```

```

call write_separator (u)
write (u, "(A,IO,A)") "Check that there are ", max_multiplicity, " particles in the last entry"
call generator%prt_queue%get_last (prt_last)
if (size (prt_last) == max_multiplicity) then
    write (u, "(A)") "SUCCESS"
else
    write (u, "(A)") "FAIL"
end if
end subroutine radiation_generator_2

```

(radiation generator: test declarations)+≡
public :: radiation_generator_3

(radiation generator: tests)+≡

```

subroutine radiation_generator_3 (u)
    integer, intent(in) :: u
    type(radiation_generator_t) :: generator
    type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model => null ()

    write (u, "(A)") "* Test output: radiation_generator_3"
    write (u, "(A)") "* Purpose: Create N+1-particle flavor structures &
        &from predefined N-particle flavor structures"
    write (u, "(A)") "* One additional electroweak coupling, no additional strong coupling"
    write (u, "(A)")
    write (u, "(A)") "* Loading radiation model: SM.mdl"

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
        (var_str ("SM"), var_str ("SM.mdl"), &
        os_data, model)
    write (u, "(A)") "* Success"

    allocate (pdg_in (2))
    pdg_in(1) = 11; pdg_in(2) = -11

    write (u, "(A)") "* Start checking processes"
    call write_separator (u)

    write (u, "(A)") "* Process 1: Tau pair-production with additional photon"
    allocate (pdg_out(3))
    pdg_out(1) = 15; pdg_out(2) = -15; pdg_out(3) = 22
    call test_process (generator, pdg_in, pdg_out, u)
    deallocate (pdg_out)

    write (u, "(A)") "* Process 2: Tau pair-production with additional leptons or photon"
    allocate (pdg_out(3))
    pdg_out(1) = 15; pdg_out(2) = -15; pdg_out(3) = [-13, 13, 22]
    call test_process (generator, pdg_in, pdg_out, u)
    deallocate (pdg_out)

```

```

write (u, "(A)") "* Process 3: Electron-positron production"
allocate (pdg_out(2))
pdg_out(1) = 11; pdg_out(2) = -11
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 4: Quark-antiquark production with additional photon"
allocate (pdg_out(3))
pdg_out(1) = 2; pdg_out(2) = -2; pdg_out(3) = 22
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 5: Z + jets "
allocate (pdg_out(3))
pdg_out(1) = 2; pdg_out(2) = -2; pdg_out(3) = 23
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 6: W + jets"
allocate (pdg_out(3))
pdg_out(1) = 1; pdg_out(2) = -2; pdg_out(3) = -24
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 7: Top Decay"
allocate (pdg_out(4))
pdg_out(1) = 24; pdg_out(2) = -24
pdg_out(3) = 5; pdg_out(4) = -5
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 8: Production of four quarks"
allocate (pdg_out(4))
pdg_out(1) = 2; pdg_out(2) = -2;
pdg_out(3) = 2; pdg_out(4) = -2
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out)

write (u, "(A)") "* Process 9: Neutrino pair-production"
allocate (pdg_out(2))
pdg_out(1) = 12; pdg_out(2) = -12
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 10: Drell-Yan lepto-production"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = 2; pdg_in(2) = -2
pdg_out(1) = 11; pdg_out(2) = -11
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 11: WZ production at hadron-colliders"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = 1; pdg_in(2) = -2

```

```

pdg_out(1) = -24; pdg_out(2) = 23
call test_process (generator, pdg_in, pdg_out, u, .true.)
deallocate (pdg_out); deallocate (pdg_in)

write (u, "(A)") "* Process 12: Positron-neutrino production"
allocate (pdg_in (2)); allocate (pdg_out (2))
pdg_in(1) = -1; pdg_in(2) = 2
pdg_out(1) = -11; pdg_out(2) = 12
call test_process (generator, pdg_in, pdg_out, u)
deallocate (pdg_out); deallocate (pdg_in)

contains
subroutine test_process (generator, pdg_in, pdg_out, u, include_initial_state)
  type(radiation_generator_t), intent(inout) :: generator
  type(pdg_array_t), dimension(:), intent(in) :: pdg_in, pdg_out
  integer, intent(in) :: u
  logical, intent(in), optional :: include_initial_state
  type(string_t), dimension(:), allocatable :: prt_strings_in
  type(string_t), dimension(:), allocatable :: prt_strings_out
  type(pdg_array_t), dimension(10) :: pdg_excluded
  logical :: yorn
  yorn = .false.
  pdg_excluded = [-4, 4, 5, -5, 6, -6, 13, -13, 15, -15]
  if (present (include_initial_state)) yorn = include_initial_state
  write (u, "(A)") "* Leading order: "
  write (u, "(A)", advance = 'no') '* Incoming: '
  call write_pdg_array (pdg_in, u)
  write (u, "(A)", advance = 'no') '* Outgoing: '
  call write_pdg_array (pdg_out, u)

  call generator%init (pdg_in, pdg_out, &
    pdg_excluded_gaugeSplittings = pdg_excluded, qcd = .false., qed = .true.)
  call generator%set_n (2, size(pdg_out), 0)
  if (yorn) call generator%set_initial_state_emissions ()
  call generator%set_constraints (.false., .false., .true., .true.)
  call generator%setup_if_table (model)
  call generator%generate (prt_strings_in, prt_strings_out)
  write (u, "(A)") "* Additional radiation: "
  write (u, "(A)") "* Incoming: "
  call write_particle_string (prt_strings_in, u)
  write (u, "(A)") "* Outgoing: "
  call write_particle_string (prt_strings_out, u)
  call write_separator(u)
  call generator%reset_resuffle_list ()
end subroutine test_process

end subroutine radiation_generator_3

<radiation_generator: test declarations>+≡
public :: radiation_generator_4

<radiation_generator: tests>+≡
subroutine radiation_generator_4 (u)
  integer, intent(in) :: u

```



```

type(radiation_generator_t) :: generator
type(pdg_array_t), dimension(:), allocatable :: pdg_in, pdg_out
type(pdg_array_t), dimension(:), allocatable :: pdg_excluded
type(os_data_t) :: os_data
type(model_list_t) :: model_list
type(model_t), pointer :: model => null ()
integer, parameter :: max_multiplicity = 10
type(string_t), dimension(:), allocatable :: prt_last

write (u, "(A)") "* Test output: radiation_generator_4"
write (u, "(A)") "* Purpose: Test the repeated application of &
    &a radiation generator splitting in QED"
write (u, "(A)") "* Only Final state emissions! "
write (u, "(A)")
write (u, "(A)") "* Loading radiation model: SM.mdl"

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
    os_data, model)
write (u, "(A)") "* Success"

allocate (pdg_in (2))
pdg_in(1) = 2; pdg_in(2) = -2
allocate (pdg_out(2))
pdg_out(1) = 11; pdg_out(2) = -11
allocate ( pdg_excluded (14))
pdg_excluded = [1, -1, 2, -2, 3, -3, 4, -4, 5, -5, 6, -6, 15, -15]

write (u, "(A)") "* Leading order"
write (u, "(A)", advance = 'no') "* Incoming: "
call write_pdg_array (pdg_in, u)
write (u, "(A)", advance = 'no') "* Outgoing: "
call write_pdg_array (pdg_out, u)

call generator%init (pdg_in, pdg_out, &
    pdg_excluded_gaugeSplittings = pdg_excluded, qcd = .false., qed = .true.)
call generator%set_n (2, 2, 0)
call generator%set_constraints (.false., .false., .true., .true.)

call write_separator (u)
write (u, "(A)") "Generate higher-multiplicity states"
write (u, "(A,IO)") "Desired multiplicity: ", max_multiplicity
call generator%generate_multiple (max_multiplicity, model)
call generator%prt_queue%write (u)
call write_separator (u)
write (u, "(A,IO)") "Number of higher-multiplicity states: ", generator%prt_queue%n_lists

write (u, "(A)") "Check that no particle state occurs twice or more"
if (.not. generator%prt_queue%check_for_same_prt_strings()) then
    write (u, "(A)") "SUCCESS"
else
    write (u, "(A)") "FAIL"

```

```

end if
call write_separator (u)
write (u, "(A,IO,A)") "Check that there are ", max_multiplicity, " particles in the last entry
call generator%prt_queue%get_last (prt_last)
if (size (prt_last) == max_multiplicity) then
    write (u, "(A)") "SUCCESS"
else
    write (u, "(A)") "FAIL"
end if
end if
end subroutine radiation_generator_4

```

28.3 Sindarin Expression Implementation

This module defines expressions of all kinds, represented in a tree structure, for repeated evaluation. This provides an implementation of the `expr_base` abstract type.

We have two flavors of expressions: one with particles and one without particles. The latter version is used for defining cut/selection criteria and for online analysis.

```
<eval_trees.f90>≡  
  <File header>  
  
  module eval_trees  
  
    use, intrinsic :: iso_c_binding !NODEP!  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use constants, only: DEGREE, IMAGO, PI  
    use format_defs, only: FMT_19  
    use numeric_utils, only: nearly_equal  
    use diagnostics  
    use lorentz  
    use md5  
    use formats  
    use sorting  
    use ifiles  
    use lexers  
    use syntax_rules  
    use parser  
    use analysis  
    use jets  
    use pdg_arrays  
    use subevents  
    use var_base  
    use expr_base  
    use variables  
    use observables  
  
    <Standard module head>  
  
    <Eval trees: public>  
  
    <Eval trees: types>  
  
    <Eval trees: interfaces>  
  
    <Eval trees: variables>  
  
    contains  
  
    <Eval trees: procedures>  
  
  end module eval_trees
```

28.3.1 Tree nodes

The evaluation tree consists of branch nodes (unary and binary) and of leaf nodes, originating from a common root. The node object should be polymorphic. For the time being, polymorphism is emulated here. This means that we have to maintain all possibilities that the node may hold, including associated procedures as pointers.

The following parameter values characterize the node. Unary and binary operators have sub-nodes. The other are leaf nodes. Possible leafs are literal constants or named-parameter references.

<Eval trees: types>≡

```
integer, parameter :: EN_UNKNOWN = 0, EN_UNARY = 1, EN_BINARY = 2
integer, parameter :: EN_CONSTANT = 3, EN_VARIABLE = 4
integer, parameter :: EN_CONDITIONAL = 5, EN_BLOCK = 6
integer, parameter :: EN_RECORD_CMD = 7
integer, parameter :: EN_OBS1_INT = 11, EN_OBS2_INT = 12
integer, parameter :: EN_OBSEV_INT = 13
integer, parameter :: EN_OBS1_REAL = 21, EN_OBS2_REAL = 22
integer, parameter :: EN_OBSEV_REAL = 23
integer, parameter :: EN_PRT_FUN_UNARY = 101, EN_PRT_FUN_BINARY = 102
integer, parameter :: EN_EVAL_FUN_UNARY = 111, EN_EVAL_FUN_BINARY = 112
integer, parameter :: EN_LOG_FUN_UNARY = 121, EN_LOG_FUN_BINARY = 122
integer, parameter :: EN_INT_FUN_UNARY = 131, EN_INT_FUN_BINARY = 132
integer, parameter :: EN_REAL_FUN_UNARY = 141, EN_REAL_FUN_BINARY = 142
integer, parameter :: EN_REAL_FUN_CUM = 151
integer, parameter :: EN_FORMAT_STR = 161
```

This is exported only for use within unit tests.

<Eval trees: public>≡

```
public :: eval_node_t
```

<Eval trees: types>+≡

```
type :: eval_node_t
private
type(string_t) :: tag
integer :: type = EN_UNKNOWN
integer :: result_type = V_NONE
type(var_list_t), pointer :: var_list => null ()
type(string_t) :: var_name
logical, pointer :: value_is_known => null ()
logical,          pointer :: lval => null ()
integer,          pointer :: ival => null ()
real(default),    pointer :: rval => null ()
complex(default), pointer :: cval => null ()
type(subvt_t),    pointer :: pval => null ()
type(pdg_array_t), pointer :: aval => null ()
type(string_t),    pointer :: sval => null ()
type(eval_node_t), pointer :: arg0 => null ()
type(eval_node_t), pointer :: arg1 => null ()
type(eval_node_t), pointer :: arg2 => null ()
type(eval_node_t), pointer :: arg3 => null ()
type(eval_node_t), pointer :: arg4 => null ()
procedure(obs_unary_int), nopass, pointer :: obs1_int => null ()
procedure(obs_unary_real), nopass, pointer :: obs1_real => null ()
```

```

procedure(obs_binary_int), nopass, pointer :: obs2_int => null ()
procedure(obs_binary_real), nopass, pointer :: obs2_real => null ()
procedure(obs_sev_int), nopass, pointer :: obsev_int => null ()
procedure(obs_sev_real), nopass, pointer :: obsev_real => null ()
integer, pointer :: prt_type => null ()
integer, pointer :: index => null ()
real(default), pointer :: tolerance => null ()
integer, pointer :: jet_algorithm => null ()
real(default), pointer :: jet_r => null ()
real(default), pointer :: jet_p => null ()
real(default), pointer :: jet_ycut => null ()
real(default), pointer :: jet_dcut => null ()
real(default), pointer :: photon_iso_eps => null ()
real(default), pointer :: photon_iso_n => null ()
real(default), pointer :: photon_iso_r0 => null ()
real(default), pointer :: photon_rec_r0 => null ()
type(prt_t), pointer :: prt1 => null ()
type(prt_t), pointer :: prt2 => null ()
procedure(unary_log), nopass, pointer :: op1_log => null ()
procedure(unary_int), nopass, pointer :: op1_int => null ()
procedure(unary_real), nopass, pointer :: op1_real => null ()
procedure(unary_cmplx), nopass, pointer :: op1_cmplx => null ()
procedure(unary_pdg), nopass, pointer :: op1_pdg => null ()
procedure(unary_sev), nopass, pointer :: op1_sev => null ()
procedure(unary_str), nopass, pointer :: op1_str => null ()
procedure(unary_cut), nopass, pointer :: op1_cut => null ()
procedure(unary_evi), nopass, pointer :: op1_evi => null ()
procedure(unary_evr), nopass, pointer :: op1_evr => null ()
procedure(binary_log), nopass, pointer :: op2_log => null ()
procedure(binary_int), nopass, pointer :: op2_int => null ()
procedure(binary_real), nopass, pointer :: op2_real => null ()
procedure(binary_cmplx), nopass, pointer :: op2_cmplx => null ()
procedure(binary_pdg), nopass, pointer :: op2_pdg => null ()
procedure(binary_sev), nopass, pointer :: op2_sev => null ()
procedure(binary_str), nopass, pointer :: op2_str => null ()
procedure(binary_cut), nopass, pointer :: op2_cut => null ()
procedure(binary_evi), nopass, pointer :: op2_evi => null ()
procedure(binary_evr), nopass, pointer :: op2_evr => null ()
procedure(cum_evi), nopass, pointer :: opcum_evi => null ()
procedure(cum_evr), nopass, pointer :: opcum_evr => null ()
contains
  <Eval trees: eval node: TBP>
end type eval_node_t

```

Finalize a node recursively. Allocated constants are deleted, pointers are ignored.

```

<Eval trees: eval node: TBP>≡
  procedure :: final_rec => eval_node_final_rec

<Eval trees: procedures>≡
  recursive subroutine eval_node_final_rec (node)
    class(eval_node_t), intent(inout) :: node
    select case (node%type)
      case (EN_UNARY)

```

```

        call eval_node_final_rec (node%arg1)
case (EN_BINARY)
    call eval_node_final_rec (node%arg1)
    call eval_node_final_rec (node%arg2)
case (EN_CONDITIONAL)
    call eval_node_final_rec (node%arg0)
    call eval_node_final_rec (node%arg1)
    call eval_node_final_rec (node%arg2)
case (EN_BLOCK)
    call eval_node_final_rec (node%arg0)
    call eval_node_final_rec (node%arg1)
case (EN_PRT_FUN_UNARY, EN_EVAL_FUN_UNARY, &
      EN_LOG_FUN_UNARY, EN_INT_FUN_UNARY, EN_REAL_FUN_UNARY)
    if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
    call eval_node_final_rec (node%arg1)
    deallocate (node%index)
    deallocate (node%prt1)
case (EN_REAL_FUN_CUM)
    if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
    call eval_node_final_rec (node%arg1)
    deallocate (node%index)
    deallocate (node%prt1)
case (EN_PRT_FUN_BINARY, EN_EVAL_FUN_BINARY, &
      EN_LOG_FUN_BINARY, EN_INT_FUN_BINARY, EN_REAL_FUN_BINARY)
    if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
    call eval_node_final_rec (node%arg1)
    call eval_node_final_rec (node%arg2)
    deallocate (node%index)
    deallocate (node%prt1)
    deallocate (node%prt2)
case (EN_FORMAT_STR)
    if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
    if (associated (node%arg1)) call eval_node_final_rec (node%arg1)
    deallocate (node%ival)
case (EN_RECORD_CMD)
    if (associated (node%arg0)) call eval_node_final_rec (node%arg0)
    if (associated (node%arg1)) call eval_node_final_rec (node%arg1)
    if (associated (node%arg2)) call eval_node_final_rec (node%arg2)
    if (associated (node%arg3)) call eval_node_final_rec (node%arg3)
    if (associated (node%arg4)) call eval_node_final_rec (node%arg4)
end select
select case (node%type)
case (EN_UNARY, EN_BINARY, EN_CONDITIONAL, EN_CONSTANT, EN_BLOCK, &
      EN_PRT_FUN_UNARY, EN_PRT_FUN_BINARY, &
      EN_EVAL_FUN_UNARY, EN_EVAL_FUN_BINARY, &
      EN_LOG_FUN_UNARY, EN_LOG_FUN_BINARY, &
      EN_INT_FUN_UNARY, EN_INT_FUN_BINARY, &
      EN_REAL_FUN_UNARY, EN_REAL_FUN_BINARY, &
      EN_REAL_FUN_CUM, &
      EN_FORMAT_STR, EN_RECORD_CMD)
    select case (node%result_type)
    case (V_LOG); deallocate (node%lval)
    case (V_INT); deallocate (node%ival)
    case (V_REAL); deallocate (node%rval)

```

```

        case (V_CMPLX); deallocate (node%cval)
        case (V_SEV); deallocate (node%pval)
        case (V_PDG); deallocate (node%aval)
        case (V_STR); deallocate (node%sval)
    end select
    deallocate (node%value_is_known)
end select
end subroutine eval_node_final_rec

```

Leaf nodes

Initialize a leaf node with a literal constant.

(Eval trees: procedures) +=

```

subroutine eval_node_init_log (node, lval)
    type(eval_node_t), intent(out) :: node
    logical, intent(in) :: lval
    node%type = EN_CONSTANT
    node%result_type = V_LOG
    allocate (node%lval, node%value_is_known)
    node%lval = lval
    node%value_is_known = .true.
end subroutine eval_node_init_log

```

```

subroutine eval_node_init_int (node, ival)
    type(eval_node_t), intent(out) :: node
    integer, intent(in) :: ival
    node%type = EN_CONSTANT
    node%result_type = V_INT
    allocate (node%ival, node%value_is_known)
    node%ival = ival
    node%value_is_known = .true.
end subroutine eval_node_init_int

```

```

subroutine eval_node_init_real (node, rval)
    type(eval_node_t), intent(out) :: node
    real(default), intent(in) :: rval
    node%type = EN_CONSTANT
    node%result_type = V_REAL
    allocate (node%rval, node%value_is_known)
    node%rval = rval
    node%value_is_known = .true.
end subroutine eval_node_init_real

```

```

subroutine eval_node_init_cmplx (node, cval)
    type(eval_node_t), intent(out) :: node
    complex(default), intent(in) :: cval
    node%type = EN_CONSTANT
    node%result_type = V_CMPLX
    allocate (node%cval, node%value_is_known)
    node%cval = cval
    node%value_is_known = .true.
end subroutine eval_node_init_cmplx

```

```

subroutine eval_node_init_subevt (node, pval)
  type(eval_node_t), intent(out) :: node
  type(subevt_t), intent(in) :: pval
  node%type = EN_CONSTANT
  node%result_type = V_SEV
  allocate (node%pval, node%value_is_known)
  node%pval = pval
  node%value_is_known = .true.
end subroutine eval_node_init_subevt

subroutine eval_node_init_pdg_array (node, aval)
  type(eval_node_t), intent(out) :: node
  type(pdg_array_t), intent(in) :: aval
  node%type = EN_CONSTANT
  node%result_type = V_PDG
  allocate (node%aval, node%value_is_known)
  node%aval = aval
  node%value_is_known = .true.
end subroutine eval_node_init_pdg_array

subroutine eval_node_init_string (node, sval)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: sval
  node%type = EN_CONSTANT
  node%result_type = V_STR
  allocate (node%sval, node%value_is_known)
  node%sval = sval
  node%value_is_known = .true.
end subroutine eval_node_init_string

```

Initialize a leaf node with a pointer to a named parameter

(Eval trees: procedures)+≡

```

subroutine eval_node_init_log_ptr (node, name, lval, is_known)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  logical, intent(in), target :: lval
  logical, intent(in), target :: is_known
  node%type = EN_VARIABLE
  node%tag = name
  node%result_type = V_LOG
  node%lval => lval
  node%value_is_known => is_known
end subroutine eval_node_init_log_ptr

subroutine eval_node_init_int_ptr (node, name, ival, is_known)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  integer, intent(in), target :: ival
  logical, intent(in), target :: is_known
  node%type = EN_VARIABLE
  node%tag = name
  node%result_type = V_INT
  node%ival => ival

```



```

    node%value_is_known => is_known
end subroutine eval_node_init_int_ptr

subroutine eval_node_init_real_ptr (node, name, rval, is_known)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name
    real(default), intent(in), target :: rval
    logical, intent(in), target :: is_known
    node%type = EN_VARIABLE
    node%tag = name
    node%result_type = V_REAL
    node%rval => rval
    node%value_is_known => is_known
end subroutine eval_node_init_real_ptr

subroutine eval_node_init_cmplx_ptr (node, name, cval, is_known)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name
    complex(default), intent(in), target :: cval
    logical, intent(in), target :: is_known
    node%type = EN_VARIABLE
    node%tag = name
    node%result_type = V_CMPLX
    node%cval => cval
    node%value_is_known => is_known
end subroutine eval_node_init_cmplx_ptr

subroutine eval_node_init_subevt_ptr (node, name, pval, is_known)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name
    type(subevt_t), intent(in), target :: pval
    logical, intent(in), target :: is_known
    node%type = EN_VARIABLE
    node%tag = name
    node%result_type = V_SEV
    node%pval => pval
    node%value_is_known => is_known
end subroutine eval_node_init_subevt_ptr

subroutine eval_node_init_pdg_array_ptr (node, name, aval, is_known)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name
    type(pdg_array_t), intent(in), target :: aval
    logical, intent(in), target :: is_known
    node%type = EN_VARIABLE
    node%tag = name
    node%result_type = V_PDG
    node%aval => aval
    node%value_is_known => is_known
end subroutine eval_node_init_pdg_array_ptr

subroutine eval_node_init_string_ptr (node, name, sval, is_known)
    type(eval_node_t), intent(out) :: node
    type(string_t), intent(in) :: name

```

```

type(string_t), intent(in), target :: sval
logical, intent(in), target :: is_known
node%type = EN_VARIABLE
node%tag = name
node%result_type = V_STR
node%sval => sval
node%value_is_known => is_known
end subroutine eval_node_init_string_ptr

```

The procedure-pointer cases:

(Eval trees: procedures)+≡

```

subroutine eval_node_init_obs1_int_ptr (node, name, obs1_iptr, p1)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  procedure(obs_unary_int), intent(in), pointer :: obs1_iptr
  type(prt_t), intent(in), target :: p1
  node%type = EN_OBS1_INT
  node%tag = name
  node%result_type = V_INT
  node%obs1_int => obs1_iptr
  node%prt1 => p1
  allocate (node%ival, node%value_is_known)
  node%value_is_known = .false.
end subroutine eval_node_init_obs1_int_ptr

subroutine eval_node_init_obs2_int_ptr (node, name, obs2_iptr, p1, p2)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  procedure(obs_binary_int), intent(in), pointer :: obs2_iptr
  type(prt_t), intent(in), target :: p1, p2
  node%type = EN_OBS2_INT
  node%tag = name
  node%result_type = V_INT
  node%obs2_int => obs2_iptr
  node%prt1 => p1
  node%prt2 => p2
  allocate (node%ival, node%value_is_known)
  node%value_is_known = .false.
end subroutine eval_node_init_obs2_int_ptr

subroutine eval_node_init_obsev_int_ptr (node, name, obsev_iptr, pval)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  procedure(obs_sev_int), intent(in), pointer :: obsev_iptr
  type(subevt_t), intent(in), target :: pval
  node%type = EN_OBSEV_INT
  node%tag = name
  node%result_type = V_INT
  node%obsev_int => obsev_iptr
  node%pval => pval
  allocate (node%rval, node%value_is_known)
  node%value_is_known = .false.
end subroutine eval_node_init_obsev_int_ptr

```

```

subroutine eval_node_init_obs1_real_ptr (node, name, obs1_rptr, p1)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  procedure(obs_unary_real), intent(in), pointer :: obs1_rptr
  type(prt_t), intent(in), target :: p1
  node%type = EN_OBS1_REAL
  node%tag = name
  node%result_type = V_REAL
  node%obs1_real => obs1_rptr
  node%prt1 => p1
  allocate (node%rval, node%value_is_known)
  node%value_is_known = .false.
end subroutine eval_node_init_obs1_real_ptr

subroutine eval_node_init_obs2_real_ptr (node, name, obs2_rptr, p1, p2)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  procedure(obs_binary_real), intent(in), pointer :: obs2_rptr
  type(prt_t), intent(in), target :: p1, p2
  node%type = EN_OBS2_REAL
  node%tag = name
  node%result_type = V_REAL
  node%obs2_real => obs2_rptr
  node%prt1 => p1
  node%prt2 => p2
  allocate (node%rval, node%value_is_known)
  node%value_is_known = .false.
end subroutine eval_node_init_obs2_real_ptr

subroutine eval_node_init_obsev_real_ptr (node, name, obsev_rptr, pval)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: name
  procedure(obs_sev_real), intent(in), pointer :: obsev_rptr
  type(subevt_t), intent(in), target :: pval
  node%type = EN_OBSEV_REAL
  node%tag = name
  node%result_type = V_REAL
  node%obsev_real => obsev_rptr
  node%pval => pval
  allocate (node%rval, node%value_is_known)
  node%value_is_known = .false.
end subroutine eval_node_init_obsev_real_ptr

```

Branch nodes

Initialize a branch node, sub-nodes are given.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_branch (node, tag, result_type, arg1, arg2)
  type(eval_node_t), intent(out) :: node
  type(string_t), intent(in) :: tag
  integer, intent(in) :: result_type
  type(eval_node_t), intent(in), target :: arg1
  type(eval_node_t), intent(in), target, optional :: arg2

```

```

    if (present (arg2)) then
        node%type = EN_BINARY
    else
        node%type = EN_UNARY
    end if
    node%tag = tag
    node%result_type = result_type
    call eval_node_allocate_value (node)
    node%arg1 => arg1
    if (present (arg2)) node%arg2 => arg2
end subroutine eval_node_init_branch

```

Allocate the node value according to the result type.

(Eval trees: procedures)+≡

```

subroutine eval_node_allocate_value (node)
    type(eval_node_t), intent(inout) :: node
    select case (node%result_type)
    case (V_LOG); allocate (node%lval)
    case (V_INT); allocate (node%ival)
    case (V_REAL); allocate (node%rval)
    case (V_CMPLX); allocate (node%cval)
    case (V_PDG); allocate (node%aval)
    case (V_SEV); allocate (node%pval)
        call subevt_init (node%pval)
    case (V_STR); allocate (node%sval)
    end select
    allocate (node%value_is_known)
    node%value_is_known = .false.
end subroutine eval_node_allocate_value

```

Initialize a block node which contains, in addition to the expression to be evaluated, a variable definition. The result type is not yet assigned, because we can compile the enclosed expression only after the var list is set up.

Note that the node always allocates a new variable list and appends it to the current one. Thus, if the variable redefines an existing one, it only shadows it but does not reset it. Any side-effects are therefore absent and need not be undone outside the block.

If the flag **new** is set, a variable is (re)declared. This must not be done for intrinsic variables. Vice versa, if the variable is not existent, the **new** flag is required.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_block (node, name, type, var_def, var_list)
    type(eval_node_t), intent(out), target :: node
    type(string_t), intent(in) :: name
    integer, intent(in) :: type
    type(eval_node_t), intent(in), target :: var_def
    type(var_list_t), intent(in), target :: var_list
    node%type = EN_BLOCK
    node%tag = "var_def"
    node%var_name = name
    node%arg1 => var_def
    allocate (node%var_list)

```

```

call node%var_list%link (var_list)
if (var_def%type == EN_CONSTANT) then
  select case (type)
    case (V_LOG)
      call var_list_append_log (node%var_list, name, var_def%lval)
    case (V_INT)
      call var_list_append_int (node%var_list, name, var_def%ival)
    case (V_REAL)
      call var_list_append_real (node%var_list, name, var_def%rval)
    case (V_CMPLX)
      call var_list_append_cmplx (node%var_list, name, var_def%cval)
    case (V_PDG)
      call var_list_append_pdg_array &
        (node%var_list, name, var_def%aval)
    case (V_SEV)
      call var_list_append_subevt &
        (node%var_list, name, var_def%pval)
    case (V_STR)
      call var_list_append_string (node%var_list, name, var_def%sval)
  end select
else
  select case (type)
    case (V_LOG); call var_list_append_log_ptr &
      (node%var_list, name, var_def%lval, var_def%value_is_known)
    case (V_INT); call var_list_append_int_ptr &
      (node%var_list, name, var_def%ival, var_def%value_is_known)
    case (V_REAL); call var_list_append_real_ptr &
      (node%var_list, name, var_def%rval, var_def%value_is_known)
    case (V_CMPLX); call var_list_append_cmplx_ptr &
      (node%var_list, name, var_def%cval, var_def%value_is_known)
    case (V_PDG); call var_list_append_pdg_array_ptr &
      (node%var_list, name, var_def%aval, var_def%value_is_known)
    case (V_SEV); call var_list_append_subevt_ptr &
      (node%var_list, name, var_def%pval, var_def%value_is_known)
    case (V_STR); call var_list_append_string_ptr &
      (node%var_list, name, var_def%sval, var_def%value_is_known)
  end select
end if
end subroutine eval_node_init_block

```

Complete block initialization by assigning the expression to evaluate to `arg0`.

(Eval trees: procedures)+≡

```

subroutine eval_node_set_expr (node, arg, result_type)
  type(eval_node_t), intent(inout) :: node
  type(eval_node_t), intent(in), target :: arg
  integer, intent(in), optional :: result_type
  if (present (result_type)) then
    node%result_type = result_type
  else
    node%result_type = arg%result_type
  end if
  call eval_node_allocate_value (node)
  node%arg0 => arg
end subroutine eval_node_set_expr

```

Initialize a conditional. There are three branches: the condition (evaluates to logical) and the two alternatives (evaluate both to the same arbitrary type).

(Eval trees: procedures)+≡

```

subroutine eval_node_init_conditional (node, result_type, cond, arg1, arg2)
  type(eval_node_t), intent(out) :: node
  integer, intent(in) :: result_type
  type(eval_node_t), intent(in), target :: cond, arg1, arg2
  node%type = EN_CONDITIONAL
  node%tag = "cond"
  node%result_type = result_type
  call eval_node_allocate_value (node)
  node%arg0 => cond
  node%arg1 => arg1
  node%arg2 => arg2
end subroutine eval_node_init_conditional

```

Initialize a recording command (which evaluates to a logical constant). The first branch is the ID of the analysis object to be filled, the optional branches 1 to 4 are the values to be recorded.

If the event-weight pointer is null, we record values with unit weight. Otherwise, we use the value pointed to as event weight.

There can be up to four arguments which represent x , y , Δy , Δx . Therefore, this is the only node type that may fill four sub-nodes.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_record_cmd &
  (node, event_weight, id, arg1, arg2, arg3, arg4)
  type(eval_node_t), intent(out) :: node
  real(default), pointer :: event_weight
  type(eval_node_t), intent(in), target :: id
  type(eval_node_t), intent(in), optional, target :: arg1, arg2, arg3, arg4
  call eval_node_init_log (node, .true.)
  node%type = EN_RECORD_CMD
  node%rval => event_weight
  node%tag = "record_cmd"
  node%arg0 => id
  if (present (arg1)) then
    node%arg1 => arg1
    if (present (arg2)) then
      node%arg2 => arg2
      if (present (arg3)) then
        node%arg3 => arg3
        if (present (arg4)) then
          node%arg4 => arg4
        end if
      end if
    end if
  end if
end if
end if
end if
end subroutine eval_node_init_record_cmd

```

Initialize a node for operations on subevents. The particle lists (one or two) are inserted as `arg1` and `arg2`. We allocated particle pointers as temporaries for

iterating over particle lists. The procedure pointer which holds the function to evaluate for the subevents (e.g., combine, select) is also initialized.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_prt_fun_unary (node, arg1, name, proc)
  type(eval_node_t), intent(out) :: node
  type(eval_node_t), intent(in), target :: arg1
  type(string_t), intent(in) :: name
  procedure(unary_sev) :: proc
  node%type = EN_PRT_FUN_UNARY
  node%tag = name
  node%result_type = V_SEV
  call eval_node_allocate_value (node)
  node%arg1 => arg1
  allocate (node%index, source = 0)
  allocate (node%prt1)
  node%op1_sev => proc
end subroutine eval_node_init_prt_fun_unary

subroutine eval_node_init_prt_fun_binary (node, arg1, arg2, name, proc)
  type(eval_node_t), intent(out) :: node
  type(eval_node_t), intent(in), target :: arg1, arg2
  type(string_t), intent(in) :: name
  procedure(binary_sev) :: proc
  node%type = EN_PRT_FUN_BINARY
  node%tag = name
  node%result_type = V_SEV
  call eval_node_allocate_value (node)
  node%arg1 => arg1
  node%arg2 => arg2
  allocate (node%index, source = 0)
  allocate (node%prt1)
  allocate (node%prt2)
  node%op2_sev => proc
end subroutine eval_node_init_prt_fun_binary

```

Similar, but for particle-list functions that evaluate to a real value.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_eval_fun_unary (node, arg1, name)
  type(eval_node_t), intent(out) :: node
  type(eval_node_t), intent(in), target :: arg1
  type(string_t), intent(in) :: name
  node%type = EN_EVAL_FUN_UNARY
  node%tag = name
  node%result_type = V_REAL
  call eval_node_allocate_value (node)
  node%arg1 => arg1
  allocate (node%index, source = 0)
  allocate (node%prt1)
end subroutine eval_node_init_eval_fun_unary

subroutine eval_node_init_eval_fun_binary (node, arg1, arg2, name)
  type(eval_node_t), intent(out) :: node
  type(eval_node_t), intent(in), target :: arg1, arg2

```

```

type(string_t), intent(in) :: name
node%type = EN_EVAL_FUN_BINARY
node%tag = name
node%result_type = V_REAL
call eval_node_allocate_value (node)
node%arg1 => arg1
node%arg2 => arg2
allocate (node%index, source = 0)
allocate (node%prt1)
allocate (node%prt2)
end subroutine eval_node_init_eval_fun_binary

```

These are for particle-list functions that evaluate to a logical value.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_log_fun_unary (node, arg1, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1
type(string_t), intent(in) :: name
procedure(unary_cut) :: proc
node%type = EN_LOG_FUN_UNARY
node%tag = name
node%result_type = V_LOG
call eval_node_allocate_value (node)
node%arg1 => arg1
allocate (node%index, source = 0)
allocate (node%prt1)
node%op1_cut => proc
end subroutine eval_node_init_log_fun_unary

subroutine eval_node_init_log_fun_binary (node, arg1, arg2, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1, arg2
type(string_t), intent(in) :: name
procedure(binary_cut) :: proc
node%type = EN_LOG_FUN_BINARY
node%tag = name
node%result_type = V_LOG
call eval_node_allocate_value (node)
node%arg1 => arg1
node%arg2 => arg2
allocate (node%index, source = 0)
allocate (node%prt1)
allocate (node%prt2)
node%op2_cut => proc
end subroutine eval_node_init_log_fun_binary

```

These are for particle-list functions that evaluate to an integer value.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_int_fun_unary (node, arg1, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1
type(string_t), intent(in) :: name
procedure(unary_evi) :: proc

```



```

node%type = EN_INT_FUN_UNARY
node%tag = name
node%result_type = V_INT
call eval_node_allocate_value (node)
node%arg1 => arg1
allocate (node%index, source = 0)
allocate (node%prt1)
node%op1_evi => proc
end subroutine eval_node_init_int_fun_unary

subroutine eval_node_init_int_fun_binary (node, arg1, arg2, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1, arg2
type(string_t), intent(in) :: name
procedure(binary_evi) :: proc
node%type = EN_INT_FUN_BINARY
node%tag = name
node%result_type = V_INT
call eval_node_allocate_value (node)
node%arg1 => arg1
node%arg2 => arg2
allocate (node%index, source = 0)
allocate (node%prt1)
allocate (node%prt2)
node%op2_evi => proc
end subroutine eval_node_init_int_fun_binary

```

These are for particle-list functions that evaluate to a real value.

(Eval trees: procedures)+≡

```

subroutine eval_node_init_real_fun_unary (node, arg1, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1
type(string_t), intent(in) :: name
procedure(unary_evr) :: proc
node%type = EN_REAL_FUN_UNARY
node%tag = name
node%result_type = V_REAL
call eval_node_allocate_value (node)
node%arg1 => arg1
allocate (node%index, source = 0)
allocate (node%prt1)
node%op1_evr => proc
end subroutine eval_node_init_real_fun_unary

subroutine eval_node_init_real_fun_binary (node, arg1, arg2, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1, arg2
type(string_t), intent(in) :: name
procedure(binary_evr) :: proc
node%type = EN_REAL_FUN_BINARY
node%tag = name
node%result_type = V_REAL
call eval_node_allocate_value (node)
node%arg1 => arg1

```

```

node%arg2 => arg2
allocate (node%index, source = 0)
allocate (node%prt1)
allocate (node%prt2)
node%op2_evr => proc
end subroutine eval_node_init_real_fun_binary

subroutine eval_node_init_real_fun_cum (node, arg1, name, proc)
type(eval_node_t), intent(out) :: node
type(eval_node_t), intent(in), target :: arg1
type(string_t), intent(in) :: name
procedure(cum_evr) :: proc
node%type = EN_REAL_FUN_CUM
node%tag = name
node%result_type = V_REAL
call eval_node_allocate_value (node)
node%arg1 => arg1
allocate (node%index, source = 0)
allocate (node%prt1)
node%opcum_evr => proc
end subroutine eval_node_init_real_fun_cum

```

Initialize a node for a string formatting function (sprintf).

(Eval trees: procedures)+≡

```

subroutine eval_node_init_format_string (node, fmt, arg, name, n_args)
type(eval_node_t), intent(out) :: node
type(eval_node_t), pointer :: fmt, arg
type(string_t), intent(in) :: name
integer, intent(in) :: n_args
node%type = EN_FORMAT_STR
node%tag = name
node%result_type = V_STR
call eval_node_allocate_value (node)
node%arg0 => fmt
node%arg1 => arg
allocate (node%ival)
node%ival = n_args
end subroutine eval_node_init_format_string

```

If particle functions depend upon a condition (or an expression is evaluated), the observables that can be evaluated for the given particles have to be thrown on the local variable stack. This is done here. Each observable is initialized with the particle pointers which have been allocated for the node.

The integer variable that is referred to by the `Index` pseudo-observable is always known when it is referred to.

(Eval trees: procedures)+≡

```

subroutine eval_node_set_observables (node, var_list)
type(eval_node_t), intent(inout) :: node
type(var_list_t), intent(in), target :: var_list
logical, save, target :: known = .true.
allocate (node%var_list)
call node%var_list%link (var_list)
allocate (node%index, source = 0)

```

```

call var_list_append_int_ptr &
  (node%var_list, var_str ("Index"), node%index, known, intrinsic=.true.)
if (.not. associated (node%prt2)) then
  call var_list_set_observables_unary &
    (node%var_list, node%prt1)
  if (associated (node%pval)) then
    call var_list_set_observables_sev &
      (node%var_list, node%pval)
  end if
else
  call var_list_set_observables_binary &
    (node%var_list, node%prt1, node%prt2)
end if
end subroutine eval_node_set_observables

```

Output

<Eval trees: eval node: TBP>+≡

```

procedure :: write => eval_node_write

```

<Eval trees: procedures>+≡

```

subroutine eval_node_write (node, unit, indent)
  class(eval_node_t), intent(in) :: node
  integer, intent(in), optional :: unit
  integer, intent(in), optional :: indent
  integer :: u, ind
  u = given_output_unit (unit); if (u < 0) return
  ind = 0; if (present (indent)) ind = indent
  write (u, "(A)", advance="no") repeat ("| ", ind) // "o "
  select case (node%type)
  case (EN_UNARY, EN_BINARY, EN_CONDITIONAL, &
    EN_PRT_FUN_UNARY, EN_PRT_FUN_BINARY, &
    EN_EVAL_FUN_UNARY, EN_EVAL_FUN_BINARY, &
    EN_LOG_FUN_UNARY, EN_LOG_FUN_BINARY, &
    EN_INT_FUN_UNARY, EN_INT_FUN_BINARY, &
    EN_REAL_FUN_UNARY, EN_REAL_FUN_BINARY, &
    EN_REAL_FUN_CUM)
    write (u, "(A)", advance="no") "[" // char (node%tag) // "]" = "
  case (EN_CONSTANT)
    write (u, "(A)", advance="no") "[const] ="
  case (EN_VARIABLE)
    write (u, "(A)", advance="no") char (node%tag) // " =>"
  case (EN_OBS1_INT, EN_OBS2_INT, EN_OBS1_REAL, EN_OBS2_REAL)
    write (u, "(A)", advance="no") char (node%tag) // " ="
  case (EN_BLOCK)
    write (u, "(A)", advance="no") "[" // char (node%tag) // "]" // &
      char (node%var_name) // " [expr] = "
  case default
    write (u, "(A)", advance="no") "[???" // "
  end select
  select case (node%result_type)
  case (V_LOG)
    if (node%value_is_known) then
      if (node%lval) then

```

```

        write (u, "(1x,A)") "true"
    else
        write (u, "(1x,A)") "false"
    end if
else
    write (u, "(1x,A)") "[unknown logical]"
end if
case (V_INT)
    if (node%value_is_known) then
        write (u, "(1x,I0)") node%ival
    else
        write (u, "(1x,A)") "[unknown integer]"
    end if
case (V_REAL)
    if (node%value_is_known) then
        write (u, "(1x," // FMT_19 // ")") node%rval
    else
        write (u, "(1x,A)") "[unknown real]"
    end if
case (V_CMPLX)
    if (node%value_is_known) then
        write (u, "(1x,'('," // FMT_19 // ",','," // &
            FMT_19 // ",')')") node%cval
    else
        write (u, "(1x,A)") "[unknown complex]"
    end if
case (V_SEV)
    if (char (node%tag) == "@evt") then
        write (u, "(1x,A)") "[event subevent]"
    else if (node%value_is_known) then
        call subevt_write &
            (node%pval, unit, prefix = repeat ("| ", ind + 1))
    else
        write (u, "(1x,A)") "[unknown subevent]"
    end if
case (V_PDG)
    write (u, "(1x)", advance="no")
    call pdg_array_write (node%aval, u); write (u, *)
case (V_STR)
    if (node%value_is_known) then
        write (u, "(A)" ' "' // char (node%sval) // "'')
    else
        write (u, "(1x,A)") "[unknown string]"
    end if
case default
    write (u, "(1x,A)") "[empty]"
end select
select case (node%type)
case (EN_OBS1_INT, EN_OBS1_REAL)
    write (u, "(A,6x,A)", advance="no") repeat ("| ", ind), "prt1 ="
    call prt_write (node%prt1, unit)
case (EN_OBS2_INT, EN_OBS2_REAL)
    write (u, "(A,6x,A)", advance="no") repeat ("| ", ind), "prt1 ="
    call prt_write (node%prt1, unit)

```

```

        write (u, "(A,6x,A)", advance="no") repeat ("| ", ind), "prt2 ="
        call prt_write (node%prt2, unit)
    end select
end subroutine eval_node_write

recursive subroutine eval_node_write_rec (node, unit, indent)
    type(eval_node_t), intent(in) :: node
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: indent
    integer :: u, ind
    u = given_output_unit (unit); if (u < 0) return
    ind = 0; if (present (indent)) ind = indent
    call eval_node_write (node, unit, indent)
    select case (node%type)
    case (EN_UNARY)
        if (associated (node%arg0)) &
            call eval_node_write_rec (node%arg0, unit, ind+1)
        call eval_node_write_rec (node%arg1, unit, ind+1)
    case (EN_BINARY)
        if (associated (node%arg0)) &
            call eval_node_write_rec (node%arg0, unit, ind+1)
        call eval_node_write_rec (node%arg1, unit, ind+1)
        call eval_node_write_rec (node%arg2, unit, ind+1)
    case (EN_BLOCK)
        call eval_node_write_rec (node%arg1, unit, ind+1)
        call eval_node_write_rec (node%arg0, unit, ind+1)
    case (EN_CONDITIONAL)
        call eval_node_write_rec (node%arg0, unit, ind+1)
        call eval_node_write_rec (node%arg1, unit, ind+1)
        call eval_node_write_rec (node%arg2, unit, ind+1)
    case (EN_PRT_FUN_UNARY, EN_EVAL_FUN_UNARY, &
        EN_LOG_FUN_UNARY, EN_INT_FUN_UNARY, EN_REAL_FUN_UNARY, &
        EN_REAL_FUN_CUM)
        if (associated (node%arg0)) &
            call eval_node_write_rec (node%arg0, unit, ind+1)
        call eval_node_write_rec (node%arg1, unit, ind+1)
    case (EN_PRT_FUN_BINARY, EN_EVAL_FUN_BINARY, &
        EN_LOG_FUN_BINARY, EN_INT_FUN_BINARY, EN_REAL_FUN_BINARY)
        if (associated (node%arg0)) &
            call eval_node_write_rec (node%arg0, unit, ind+1)
        call eval_node_write_rec (node%arg1, unit, ind+1)
        call eval_node_write_rec (node%arg2, unit, ind+1)
    case (EN_RECORD_CMD)
        if (associated (node%arg1)) then
            call eval_node_write_rec (node%arg1, unit, ind+1)
        if (associated (node%arg2)) then
            call eval_node_write_rec (node%arg2, unit, ind+1)
        if (associated (node%arg3)) then
            call eval_node_write_rec (node%arg3, unit, ind+1)
        if (associated (node%arg4)) then
            call eval_node_write_rec (node%arg4, unit, ind+1)
        end if
        end if
    end if
end if
end if

```

```

        end if
    end select
end subroutine eval_node_write_rec

```

28.3.2 Operation types

For the operations associated to evaluation tree nodes, we define abstract interfaces for all cases.

Particles/subevents are transferred by-reference, to avoid unnecessary copying. Therefore, subroutines instead of functions.

(Eval trees: interfaces)≡

```

abstract interface
    logical function unary_log (arg)
        import eval_node_t
        type(eval_node_t), intent(in) :: arg
    end function unary_log
end interface
abstract interface
    integer function unary_int (arg)
        import eval_node_t
        type(eval_node_t), intent(in) :: arg
    end function unary_int
end interface
abstract interface
    real(default) function unary_real (arg)
        import default
        import eval_node_t
        type(eval_node_t), intent(in) :: arg
    end function unary_real
end interface
abstract interface
    complex(default) function unary_cmplx (arg)
        import default
        import eval_node_t
        type(eval_node_t), intent(in) :: arg
    end function unary_cmplx
end interface
abstract interface
    subroutine unary_pdg (pdg_array, arg)
        import pdg_array_t
        import eval_node_t
        type(pdg_array_t), intent(out) :: pdg_array
        type(eval_node_t), intent(in) :: arg
    end subroutine unary_pdg
end interface
abstract interface
    subroutine unary_sev (subevt, arg, arg0)
        import subevt_t
        import eval_node_t
        type(subevt_t), intent(inout) :: subevt
        type(eval_node_t), intent(in) :: arg
        type(eval_node_t), intent(inout), optional :: arg0
    end subroutine unary_sev
end interface

```

```

        end subroutine unary_sev
    end interface
    abstract interface
        subroutine unary_str (string, arg)
            import string_t
            import eval_node_t
            type(string_t), intent(out) :: string
            type(eval_node_t), intent(in) :: arg
        end subroutine unary_str
    end interface
    abstract interface
        logical function unary_cut (arg1, arg0)
            import eval_node_t
            type(eval_node_t), intent(in) :: arg1
            type(eval_node_t), intent(inout) :: arg0
        end function unary_cut
    end interface
    abstract interface
        subroutine unary_evi (ival, arg1, arg0)
            import eval_node_t
            integer, intent(out) :: ival
            type(eval_node_t), intent(in) :: arg1
            type(eval_node_t), intent(inout), optional :: arg0
        end subroutine unary_evi
    end interface
    abstract interface
        subroutine unary_evr (rval, arg1, arg0)
            import eval_node_t, default
            real(default), intent(out) :: rval
            type(eval_node_t), intent(in) :: arg1
            type(eval_node_t), intent(inout), optional :: arg0
        end subroutine unary_evr
    end interface
    abstract interface
        logical function binary_log (arg1, arg2)
            import eval_node_t
            type(eval_node_t), intent(in) :: arg1, arg2
        end function binary_log
    end interface
    abstract interface
        integer function binary_int (arg1, arg2)
            import eval_node_t
            type(eval_node_t), intent(in) :: arg1, arg2
        end function binary_int
    end interface
    abstract interface
        real(default) function binary_real (arg1, arg2)
            import default
            import eval_node_t
            type(eval_node_t), intent(in) :: arg1, arg2
        end function binary_real
    end interface
    abstract interface
        complex(default) function binary_cmplx (arg1, arg2)

```

```

        import default
        import eval_node_t
        type(eval_node_t), intent(in) :: arg1, arg2
    end function binary_cmplx
end interface
abstract interface
    subroutine binary_pdg (pdg_array, arg1, arg2)
        import pdg_array_t
        import eval_node_t
        type(pdg_array_t), intent(out) :: pdg_array
        type(eval_node_t), intent(in) :: arg1, arg2
    end subroutine binary_pdg
end interface
abstract interface
    subroutine binary_sev (subevt, arg1, arg2, arg0)
        import subevt_t
        import eval_node_t
        type(subevt_t), intent(inout) :: subevt
        type(eval_node_t), intent(in) :: arg1, arg2
        type(eval_node_t), intent(inout), optional :: arg0
    end subroutine binary_sev
end interface
abstract interface
    subroutine binary_str (string, arg1, arg2)
        import string_t
        import eval_node_t
        type(string_t), intent(out) :: string
        type(eval_node_t), intent(in) :: arg1, arg2
    end subroutine binary_str
end interface
abstract interface
    logical function binary_cut (arg1, arg2, arg0)
        import eval_node_t
        type(eval_node_t), intent(in) :: arg1, arg2
        type(eval_node_t), intent(inout) :: arg0
    end function binary_cut
end interface
abstract interface
    subroutine binary_evi (ival, arg1, arg2, arg0)
        import eval_node_t
        integer, intent(out) :: ival
        type(eval_node_t), intent(in) :: arg1, arg2
        type(eval_node_t), intent(inout), optional :: arg0
    end subroutine binary_evi
end interface
abstract interface
    subroutine binary_evr (rval, arg1, arg2, arg0)
        import eval_node_t, default
        real(default), intent(out) :: rval
        type(eval_node_t), intent(in) :: arg1, arg2
        type(eval_node_t), intent(inout), optional :: arg0
    end subroutine binary_evr
end interface
abstract interface

```



```

integer function cum_evi (arg1, arg0)
import eval_node_t
type(eval_node_t), intent(in) :: arg1
type(eval_node_t), intent(inout) :: arg0
end function cum_evi
end interface
abstract interface
real(default) function cum_evr (arg1, arg0)
import eval_node_t, default
type(eval_node_t), intent(in) :: arg1
type(eval_node_t), intent(inout) :: arg0
end function cum_evr
end interface

```

The following subroutines set the procedure pointer:

(Eval trees: procedures) +≡

```

subroutine eval_node_set_op1_log (en, op)
type(eval_node_t), intent(inout) :: en
procedure(unary_log) :: op
en%op1_log => op
end subroutine eval_node_set_op1_log

subroutine eval_node_set_op1_int (en, op)
type(eval_node_t), intent(inout) :: en
procedure(unary_int) :: op
en%op1_int => op
end subroutine eval_node_set_op1_int

subroutine eval_node_set_op1_real (en, op)
type(eval_node_t), intent(inout) :: en
procedure(unary_real) :: op
en%op1_real => op
end subroutine eval_node_set_op1_real

subroutine eval_node_set_op1_cmplx (en, op)
type(eval_node_t), intent(inout) :: en
procedure(unary_cmplx) :: op
en%op1_cmplx => op
end subroutine eval_node_set_op1_cmplx

subroutine eval_node_set_op1_pdg (en, op)
type(eval_node_t), intent(inout) :: en
procedure(unary_pdg) :: op
en%op1_pdg => op
end subroutine eval_node_set_op1_pdg

subroutine eval_node_set_op1_sev (en, op)
type(eval_node_t), intent(inout) :: en
procedure(unary_sev) :: op
en%op1_sev => op
end subroutine eval_node_set_op1_sev

subroutine eval_node_set_op1_str (en, op)
type(eval_node_t), intent(inout) :: en

```

```

    procedure(unary_str) :: op
    en%op1_str => op
end subroutine eval_node_set_op1_str

subroutine eval_node_set_op2_log (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(binary_log) :: op
    en%op2_log => op
end subroutine eval_node_set_op2_log

subroutine eval_node_set_op2_int (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(binary_int) :: op
    en%op2_int => op
end subroutine eval_node_set_op2_int

subroutine eval_node_set_op2_real (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(binary_real) :: op
    en%op2_real => op
end subroutine eval_node_set_op2_real

subroutine eval_node_set_op2_cmplx (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(binary_cmplx) :: op
    en%op2_cmplx => op
end subroutine eval_node_set_op2_cmplx

subroutine eval_node_set_op2_pdg (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(binary_pdg) :: op
    en%op2_pdg => op
end subroutine eval_node_set_op2_pdg

subroutine eval_node_set_op2_sev (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(binary_sev) :: op
    en%op2_sev => op
end subroutine eval_node_set_op2_sev

subroutine eval_node_set_op2_str (en, op)
    type(eval_node_t), intent(inout) :: en
    procedure(binary_str) :: op
    en%op2_str => op
end subroutine eval_node_set_op2_str

```

28.3.3 Specific operators

Our expression syntax contains all Fortran functions that make sense. These functions have to be provided in a form that they can be used in procedures pointers, and have the abstract interfaces above. For some intrinsic functions, we could use specific versions provided by Fortran directly. However, this has

two drawbacks: (i) We should work with the values instead of the eval-nodes as argument, which complicates the interface; (ii) more importantly, the `default` real type need not be equivalent to double precision. This would, at least, introduce system dependencies. Finally, for operators there are no specific versions.

Therefore, we write wrappers for all possible functions, at the expense of some overhead.

Binary numerical functions

```

<Eval trees: procedures>+≡
integer function add_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival + en2%ival
end function add_ii
real(default) function add_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival + en2%rval
end function add_ir
complex(default) function add_ic (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival + en2%cval
end function add_ic
real(default) function add_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval + en2%ival
end function add_ri
complex(default) function add_ci (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%cval + en2%ival
end function add_ci
complex(default) function add_cr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%cval + en2%rval
end function add_cr
complex(default) function add_rc (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval + en2%cval
end function add_rc
real(default) function add_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%rval + en2%rval
end function add_rr
complex(default) function add_cc (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%cval + en2%cval
end function add_cc

integer function sub_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival - en2%ival
end function sub_ii
real(default) function sub_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  y = en1%ival - en2%rval

```

```

end function sub_ir
real(default) function sub_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval - en2%ival
end function sub_ri
complex(default) function sub_ic (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival - en2%cval
end function sub_ic
complex(default) function sub_ci (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval - en2%ival
end function sub_ci
complex(default) function sub_cr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval - en2%rval
end function sub_cr
complex(default) function sub_rc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval - en2%cval
end function sub_rc
real(default) function sub_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval - en2%rval
end function sub_rr
complex(default) function sub_cc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval - en2%cval
end function sub_cc

integer function mul_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival * en2%ival
end function mul_ii
real(default) function mul_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival * en2%rval
end function mul_ir
real(default) function mul_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval * en2%ival
end function mul_ri
complex(default) function mul_ic (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival * en2%cval
end function mul_ic
complex(default) function mul_ci (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval * en2%ival
end function mul_ci
complex(default) function mul_rc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval * en2%cval
end function mul_rc

```

```

complex(default) function mul_cr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval * en2%rval
end function mul_cr
real(default) function mul_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval * en2%rval
end function mul_rr
complex(default) function mul_cc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval * en2%cval
end function mul_cc

integer function div_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (en2%ival == 0) then
        if (en1%ival >= 0) then
            call msg_warning ("division by zero: " // int2char (en1%ival) // &
                " / 0 ; result set to 0")
        else
            call msg_warning ("division by zero: (" // int2char (en1%ival) // &
                ") / 0 ; result set to 0")
        end if
        y = 0
        return
    end if
    y = en1%ival / en2%ival
end function div_ii
real(default) function div_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival / en2%rval
end function div_ir
real(default) function div_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval / en2%ival
end function div_ri
complex(default) function div_ic (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival / en2%cval
end function div_ic
complex(default) function div_ci (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval / en2%ival
end function div_ci
complex(default) function div_rc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval / en2%cval
end function div_rc
complex(default) function div_cr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval / en2%rval
end function div_cr
real(default) function div_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2

```

```

        y = en1%rval / en2%rval
    end function div_rr
    complex(default) function div_cc (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%cval / en2%cval
    end function div_cc

    integer function pow_ii (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        integer :: a, b
        real(default) :: rres
        a = en1%ival
        b = en2%ival
        if ((a == 0) .and. (b < 0)) then
            call msg_warning ("division by zero: " // int2char (a) // &
                " ^ (" // int2char (b) // ") ; result set to 0")
            y = 0
            return
        end if
        rres = real(a, default) ** b
        y = rres
        if (real(y, default) /= rres) then
            if (b < 0) then
                call msg_warning ("result of all-integer operation " // &
                    int2char (a) // " ^ (" // int2char (b) // &
                    ") has been truncated to " // int2char (y), &
                    [ var_str ("Chances are that you want to use " // &
                        "reals instead of integers at this point.") ])
            else
                call msg_warning ("integer overflow in " // int2char (a) // &
                    " ^ " // int2char (b) // " ; result is " // int2char (y), &
                    [ var_str ("Using reals instead of integers might help.") ])
            end if
        end if
    end function pow_ii
    real(default) function pow_ri (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval ** en2%ival
    end function pow_ri
    complex(default) function pow_ci (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%cval ** en2%ival
    end function pow_ci
    real(default) function pow_ir (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%ival ** en2%rval
    end function pow_ir
    real(default) function pow_rr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%rval ** en2%rval
    end function pow_rr
    complex(default) function pow_cr (en1, en2) result (y)
        type(eval_node_t), intent(in) :: en1, en2
        y = en1%cval ** en2%rval

```

```

end function pow_cr
complex(default) function pow_ic (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival ** en2%cval
end function pow_ic
complex(default) function pow_rc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval ** en2%cval
end function pow_rc
complex(default) function pow_cc (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%cval ** en2%cval
end function pow_cc

integer function max_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = max (en1%ival, en2%ival)
end function max_ii
real(default) function max_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = max (real (en1%ival, default), en2%rval)
end function max_ir
real(default) function max_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = max (en1%rval, real (en2%ival, default))
end function max_ri
real(default) function max_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = max (en1%rval, en2%rval)
end function max_rr
integer function min_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = min (en1%ival, en2%ival)
end function min_ii
real(default) function min_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = min (real (en1%ival, default), en2%rval)
end function min_ir
real(default) function min_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = min (en1%rval, real (en2%ival, default))
end function min_ri
real(default) function min_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = min (en1%rval, en2%rval)
end function min_rr

integer function mod_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = mod (en1%ival, en2%ival)
end function mod_ii
real(default) function mod_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = mod (real (en1%ival, default), en2%rval)

```

```

end function mod_ir
real(default) function mod_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = mod (en1%rval, real (en2%ival, default))
end function mod_ri
real(default) function mod_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = mod (en1%rval, en2%rval)
end function mod_rr
integer function modulo_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = modulo (en1%ival, en2%ival)
end function modulo_ii
real(default) function modulo_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = modulo (real (en1%ival, default), en2%rval)
end function modulo_ir
real(default) function modulo_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = modulo (en1%rval, real (en2%ival, default))
end function modulo_ri
real(default) function modulo_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = modulo (en1%rval, en2%rval)
end function modulo_rr

```

Unary numeric functions

<Eval trees: procedures>+≡

```

real(default) function real_i (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = en%ival
end function real_i
real(default) function real_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = en%cval
end function real_c
integer function int_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = en%rval
end function int_r
complex(default) function cmplx_i (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = en%ival
end function cmplx_i
integer function int_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = en%cval
end function int_c
complex(default) function cmplx_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = en%rval
end function cmplx_r

```



```

integer function nint_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = nint (en%rval)
end function nint_r
integer function floor_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = floor (en%rval)
end function floor_r
integer function ceiling_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = ceiling (en%rval)
end function ceiling_r

integer function neg_i (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = - en%ival
end function neg_i
real(default) function neg_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = - en%rval
end function neg_r
complex(default) function neg_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = - en%cval
end function neg_c
integer function abs_i (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = abs (en%ival)
end function abs_i
real(default) function abs_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = abs (en%rval)
end function abs_r
real(default) function abs_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = abs (en%cval)
end function abs_c
integer function conjg_i (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = en%ival
end function conjg_i
real(default) function conjg_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = en%rval
end function conjg_r
complex(default) function conjg_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = conjg (en%cval)
end function conjg_c
integer function sgn_i (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = sign (1, en%ival)
end function sgn_i
real(default) function sgn_r (en) result (y)

```

```

        type(eval_node_t), intent(in) :: en
        y = sign (1._default, en%rval)
    end function sgn_r

real(default) function sqrt_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = sqrt (en%rval)
end function sqrt_r
real(default) function exp_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = exp (en%rval)
end function exp_r
real(default) function log_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = log (en%rval)
end function log_r
real(default) function log10_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = log10 (en%rval)
end function log10_r

complex(default) function sqrt_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = sqrt (en%cval)
end function sqrt_c
complex(default) function exp_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = exp (en%cval)
end function exp_c
complex(default) function log_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = log (en%cval)
end function log_c

real(default) function sin_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = sin (en%rval)
end function sin_r
real(default) function cos_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = cos (en%rval)
end function cos_r
real(default) function tan_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = tan (en%rval)
end function tan_r
real(default) function asin_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = asin (en%rval)
end function asin_r
real(default) function acos_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = acos (en%rval)
end function acos_r

```

```

real(default) function atan_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = atan (en%rval)
end function atan_r

complex(default) function sin_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = sin (en%cval)
end function sin_c
complex(default) function cos_c (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = cos (en%cval)
end function cos_c

real(default) function sinh_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = sinh (en%rval)
end function sinh_r
real(default) function cosh_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = cosh (en%rval)
end function cosh_r
real(default) function tanh_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = tanh (en%rval)
end function tanh_r
real(default) function asinh_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = asinh (en%rval)
end function asinh_r
real(default) function acosh_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = acosh (en%rval)
end function acosh_r
real(default) function atanh_r (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = atanh (en%rval)
end function atanh_r

```

Binary logical functions

Logical expressions:

$\langle \text{Eval trees: procedures} \rangle + \equiv$

```

logical function ignore_first_ll (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en2%lval
end function ignore_first_ll
logical function or_ll (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%lval .or. en2%lval
end function or_ll
logical function and_ll (en1, en2) result (y)

```

```

    type(eval_node_t), intent(in) :: en1, en2
    y = en1%lval .and. en2%lval
end function and_ll

```

Comparisons:

<Eval trees: procedures>+≡

```

logical function comp_lt_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival < en2%ival
end function comp_lt_ii
logical function comp_lt_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival < en2%rval
end function comp_lt_ir
logical function comp_lt_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval < en2%ival
end function comp_lt_ri
logical function comp_lt_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval < en2%rval
end function comp_lt_rr

logical function comp_gt_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival > en2%ival
end function comp_gt_ii
logical function comp_gt_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival > en2%rval
end function comp_gt_ir
logical function comp_gt_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval > en2%ival
end function comp_gt_ri
logical function comp_gt_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval > en2%rval
end function comp_gt_rr

logical function comp_le_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival <= en2%ival
end function comp_le_ii
logical function comp_le_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival <= en2%rval
end function comp_le_ir
logical function comp_le_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval <= en2%ival
end function comp_le_ri
logical function comp_le_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2

```

```

    y = en1%rval <= en2%rval
end function comp_le_rr

logical function comp_ge_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival >= en2%ival
end function comp_ge_ii
logical function comp_ge_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival >= en2%rval
end function comp_ge_ir
logical function comp_ge_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval >= en2%ival
end function comp_ge_ri
logical function comp_ge_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval >= en2%rval
end function comp_ge_rr

logical function comp_eq_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival == en2%ival
end function comp_eq_ii
logical function comp_eq_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival == en2%rval
end function comp_eq_ir
logical function comp_eq_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval == en2%ival
end function comp_eq_ri
logical function comp_eq_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval == en2%rval
end function comp_eq_rr
logical function comp_eq_ss (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%sval == en2%sval
end function comp_eq_ss

logical function comp_ne_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival /= en2%ival
end function comp_ne_ii
logical function comp_ne_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%ival /= en2%rval
end function comp_ne_ir
logical function comp_ne_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval /= en2%ival
end function comp_ne_ri
logical function comp_ne_rr (en1, en2) result (y)

```

```

    type(eval_node_t), intent(in) :: en1, en2
    y = en1%rval /= en2%rval
end function comp_ne_rr
logical function comp_ne_ss (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    y = en1%sval /= en2%sval
end function comp_ne_ss

```

Comparisons with tolerance:

(Eval trees: procedures)+≡

```

logical function comp_se_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = abs (en1%ival - en2%ival) <= en1%tolerance
    else
        y = en1%ival == en2%ival
    end if
end function comp_se_ii
logical function comp_se_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = abs (en1%rval - en2%ival) <= en1%tolerance
    else
        y = en1%rval == en2%ival
    end if
end function comp_se_ri
logical function comp_se_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = abs (en1%ival - en2%rval) <= en1%tolerance
    else
        y = en1%ival == en2%rval
    end if
end function comp_se_ir
logical function comp_se_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = abs (en1%rval - en2%rval) <= en1%tolerance
    else
        y = en1%rval == en2%rval
    end if
end function comp_se_rr
logical function comp_ns_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = abs (en1%ival - en2%ival) > en1%tolerance
    else
        y = en1%ival /= en2%ival
    end if
end function comp_ns_ii
logical function comp_ns_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = abs (en1%rval - en2%ival) > en1%tolerance

```

```

else
    y = en1%rval /= en2%ival
end if
end function comp_ns_ri
logical function comp_ns_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = abs (en1%ival - en2%rval) > en1%tolerance
    else
        y = en1%ival /= en2%rval
    end if
end function comp_ns_ir
logical function comp_ns_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = abs (en1%rval - en2%rval) > en1%tolerance
    else
        y = en1%rval /= en2%rval
    end if
end function comp_ns_rr

logical function comp_ls_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival <= en2%ival + en1%tolerance
    else
        y = en1%ival <= en2%ival
    end if
end function comp_ls_ii
logical function comp_ls_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval <= en2%ival + en1%tolerance
    else
        y = en1%rval <= en2%ival
    end if
end function comp_ls_ri
logical function comp_ls_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival <= en2%rval + en1%tolerance
    else
        y = en1%ival <= en2%rval
    end if
end function comp_ls_ir
logical function comp_ls_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval <= en2%rval + en1%tolerance
    else
        y = en1%rval <= en2%rval
    end if
end function comp_ls_rr

```

```

logical function comp_ll_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = en1%ival < en2%ival - en1%tolerance
  else
    y = en1%ival < en2%ival
  end if
end function comp_ll_ii
logical function comp_ll_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = en1%rval < en2%ival - en1%tolerance
  else
    y = en1%rval < en2%ival
  end if
end function comp_ll_ri
logical function comp_ll_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = en1%ival < en2%rval - en1%tolerance
  else
    y = en1%ival < en2%rval
  end if
end function comp_ll_ir
logical function comp_ll_rr (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = en1%rval < en2%rval - en1%tolerance
  else
    y = en1%rval < en2%rval
  end if
end function comp_ll_rr

logical function comp_gs_ii (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = en1%ival >= en2%ival - en1%tolerance
  else
    y = en1%ival >= en2%ival
  end if
end function comp_gs_ii
logical function comp_gs_ri (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = en1%rval >= en2%ival - en1%tolerance
  else
    y = en1%rval >= en2%ival
  end if
end function comp_gs_ri
logical function comp_gs_ir (en1, en2) result (y)
  type(eval_node_t), intent(in) :: en1, en2
  if (associated (en1%tolerance)) then
    y = en1%ival >= en2%rval - en1%tolerance
  else

```



```

        y = en1%ival >= en2%rval
    end if
end function comp_gs_ir
logical function comp_gs_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval >= en2%rval - en1%tolerance
    else
        y = en1%rval >= en2%rval
    end if
end function comp_gs_rr

logical function comp_gg_ii (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival > en2%ival + en1%tolerance
    else
        y = en1%ival > en2%ival
    end if
end function comp_gg_ii
logical function comp_gg_ri (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval > en2%ival + en1%tolerance
    else
        y = en1%rval > en2%ival
    end if
end function comp_gg_ri
logical function comp_gg_ir (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%ival > en2%rval + en1%tolerance
    else
        y = en1%ival > en2%rval
    end if
end function comp_gg_ir
logical function comp_gg_rr (en1, en2) result (y)
    type(eval_node_t), intent(in) :: en1, en2
    if (associated (en1%tolerance)) then
        y = en1%rval > en2%rval + en1%tolerance
    else
        y = en1%rval > en2%rval
    end if
end function comp_gg_rr

```

Unary logical functions

(Eval trees: procedures)+≡

```

logical function not_1 (en) result (y)
    type(eval_node_t), intent(in) :: en
    y = .not. en%lval
end function not_1

```

Unary PDG-array functions

Make a PDG-array object from an integer.

```
<Eval trees: procedures>+≡  
  subroutine pdg_i (pdg_array, en)  
    type(pdg_array_t), intent(out) :: pdg_array  
    type(eval_node_t), intent(in) :: en  
    pdg_array = en%ival  
  end subroutine pdg_i
```

Binary PDG-array functions

Concatenate two PDG-array objects.

```
<Eval trees: procedures>+≡  
  subroutine concat_cc (pdg_array, en1, en2)  
    type(pdg_array_t), intent(out) :: pdg_array  
    type(eval_node_t), intent(in) :: en1, en2  
    pdg_array = en1%aval // en2%aval  
  end subroutine concat_cc
```

Unary particle-list functions

Combine all particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test.

```
<Eval trees: procedures>+≡  
  subroutine collect_p (subevt, en1, en0)  
    type(subevt_t), intent(inout) :: subevt  
    type(eval_node_t), intent(in) :: en1  
    type(eval_node_t), intent(inout), optional :: en0  
    logical, dimension(:), allocatable :: mask1  
    integer :: n, i  
    n = subevt_get_length (en1%pval)  
    allocate (mask1 (n))  
    if (present (en0)) then  
      do i = 1, n  
        en0%index = i  
        en0%prt1 = subevt_get_prt (en1%pval, i)  
        call eval_node_evaluate (en0)  
        mask1(i) = en0%lval  
      end do  
    else  
      mask1 = .true.  
    end if  
    call subevt_collect (subevt, en1%pval, mask1)  
  end subroutine collect_p
```

Cluster the particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test.

```
<Eval trees: procedures>+≡  
  subroutine cluster_p (subevt, en1, en0)
```

```

type(subevt_t), intent(inout) :: subevt
type(eval_node_t), intent(in) :: en1
type(eval_node_t), intent(inout), optional :: en0
logical, dimension(:), allocatable :: mask1
integer :: n, i
!!! Should not be initialized for every event
type(jet_definition_t) :: jet_def
logical :: keep_jets, exclusive
call jet_def%init (en1%jet_algorithm, en1%jet_r, en1%jet_p, en1%jet_ycut)
n = subevt_get_length (en1%pval)
allocate (mask1 (n))
if (present (en0)) then
  do i = 1, n
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    mask1(i) = en0%lval
  end do
else
  mask1 = .true.
end if
if (associated (en1%var_list)) then
  keep_jets = en1%var_list%get_lval (var_str("?keep_flavors_when_clustering"))
else
  keep_jets = .false.
end if
exclusive = .false.
select case (en1%jet_algorithm)
case (ee_kt_algorithm)
  exclusive = .true.
case (ee_genkt_algorithm)
  if (en1%jet_r > Pi) exclusive = .true.
end select
call subevt_cluster (subevt, en1%pval, en1%jet_dcut, mask1, &
  jet_def, keep_jets, exclusive)
call jet_def%final ()
end subroutine cluster_p

```

Recombine photons with other particles (usually charged leptons and maybe quarks) given in the same subevent. If `en0` is present, create a mask which is true only for those particles that pass the test.

<Eval trees: procedures>+≡

```

subroutine photon_recombination_p (subevt, en1, en0)
type(subevt_t), intent(inout) :: subevt
type(eval_node_t), intent(in) :: en1
type(eval_node_t), intent(inout), optional :: en0
logical, dimension(:), allocatable :: mask1
type(prt_t), dimension(:), allocatable :: prt
integer :: n, i
real(default) :: reco_r0
logical :: keep_flv
reco_r0 = en1%photon_rec_r0
n = subevt_get_length (en1%pval)

```

```

allocate (prt (n))
do i = 1, n
  prt(i) = subevt_get_prt (en1%pval, i)
  if (.not. prt_is_recombinable (prt (i))) then
    call msg_fatal ("Only charged leptons, quarks, and " // &
      "photons can be included in photon recombination.")
  end if
end do
if (count (prt_is_photon (prt)) > 1) &
  call msg_fatal ("Photon recombination is supported " // &
    "only for single photons.")
allocate (mask1 (n))
if (present (en0)) then
  do i = 1, n
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    mask1(i) = en0%lval
  end do
else
  mask1 = .true.
end if
if (associated (en1%var_list)) then
  keep_flg = en1%var_list%get_lval &
    (var_str("?keep_flavors_when_recombining"))
else
  keep_flg = .false.
end if
call subevt_recombine &
  (subevt, en1%pval, mask1, reco_r0, keep_flg)
end subroutine photon_recombination_p

```

Select all particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test.

(Eval trees: procedures)+≡

```

subroutine select_p (subevt, en1, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout), optional :: en0
  logical, dimension(:), allocatable :: mask1
  integer :: n, i
  n = subevt_get_length (en1%pval)
  allocate (mask1 (n))
  if (present (en0)) then
    do i = 1, subevt_get_length (en1%pval)
      en0%index = i
      en0%prt1 = subevt_get_prt (en1%pval, i)
      call eval_node_evaluate (en0)
      mask1(i) = en0%lval
    end do
  else
    mask1 = .true.
  end if
end if

```

```

        call subevt_select (subevt, en1%pval, mask1)
    end subroutine select_p

```

`select_b_jet_p`, `select_non_b_jet_p`, `select_c_jet_p`, and `select_light_jet_p` are special selection function acting on a subevent of combined particles (jets) and result in a list of *b* jets, non-*b* jets (i.e. *c* and light jets), *c* jets, and light jets, respectively.

(Eval trees: procedures)+≡

```

subroutine select_b_jet_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: n, i
    n = subevt_get_length (en1%pval)
    allocate (mask1 (n))
    do i = 1, subevt_get_length (en1%pval)
        mask1(i) = prt_is_b_jet (subevt_get_prt (en1%pval, i))
        if (present (en0)) then
            en0%index = i
            en0%prt1 = subevt_get_prt (en1%pval, i)
            call eval_node_evaluate (en0)
            mask1(i) = en0%lval .and. mask1(i)
        end if
    end do
    call subevt_select (subevt, en1%pval, mask1)
end subroutine select_b_jet_p

```

(Eval trees: procedures)+≡

```

subroutine select_non_b_jet_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: n, i
    n = subevt_get_length (en1%pval)
    allocate (mask1 (n))
    do i = 1, subevt_get_length (en1%pval)
        mask1(i) = .not. prt_is_b_jet (subevt_get_prt (en1%pval, i))
        if (present (en0)) then
            en0%index = i
            en0%prt1 = subevt_get_prt (en1%pval, i)
            call eval_node_evaluate (en0)
            mask1(i) = en0%lval .and. mask1(i)
        end if
    end do
    call subevt_select (subevt, en1%pval, mask1)
end subroutine select_non_b_jet_p

```

(Eval trees: procedures)+≡

```

subroutine select_c_jet_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1

```

```

type(eval_node_t), intent(inout), optional :: en0
logical, dimension(:), allocatable :: mask1
integer :: n, i
n = subevt_get_length (en1%pval)
allocate (mask1 (n))
do i = 1, subevt_get_length (en1%pval)
  mask1(i) = .not. prt_is_b_jet (subevt_get_prt (en1%pval, i)) &
    .and. prt_is_c_jet (subevt_get_prt (en1%pval, i))
  if (present (en0)) then
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    mask1(i) = en0%lval .and. mask1(i)
  end if
end do
call subevt_select (subevt, en1%pval, mask1)
end subroutine select_c_jet_p

```

(Eval trees: procedures)+≡

```

subroutine select_light_jet_p (subevt, en1, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout), optional :: en0
  logical, dimension(:), allocatable :: mask1
  integer :: n, i
  n = subevt_get_length (en1%pval)
  allocate (mask1 (n))
  do i = 1, subevt_get_length (en1%pval)
    mask1(i) = .not. prt_is_b_jet (subevt_get_prt (en1%pval, i)) &
      .and. .not. prt_is_c_jet (subevt_get_prt (en1%pval, i))
    if (present (en0)) then
      en0%index = i
      en0%prt1 = subevt_get_prt (en1%pval, i)
      call eval_node_evaluate (en0)
      mask1(i) = en0%lval .and. mask1(i)
    end if
  end do
  call subevt_select (subevt, en1%pval, mask1)
end subroutine select_light_jet_p

```

Extract the particle with index given by `en0` from the argument list. Negative indices count from the end. If `en0` is absent, extract the first particle. The result is a list with a single entry, or no entries if the original list was empty or if the index is out of range.

This function has no counterpart with two arguments.

(Eval trees: procedures)+≡

```

subroutine extract_p (subevt, en1, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout), optional :: en0
  integer :: index
  if (present (en0)) then
    call eval_node_evaluate (en0)
  end if

```

```

        select case (en0%result_type)
        case (V_INT); index = en0%ival
        case default
            call eval_node_write (en0)
            call msg_fatal (" Index parameter of 'extract' must be integer.")
        end select
    else
        index = 1
    end if
    call subevt_extract (subevt, en1%pval, index)
end subroutine extract_p

```

Sort the subevent according to the result of evaluating `en0`. If `en0` is absent, sort by default method (PDG code, particles before antiparticles).

(Eval trees: procedures)+≡

```

subroutine sort_p (subevt, en1, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout), optional :: en0
    integer, dimension(:), allocatable :: ival
    real(default), dimension(:), allocatable :: rval
    integer :: i, n
    n = subevt_get_length (en1%pval)
    if (present (en0)) then
        select case (en0%result_type)
        case (V_INT); allocate (ival (n))
        case (V_REAL); allocate (rval (n))
        end select
        do i = 1, n
            en0%index = i
            en0%prt1 = subevt_get_prt (en1%pval, i)
            call eval_node_evaluate (en0)
            select case (en0%result_type)
            case (V_INT); ival(i) = en0%ival
            case (V_REAL); rval(i) = en0%rval
            end select
        end do
        select case (en0%result_type)
        case (V_INT); call subevt_sort (subevt, en1%pval, ival)
        case (V_REAL); call subevt_sort (subevt, en1%pval, rval)
        end select
    else
        call subevt_sort (subevt, en1%pval)
    end if
end subroutine sort_p

```

The following functions return a logical value. `all` evaluates to true if the condition `en0` is true for all elements of the subevent. `any` and `no` are analogous.

(Eval trees: procedures)+≡

```

function all_p (en1, en0) result (lval)
    logical :: lval
    type(eval_node_t), intent(in) :: en1
    type(eval_node_t), intent(inout) :: en0

```

```

integer :: i, n
n = subevt_get_length (en1%pval)
lval = .true.
do i = 1, n
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    lval = en0%lval
    if (.not. lval) exit
end do
end function all_p

function any_p (en1, en0) result (lval)
logical :: lval
type(eval_node_t), intent(in) :: en1
type(eval_node_t), intent(inout) :: en0
integer :: i, n
n = subevt_get_length (en1%pval)
lval = .false.
do i = 1, n
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    lval = en0%lval
    if (lval) exit
end do
end function any_p

function no_p (en1, en0) result (lval)
logical :: lval
type(eval_node_t), intent(in) :: en1
type(eval_node_t), intent(inout) :: en0
integer :: i, n
n = subevt_get_length (en1%pval)
lval = .true.
do i = 1, n
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    lval = .not. en0%lval
    if (lval) exit
end do
end function no_p

```

The following function returns an integer value, namely the number of particles for which the condition is true. If there is no condition, it returns simply the length of the subevent.

(Eval trees: procedures)+≡

```

subroutine count_a (ival, en1, en0)
integer, intent(out) :: ival
type(eval_node_t), intent(in) :: en1
type(eval_node_t), intent(inout), optional :: en0
integer :: i, n, count

```



```

n = subevt_get_length (en1%pval)
if (present (en0)) then
  count = 0
  do i = 1, n
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    if (en0%lval) count = count + 1
  end do
  ival = count
else
  ival = n
end if
end subroutine count_a

```

The following functions return either an integer or a real value, namely the sum or the product of the values of the corresponding expression.

(Eval trees: procedures) +≡

```

function sum_a (en1, en0) result (rval)
  real(default) :: rval
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout) :: en0
  integer :: i, n
  n = subevt_get_length (en1%pval)
  rval = 0._default
  do i = 1, n
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    rval = rval + en0%rval
  end do
end function sum_a

function prod_a (en1, en0) result (rval)
  real(default) :: rval
  type(eval_node_t), intent(in) :: en1
  type(eval_node_t), intent(inout) :: en0
  integer :: i, n
  n = subevt_get_length (en1%pval)
  rval = 1._default
  do i = 1, n
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    call eval_node_evaluate (en0)
    rval = rval * en0%rval
  end do
end function prod_a

```

Binary particle-list functions

This joins two subevents, stored in the evaluation nodes **en1** and **en2**. If **en0** is also present, it amounts to a logical test returning true or false for every pair

of particles. A particle of the second list gets a mask entry only if it passes the test for all particles of the first list.

(Eval trees: procedures)+≡

```

subroutine join_pp (subevt, en1, en2, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout), optional :: en0
  logical, dimension(:), allocatable :: mask2
  integer :: i, j, n1, n2
  n1 = subevt_get_length (en1%pval)
  n2 = subevt_get_length (en2%pval)
  allocate (mask2 (n2))
  mask2 = .true.
  if (present (en0)) then
    do i = 1, n1
      en0%index = i
      en0%prt1 = subevt_get_prt (en1%pval, i)
      do j = 1, n2
        en0%prt2 = subevt_get_prt (en2%pval, j)
        call eval_node_evaluate (en0)
        mask2(j) = mask2(j) .and. en0%lval
      end do
    end do
  end if
  call subevt_join (subevt, en1%pval, en2%pval, mask2)
end subroutine join_pp

```

Combine two subevents, i.e., make a list of composite particles built from all possible particle pairs from the two lists. If `en0` is present, create a mask which is true only for those pairs that pass the test.

(Eval trees: procedures)+≡

```

subroutine combine_pp (subevt, en1, en2, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout), optional :: en0
  logical, dimension(:,:), allocatable :: mask12
  integer :: i, j, n1, n2
  n1 = subevt_get_length (en1%pval)
  n2 = subevt_get_length (en2%pval)
  if (present (en0)) then
    allocate (mask12 (n1, n2))
    do i = 1, n1
      en0%index = i
      en0%prt1 = subevt_get_prt (en1%pval, i)
      do j = 1, n2
        en0%prt2 = subevt_get_prt (en2%pval, j)
        call eval_node_evaluate (en0)
        mask12(i,j) = en0%lval
      end do
    end do
    call subevt_combine (subevt, en1%pval, en2%pval, mask12)
  else
    call subevt_combine (subevt, en1%pval, en2%pval)
  end if
end subroutine combine_pp

```

```

        end if
    end subroutine combine_pp

```

Combine all particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test w.r.t. all particles in the second argument. If `en0` is absent, the second argument is ignored.

(Eval trees: procedures)+≡

```

subroutine collect_pp (subevt, en1, en2, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: i, j, n1, n2
    n1 = subevt_get_length (en1%pval)
    n2 = subevt_get_length (en2%pval)
    allocate (mask1 (n1))
    mask1 = .true.
    if (present (en0)) then
        do i = 1, n1
            en0%index = i
            en0%prt1 = subevt_get_prt (en1%pval, i)
            do j = 1, n2
                en0%prt2 = subevt_get_prt (en2%pval, j)
                call eval_node_evaluate (en0)
                mask1(i) = mask1(i) .and. en0%lval
            end do
        end do
    end if
    call subevt_collect (subevt, en1%pval, mask1)
end subroutine collect_pp

```

Select all particles of the first argument. If `en0` is present, create a mask which is true only for those particles that pass the test w.r.t. all particles in the second argument. If `en0` is absent, the second argument is ignored, and the first argument is transferred unchanged. (This case is not very useful, of course.)

(Eval trees: procedures)+≡

```

subroutine select_pp (subevt, en1, en2, en0)
    type(subevt_t), intent(inout) :: subevt
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout), optional :: en0
    logical, dimension(:), allocatable :: mask1
    integer :: i, j, n1, n2
    n1 = subevt_get_length (en1%pval)
    n2 = subevt_get_length (en2%pval)
    allocate (mask1 (n1))
    mask1 = .true.
    if (present (en0)) then
        do i = 1, n1
            en0%index = i
            en0%prt1 = subevt_get_prt (en1%pval, i)
            do j = 1, n2
                en0%prt2 = subevt_get_prt (en2%pval, j)
                call eval_node_evaluate (en0)
            end do
        end do
    end if
    call subevt_collect (subevt, en1%pval, mask1)
end subroutine select_pp

```

```

        mask1(i) = mask1(i) .and. en0%lval
    end do
end do
end if
call subevt_select (subevt, en1%pval, mask1)
end subroutine select_pp

```

Sort the first subevent according to the result of evaluating `en0`. From the second subevent, only the first element is taken as reference. If `en0` is absent, we sort by default method (PDG code, particles before antiparticles).

(Eval trees: procedures)+≡

```

subroutine sort_pp (subevt, en1, en2, en0)
  type(subvt_t), intent(inout) :: subvt
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout), optional :: en0
  integer, dimension(:), allocatable :: ival
  real(default), dimension(:), allocatable :: rval
  integer :: i, n1
  n1 = subvt_get_length (en1%pval)
  if (present (en0)) then
    select case (en0%result_type)
    case (V_INT); allocate (ival (n1))
    case (V_REAL); allocate (rval (n1))
    end select
    do i = 1, n1
      en0%index = i
      en0%prt1 = subvt_get_prt (en1%pval, i)
      en0%prt2 = subvt_get_prt (en2%pval, 1)
      call eval_node_evaluate (en0)
      select case (en0%result_type)
      case (V_INT); ival(i) = en0%ival
      case (V_REAL); rval(i) = en0%rval
      end select
    end do
    select case (en0%result_type)
    case (V_INT); call subvt_sort (subvt, en1%pval, ival)
    case (V_REAL); call subvt_sort (subvt, en1%pval, rval)
    end select
  else
    call subvt_sort (subvt, en1%pval)
  end if
end subroutine sort_pp

```

The following functions return a logical value. `all` evaluates to true if the condition `en0` is true for all valid element pairs of both subevents. Invalid pairs (with common `src` entry) are ignored.

`any` and `no` are analogous.

(Eval trees: procedures)+≡

```

function all_pp (en1, en2, en0) result (lval)
  logical :: lval
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout) :: en0
  integer :: i, j, n1, n2

```

```

n1 = subevt_get_length (en1%pval)
n2 = subevt_get_length (en2%pval)
lval = .true.
LOOP1: do i = 1, n1
  en0%index = i
  en0%prt1 = subevt_get_prt (en1%pval, i)
  do j = 1, n2
    en0%prt2 = subevt_get_prt (en2%pval, j)
    if (are_disjoint (en0%prt1, en0%prt2)) then
      call eval_node_evaluate (en0)
      lval = en0%lval
      if (.not. lval) exit LOOP1
    end if
  end do
end do LOOP1
end function all_pp

function any_pp (en1, en2, en0) result (lval)
  logical :: lval
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout) :: en0
  integer :: i, j, n1, n2
  n1 = subevt_get_length (en1%pval)
  n2 = subevt_get_length (en2%pval)
  lval = .false.
  LOOP1: do i = 1, n1
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    do j = 1, n2
      en0%prt2 = subevt_get_prt (en2%pval, j)
      if (are_disjoint (en0%prt1, en0%prt2)) then
        call eval_node_evaluate (en0)
        lval = en0%lval
        if (lval) exit LOOP1
      end if
    end do
  end do LOOP1
end function any_pp

function no_pp (en1, en2, en0) result (lval)
  logical :: lval
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout) :: en0
  integer :: i, j, n1, n2
  n1 = subevt_get_length (en1%pval)
  n2 = subevt_get_length (en2%pval)
  lval = .true.
  LOOP1: do i = 1, n1
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)
    do j = 1, n2
      en0%prt2 = subevt_get_prt (en2%pval, j)
      if (are_disjoint (en0%prt1, en0%prt2)) then
        call eval_node_evaluate (en0)

```

```

        lval = .not. en0%lval
        if (lval) exit LOOP1
    end if
end do
end do LOOP1
end function no_pp

```

The conditional restriction encoded in the `eval_node_t en_0` is applied only to the photons from `en1`, not to the objects being isolated from in `en2`.

(*Eval trees: procedures*) +=

```

function photon_isolation_pp (en1, en2, en0) result (lval)
    logical :: lval
    type(eval_node_t), intent(in) :: en1, en2
    type(eval_node_t), intent(inout) :: en0
    type(prt_t) :: prt
    type(prt_t), dimension(:), allocatable :: prt_gam0, prt_lep
    type(vector4_t), dimension(:), allocatable :: &
        p_gam0, p_lep0, p_lep, p_par
    integer :: i, j, n1, n2, n_par, n_lep, n_gam, n_delta
    real(default), dimension(:), allocatable :: delta_r, et_sum
    integer, dimension(:), allocatable :: index
    real(default) :: eps, iso_n, r0, pt_gam
    logical, dimension(:,:), allocatable :: photon_mask
    n1 = subevt_get_length (en1%pval)
    n2 = subevt_get_length (en2%pval)
    allocate (p_gam0 (n1), prt_gam0 (n1))
    eps = en1%photon_iso_eps
    iso_n = en1%photon_iso_n
    r0 = en1%photon_iso_r0
    lval = .true.
    do i = 1, n1
        en0%index = i
        prt = subevt_get_prt (en1%pval, i)
        prt_gam0(i) = prt
        if (.not. prt_is_photon (prt_gam0(i))) &
            call msg_fatal ("Photon isolation can only " // &
                "be applied to photons.")
        p_gam0(i) = prt_get_momentum (prt_gam0(i))
        en0%prt1 = prt
        call eval_node_evaluate (en0)
        lval = en0%lval
        if (.not. lval) return
    end do
    if (n1 == 0) then
        call msg_fatal ("Photon isolation applied on empty photon sample.")
    end if
    n_par = 0
    n_lep = 0
    n_gam = 0
    do i = 1, n2
        prt = subevt_get_prt (en2%pval, i)
        if (prt_is_parton (prt) .or. prt_is_clustered (prt)) then
            n_par = n_par + 1

```

```

end if
if (prt_is_lepton (prt)) then
  n_lep = n_lep + 1
end if
if (prt_is_photon (prt)) then
  n_gam = n_gam + 1
end if
end do
if (n_lep > 0 .and. n_gam == 0) then
  call msg_fatal ("Photon isolation from EM energy: photons " // &
    "have to be included.")
end if
if (n_lep > 0 .and. n_gam /= n1) then
  call msg_fatal ("Photon isolation: photon samples do not match.")
end if
allocate (p_par (n_par))
allocate (p_lep0 (n_gam+n_lep), prt_lep(n_gam+n_lep))
n_par = 0
n_lep = 0
do i = 1, n2
  prt = subevt_get_prt (en2%pval, i)
  if (prt_is_parton (prt) .or. prt_is_clustered (prt)) then
    n_par = n_par + 1
    p_par(n_par) = prt_get_momentum (prt)
  end if
  if (prt_is_lepton (prt) .or. prt_is_photon(prt)) then
    n_lep = n_lep + 1
    prt_lep(n_lep) = prt
    p_lep0(n_lep) = prt_get_momentum (prt_lep(n_lep))
  end if
end do
if (n_par > 0) then
  allocate (delta_r (n_par), index (n_par))
  HADRON_ISOLATION: do i = 1, n1
    pt_gam = transverse_part (p_gam0(i))
    delta_r(1:n_par) = sort (eta_phi_distance (p_gam0(i), p_par(1:n_par)))
    index(1:n_par) = order (eta_phi_distance (p_gam0(i), p_par(1:n_par)))
    n_delta = count (delta_r < r0)
    allocate (et_sum(n_delta))
    do j = 1, n_delta
      et_sum(j) = sum (transverse_part (p_par (index (1:j))))
      if (.not. et_sum(j) <= &
        iso_chi_gamma (delta_r(j), r0, iso_n, eps, pt_gam)) then
        lval = .false.
      end if
    end do
    return
  end do
  deallocate (et_sum)
end do HADRON_ISOLATION
deallocate (delta_r)
deallocate (index)
end if
if (n_lep > 0) then
  allocate (photon_mask(n1,n_lep))

```

```

do i = 1, n1
  photon_mask(i,:) = .not. (prt_gam0(i) .match. prt_lep(:))
end do
allocate (delta_r (n_lep-1), index (n_lep-1), p_lep(n_lep-1))
EM_ISOLATION: do i = 1, n1
  pt_gam = transverse_part (p_gam0(i))
  p_lep = pack (p_lep0, photon_mask(i,:))
  delta_r(1:n_lep-1) = sort (eta_phi_distance (p_gam0(i), p_lep(1:n_lep-1)))
  index(1:n_lep-1) = order (eta_phi_distance (p_gam0(i), p_lep(1:n_lep-1)))
  n_delta = count (delta_r < r0)
  allocate (et_sum(n_delta))
  do j = 1, n_delta
    et_sum(j) = sum (transverse_part (p_lep (index(1:j))))
    if (.not. et_sum(j) <= &
        iso_chi_gamma (delta_r(j), r0, iso_n, eps, pt_gam)) then
      lval = .false.
      return
    end if
  end do
  deallocate (et_sum)
end do EM_ISOLATION
deallocate (delta_r)
deallocate (index)
end if
contains
function iso_chi_gamma (dr, r0_gam, n_gam, eps_gam, pt_gam) result (iso)
  real(default) :: iso
  real(default), intent(in) :: dr, r0_gam, n_gam, eps_gam, pt_gam
  iso = eps_gam * pt_gam
  if (.not. nearly_equal (abs(n_gam), 0._default)) then
    iso = iso * ((1._default - cos(dr)) / &
        (1._default - cos(r0_gam)))*abs(n_gam)
  end if
end function iso_chi_gamma
end function photon_isolation_pp

```

This function evaluates an observable for a pair of particles. From the two particle lists, we take the first pair without src overlap. If there is no valid pair, we revert the status of the value to unknown.

(Eval trees: procedures)+≡

```

subroutine eval_pp (en1, en2, en0, rval, is_known)
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout) :: en0
  real(default), intent(out) :: rval
  logical, intent(out) :: is_known
  integer :: i, j, n1, n2
  n1 = subevt_get_length (en1%pval)
  n2 = subevt_get_length (en2%pval)
  rval = 0
  is_known = .false.
  LOOP1: do i = 1, n1
    en0%index = i
    en0%prt1 = subevt_get_prt (en1%pval, i)

```



```

do j = 1, n2
  en0%prt2 = subevt_get_prt (en2%pval, j)
  if (are_disjoint (en0%prt1, en0%prt2)) then
    call eval_node_evaluate (en0)
    rval = en0%rval
    is_known = .true.
    exit LOOP1
  end if
end do
end do LOOP1
end subroutine eval_pp

```

The following function returns an integer value, namely the number of valid particle-pairs from both lists for which the condition is true. Invalid pairs (with common `src` entry) are ignored. If there is no condition, it returns the number of valid particle pairs.

(Eval trees: procedures)+≡

```

subroutine count_pp (ival, en1, en2, en0)
  integer, intent(out) :: ival
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout), optional :: en0
  integer :: i, j, n1, n2, count
  n1 = subevt_get_length (en1%pval)
  n2 = subevt_get_length (en2%pval)
  if (present (en0)) then
    count = 0
    do i = 1, n1
      en0%index = i
      en0%prt1 = subevt_get_prt (en1%pval, i)
      do j = 1, n2
        en0%prt2 = subevt_get_prt (en2%pval, j)
        if (are_disjoint (en0%prt1, en0%prt2)) then
          call eval_node_evaluate (en0)
          if (en0%lval) count = count + 1
        end if
      end do
    end do
  else
    count = 0
    do i = 1, n1
      do j = 1, n2
        if (are_disjoint (subevt_get_prt (en1%pval, i), &
                               subevt_get_prt (en2%pval, j))) then
          count = count + 1
        end if
      end do
    end do
  end if
  ival = count
end subroutine count_pp

```

This function makes up a subevent from the second argument which consists only of particles which match the PDG code array (first argument).

```

<Eval trees: procedures>+≡
subroutine select_pdg_ca (subevt, en1, en2, en0)
  type(subevt_t), intent(inout) :: subevt
  type(eval_node_t), intent(in) :: en1, en2
  type(eval_node_t), intent(inout), optional :: en0
  if (present (en0)) then
    call subevt_select_pdg_code (subevt, en1%aval, en2%pval, en0%ival)
  else
    call subevt_select_pdg_code (subevt, en1%aval, en2%pval)
  end if
end subroutine select_pdg_ca

```

Binary string functions

Currently, the only string operation is concatenation.

```

<Eval trees: procedures>+≡
subroutine concat_ss (string, en1, en2)
  type(string_t), intent(out) :: string
  type(eval_node_t), intent(in) :: en1, en2
  string = en1%sval // en2%sval
end subroutine concat_ss

```

28.3.4 Compiling the parse tree

The evaluation tree is built recursively by following a parse tree. Evaluate an expression. The requested type is given as an optional argument; default is numeric (integer or real).

```

<Eval trees: procedures>+≡
recursive subroutine eval_node_compile_genexpr &
  (en, pn, var_list, result_type)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  integer, intent(in), optional :: result_type
  if (debug_active (D_MODEL_F)) then
    print *, "read genexpr"; call parse_node_write (pn)
  end if
  if (present (result_type)) then
    select case (result_type)
    case (V_INT, V_REAL, V_CMPLX)
      call eval_node_compile_expr (en, pn, var_list)
    case (V_LOG)
      call eval_node_compile_lexpr (en, pn, var_list)
    case (V_SEV)
      call eval_node_compile_pexpr (en, pn, var_list)
    case (V_PDG)
      call eval_node_compile_cexpr (en, pn, var_list)
    case (V_STR)
      call eval_node_compile_sexpr (en, pn, var_list)
    end select
  else

```

```

        call eval_node_compile_expr (en, pn, var_list)
    end if
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done genexpr"
    end if
end subroutine eval_node_compile_genexpr

```

Numeric expressions

This procedure compiles a numerical expression. This is a single term or a sum or difference of terms. We have to account for all combinations of integer and real arguments. If both are constant, we immediately do the calculation and allocate a constant node.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_expr (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_term, pn_addition, pn_op, pn_arg
    type(eval_node_t), pointer :: en1, en2
    type(string_t) :: key
    integer :: t1, t2, t
    if (debug_active (D_MODEL_F)) then
        print *, "read expr"; call parse_node_write (pn)
    end if
    pn_term => parse_node_get_sub_ptr (pn)
    select case (char (parse_node_get_rule_key (pn_term)))
    case ("term")
        call eval_node_compile_term (en, pn_term, var_list)
        pn_addition => parse_node_get_next_ptr (pn_term, tag="addition")
    case ("addition")
        en => null ()
        pn_addition => pn_term
    case default
        call parse_node_mismatch ("term|addition", pn)
    end select
    do while (associated (pn_addition))
        pn_op => parse_node_get_sub_ptr (pn_addition)
        pn_arg => parse_node_get_next_ptr (pn_op, tag="term")
        call eval_node_compile_term (en2, pn_arg, var_list)
        t2 = en2%result_type
        if (associated (en)) then
            en1 => en
            t1 = en1%result_type
        else
            allocate (en1)
            select case (t2)
            case (V_INT); call eval_node_init_int (en1, 0)
            case (V_REAL); call eval_node_init_real (en1, 0._default)
            case (V_CMPLX); call eval_node_init_cmplx (en1, cmplx &
                (0._default, 0._default, kind=default))
            end select
        end if
        call eval_node_compile_expr (en1, pn_addition, var_list)
        call eval_node_init_int (en1, 0)
    end do
end subroutine eval_node_compile_expr

```

```

        end select
        t1 = t2
    end if
    t = numeric_result_type (t1, t2)
    allocate (en)
    key = parse_node_get_key (pn_op)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
        select case (char (key))
        case ("+")
            select case (t1)
            case (V_INT)
                select case (t2)
                case (V_INT); call eval_node_init_int (en, add_ii (en1, en2))
                case (V_REAL); call eval_node_init_real (en, add_ir (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, add_ic (en1, en2))
                end select
            case (V_REAL)
                select case (t2)
                case (V_INT); call eval_node_init_real (en, add_ri (en1, en2))
                case (V_REAL); call eval_node_init_real (en, add_rr (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, add_rc (en1, en2))
                end select
            case (V_CMPLX)
                select case (t2)
                case (V_INT); call eval_node_init_cmplx (en, add_ci (en1, en2))
                case (V_REAL); call eval_node_init_cmplx (en, add_cr (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, add_cc (en1, en2))
                end select
            end select
        case ("-")
            select case (t1)
            case (V_INT)
                select case (t2)
                case (V_INT); call eval_node_init_int (en, sub_ii (en1, en2))
                case (V_REAL); call eval_node_init_real (en, sub_ir (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, sub_ic (en1, en2))
                end select
            case (V_REAL)
                select case (t2)
                case (V_INT); call eval_node_init_real (en, sub_ri (en1, en2))
                case (V_REAL); call eval_node_init_real (en, sub_rr (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, sub_rc (en1, en2))
                end select
            case (V_CMPLX)
                select case (t2)
                case (V_INT); call eval_node_init_cmplx (en, sub_ci (en1, en2))
                case (V_REAL); call eval_node_init_cmplx (en, sub_cr (en1, en2))
                case (V_CMPLX); call eval_node_init_cmplx (en, sub_cc (en1, en2))
                end select
            end select
        end select
    end select
    call eval_node_final_rec (en1)
    call eval_node_final_rec (en2)
    deallocate (en1, en2)

```

```

else
  call eval_node_init_branch (en, key, t, en1, en2)
  select case (char (key))
  case ("+")
    select case (t1)
    case (V_INT)
      select case (t2)
      case (V_INT);   call eval_node_set_op2_int  (en, add_ii)
      case (V_REAL);  call eval_node_set_op2_real (en, add_ir)
      case (V_CMPLX); call eval_node_set_op2_cmplx (en, add_ic)
      end select
    case (V_REAL)
      select case (t2)
      case (V_INT);   call eval_node_set_op2_real (en, add_ri)
      case (V_REAL);  call eval_node_set_op2_real (en, add_rr)
      case (V_CMPLX); call eval_node_set_op2_cmplx (en, add_rc)
      end select
    case (V_CMPLX)
      select case (t2)
      case (V_INT);   call eval_node_set_op2_cmplx (en, add_ci)
      case (V_REAL);  call eval_node_set_op2_cmplx (en, add_cr)
      case (V_CMPLX); call eval_node_set_op2_cmplx (en, add_cc)
      end select
    end select
  case ("-")
    select case (t1)
    case (V_INT)
      select case (t2)
      case (V_INT);   call eval_node_set_op2_int  (en, sub_ii)
      case (V_REAL);  call eval_node_set_op2_real (en, sub_ir)
      case (V_CMPLX); call eval_node_set_op2_cmplx (en, sub_ic)
      end select
    case (V_REAL)
      select case (t2)
      case (V_INT);   call eval_node_set_op2_real (en, sub_ri)
      case (V_REAL);  call eval_node_set_op2_real (en, sub_rr)
      case (V_CMPLX); call eval_node_set_op2_cmplx (en, sub_rc)
      end select
    case (V_CMPLX)
      select case (t2)
      case (V_INT);   call eval_node_set_op2_cmplx (en, sub_ci)
      case (V_REAL);  call eval_node_set_op2_cmplx (en, sub_cr)
      case (V_CMPLX); call eval_node_set_op2_cmplx (en, sub_cc)
      end select
    end select
  end select
end if
pn_addition => parse_node_get_next_ptr (pn_addition)
end do
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done expr"
end if
end subroutine eval_node_compile_expr

```

<Eval trees: procedures>+≡

```

recursive subroutine eval_node_compile_term (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_factor, pn_multiplication, pn_op, pn_arg
  type(eval_node_t), pointer :: en1, en2
  type(string_t) :: key
  integer :: t1, t2, t
  if (debug_active (D_MODEL_F)) then
    print *, "read term"; call parse_node_write (pn)
  end if
  pn_factor => parse_node_get_sub_ptr (pn, tag="factor")
  call eval_node_compile_factor (en, pn_factor, var_list)
  pn_multiplication => &
    parse_node_get_next_ptr (pn_factor, tag="multiplication")
  do while (associated (pn_multiplication))
    pn_op => parse_node_get_sub_ptr (pn_multiplication)
    pn_arg => parse_node_get_next_ptr (pn_op, tag="factor")
    en1 => en
    call eval_node_compile_factor (en2, pn_arg, var_list)
    t1 = en1%result_type
    t2 = en2%result_type
    t = numeric_result_type (t1, t2)
    allocate (en)
    key = parse_node_get_key (pn_op)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
      select case (char (key))
        case ("*")
          select case (t1)
            case (V_INT)
              select case (t2)
                case (V_INT); call eval_node_init_int (en, mul_ii (en1, en2))
                case (V_REAL); call eval_node_init_real (en, mul_ir (en1, en2))
                case (V_CMLPX); call eval_node_init_cmlpx (en, mul_ic (en1, en2))
              end select
            case (V_REAL)
              select case (t2)
                case (V_INT); call eval_node_init_real (en, mul_ri (en1, en2))
                case (V_REAL); call eval_node_init_real (en, mul_rr (en1, en2))
                case (V_CMLPX); call eval_node_init_cmlpx (en, mul_rc (en1, en2))
              end select
            case (V_CMLPX)
              select case (t2)
                case (V_INT); call eval_node_init_cmlpx (en, mul_ci (en1, en2))
                case (V_REAL); call eval_node_init_cmlpx (en, mul_cr (en1, en2))
                case (V_CMLPX); call eval_node_init_cmlpx (en, mul_cc (en1, en2))
              end select
            end select
          case ("/")
            select case (t1)
              case (V_INT)
                select case (t2)

```

```

        case (V_INT); call eval_node_init_int (en, div_ii (en1, en2))
        case (V_REAL); call eval_node_init_real (en, div_ir (en1, en2))
        case (V_CMPLX); call eval_node_init_real (en, div_ir (en1, en2))
    end select
case (V_REAL)
    select case (t2)
        case (V_INT); call eval_node_init_real (en, div_ri (en1, en2))
        case (V_REAL); call eval_node_init_real (en, div_rr (en1, en2))
        case (V_CMPLX); call eval_node_init_cmplx (en, div_rc (en1, en2))
    end select
case (V_CMPLX)
    select case (t2)
        case (V_INT); call eval_node_init_cmplx (en, div_ci (en1, en2))
        case (V_REAL); call eval_node_init_cmplx (en, div_cr (en1, en2))
        case (V_CMPLX); call eval_node_init_cmplx (en, div_cc (en1, en2))
    end select
end select
call eval_node_final_rec (en1)
call eval_node_final_rec (en2)
deallocate (en1, en2)
else
call eval_node_init_branch (en, key, t, en1, en2)
select case (char (key))
case ("*")
    select case (t1)
        case (V_INT)
            select case (t2)
                case (V_INT); call eval_node_set_op2_int (en, mul_ii)
                case (V_REAL); call eval_node_set_op2_real (en, mul_ir)
                case (V_CMPLX); call eval_node_set_op2_cmplx (en, mul_ic)
            end select
        case (V_REAL)
            select case (t2)
                case (V_INT); call eval_node_set_op2_real (en, mul_ri)
                case (V_REAL); call eval_node_set_op2_real (en, mul_rr)
                case (V_CMPLX); call eval_node_set_op2_cmplx (en, mul_rc)
            end select
        case (V_CMPLX)
            select case (t2)
                case (V_INT); call eval_node_set_op2_cmplx (en, mul_ci)
                case (V_REAL); call eval_node_set_op2_cmplx (en, mul_cr)
                case (V_CMPLX); call eval_node_set_op2_cmplx (en, mul_cc)
            end select
        end select
case ("/")
    select case (t1)
        case (V_INT)
            select case (t2)
                case (V_INT); call eval_node_set_op2_int (en, div_ii)
                case (V_REAL); call eval_node_set_op2_real (en, div_ir)
                case (V_CMPLX); call eval_node_set_op2_cmplx (en, div_ic)
            end select
        case (V_REAL)

```

```

        select case (t2)
        case (V_INT);    call eval_node_set_op2_real (en, div_ri)
        case (V_REAL);   call eval_node_set_op2_real (en, div_rr)
        case (V_CMPLX);  call eval_node_set_op2_cmplx (en, div_rc)
        end select
    case (V_CMPLX)
        select case (t2)
        case (V_INT);    call eval_node_set_op2_cmplx (en, div_ci)
        case (V_REAL);   call eval_node_set_op2_cmplx (en, div_cr)
        case (V_CMPLX);  call eval_node_set_op2_cmplx (en, div_cc)
        end select
    end select
end select
end if
pn_multiplication => parse_node_get_next_ptr (pn_multiplication)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done term"
end if
end subroutine eval_node_compile_term

```

<Eval trees: procedures>+≡

```

recursive subroutine eval_node_compile_factor (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_value, pn_exponentiation, pn_op, pn_arg
    type(eval_node_t), pointer :: en1, en2
    type(string_t) :: key
    integer :: t1, t2, t
    if (debug_active (D_MODEL_F)) then
        print *, "read factor"; call parse_node_write (pn)
    end if
    pn_value => parse_node_get_sub_ptr (pn)
    call eval_node_compile_signed_value (en, pn_value, var_list)
    pn_exponentiation => &
        parse_node_get_next_ptr (pn_value, tag="exponentiation")
    if (associated (pn_exponentiation)) then
        pn_op => parse_node_get_sub_ptr (pn_exponentiation)
        pn_arg => parse_node_get_next_ptr (pn_op)
        en1 => en
        call eval_node_compile_signed_value (en2, pn_arg, var_list)
        t1 = en1%result_type
        t2 = en2%result_type
        t = numeric_result_type (t1, t2)
        allocate (en)
        key = parse_node_get_key (pn_op)
        if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
            select case (t1)
            case (V_INT)
                select case (t2)
                case (V_INT);    call eval_node_init_int    (en, pow_ii (en1, en2))
                case (V_REAL);   call eval_node_init_real   (en, pow_ir (en1, en2))

```



```

        case (V_CMPLX); call eval_node_init_cmplx (en, pow_ic (en1, en2))
    end select
case (V_REAL)
    select case (t2)
        case (V_INT);   call eval_node_init_real  (en, pow_ri (en1, en2))
        case (V_REAL);  call eval_node_init_real  (en, pow_rr (en1, en2))
        case (V_CMPLX); call eval_node_init_cmplx (en, pow_rc (en1, en2))
    end select
case (V_CMPLX)
    select case (t2)
        case (V_INT);   call eval_node_init_cmplx (en, pow_ci (en1, en2))
        case (V_REAL);  call eval_node_init_cmplx (en, pow_cr (en1, en2))
        case (V_CMPLX); call eval_node_init_cmplx (en, pow_cc (en1, en2))
    end select
end select
call eval_node_final_rec (en1)
call eval_node_final_rec (en2)
deallocate (en1, en2)
else
    call eval_node_init_branch (en, key, t, en1, en2)
    select case (t1)
        case (V_INT)
            select case (t2)
                case (V_INT);   call eval_node_set_op2_int  (en, pow_ii)
                case (V_REAL,V_CMPLX); call eval_type_error (pn, "exponentiation", t1)
            end select
        case (V_REAL)
            select case (t2)
                case (V_INT);   call eval_node_set_op2_real (en, pow_ri)
                case (V_REAL);  call eval_node_set_op2_real (en, pow_rr)
                case (V_CMPLX); call eval_type_error (pn, "exponentiation", t1)
            end select
        case (V_CMPLX)
            select case (t2)
                case (V_INT);   call eval_node_set_op2_cmplx (en, pow_ci)
                case (V_REAL);  call eval_node_set_op2_cmplx (en, pow_cr)
                case (V_CMPLX); call eval_node_set_op2_cmplx (en, pow_cc)
            end select
    end select
end if
end if
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done factor"
end if
end subroutine eval_node_compile_factor

```

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_signed_value (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_arg
    type(eval_node_t), pointer :: en1

```

```

integer :: t
if (debug_active (D_MODEL_F)) then
    print *, "read signed value"; call parse_node_write (pn)
end if
select case (char (parse_node_get_rule_key (pn)))
case ("signed_value")
    pn_arg => parse_node_get_sub_ptr (pn, 2)
    call eval_node_compile_value (en1, pn_arg, var_list)
    t = en1%result_type
    allocate (en)
    if (en1%type == EN_CONSTANT) then
        select case (t)
        case (V_INT); call eval_node_init_int (en, neg_i (en1))
        case (V_REAL); call eval_node_init_real (en, neg_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, neg_c (en1))
        end select
        call eval_node_final_rec (en1)
        deallocate (en1)
    else
        call eval_node_init_branch (en, var_str ("-"), t, en1)
        select case (t)
        case (V_INT); call eval_node_set_op1_int (en, neg_i)
        case (V_REAL); call eval_node_set_op1_real (en, neg_r)
        case (V_CMPLX); call eval_node_set_op1_cmplx (en, neg_c)
        end select
    end if
case default
    call eval_node_compile_value (en, pn, var_list)
end select
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done signed value"
end if
end subroutine eval_node_compile_signed_value

```

Integer, real and complex values have an optional unit. The unit is extracted and applied immediately. An integer with unit evaluates to a real constant.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_value (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    if (debug_active (D_MODEL_F)) then
        print *, "read value"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("integer_value", "real_value", "complex_value")
        call eval_node_compile_numeric_value (en, pn)
    case ("pi")
        call eval_node_compile_constant (en, pn)
    case ("I")
        call eval_node_compile_constant (en, pn)
    case ("variable")

```

```

        call eval_node_compile_variable (en, pn, var_list)
case ("result")
    call eval_node_compile_result (en, pn, var_list)
case ("expr")
    call eval_node_compile_expr (en, pn, var_list)
case ("block_expr")
    call eval_node_compile_block_expr (en, pn, var_list)
case ("conditional_expr")
    call eval_node_compile_conditional (en, pn, var_list)
case ("unary_function")
    call eval_node_compile_unary_function (en, pn, var_list)
case ("binary_function")
    call eval_node_compile_binary_function (en, pn, var_list)
case ("eval_fun")
    call eval_node_compile_eval_function (en, pn, var_list)
case ("count_fun")
    call eval_node_compile_count_function (en, pn, var_list)
case ("sum_fun", "prod_fun")
    call eval_node_compile_numeric_function (en, pn, var_list)
case default
    call parse_node_mismatch &
        ("integer|real|complex|constant|variable|" // &
         "expr|block_expr|conditional_expr|" // &
         "unary_function|binary_function|numeric_pexpr", pn)
end select
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done value"
end if
end subroutine eval_node_compile_value

```

Real, complex and integer values are numeric literals with an optional unit attached. In case of an integer, the unit actually makes it a real value in disguise. The signed version of real values is not possible in generic expressions; it is a special case for numeric constants in model files (see below). We do not introduce signed versions of complex values.

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_numeric_value (en, pn)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in), target :: pn
    type(parse_node_t), pointer :: pn_val, pn_unit
    allocate (en)
    pn_val => parse_node_get_sub_ptr (pn)
    pn_unit => parse_node_get_next_ptr (pn_val)
    select case (char (parse_node_get_rule_key (pn)))
    case ("integer_value")
        if (associated (pn_unit)) then
            call eval_node_init_real (en, &
                parse_node_get_integer (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_int (en, parse_node_get_integer (pn_val))
        end if
    case ("real_value")

```

```

        if (associated (pn_unit)) then
            call eval_node_init_real (en, &
                parse_node_get_real (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_real (en, parse_node_get_real (pn_val))
        end if
    case ("complex_value")
        if (associated (pn_unit)) then
            call eval_node_init_cmplx (en, &
                parse_node_get_cmplx (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_cmplx (en, parse_node_get_cmplx (pn_val))
        end if
    case ("neg_real_value")
        pn_val => parse_node_get_sub_ptr (parse_node_get_sub_ptr (pn, 2))
        pn_unit => parse_node_get_next_ptr (pn_val)
        if (associated (pn_unit)) then
            call eval_node_init_real (en, &
                - parse_node_get_real (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_real (en, - parse_node_get_real (pn_val))
        end if
    case ("pos_real_value")
        pn_val => parse_node_get_sub_ptr (parse_node_get_sub_ptr (pn, 2))
        pn_unit => parse_node_get_next_ptr (pn_val)
        if (associated (pn_unit)) then
            call eval_node_init_real (en, &
                parse_node_get_real (pn_val) * parse_node_get_unit (pn_unit))
        else
            call eval_node_init_real (en, parse_node_get_real (pn_val))
        end if
    case default
        call parse_node_mismatch &
            ("integer_value|real_value|complex_value|neg_real_value|pos_real_value", pn)
    end select
end subroutine eval_node_compile_numeric_value

```

These are the units, predefined and hardcoded. The default energy unit is GeV, the default angular unit is radians. We include units for observables of dimension energy squared. Luminosities are normalized in inverse femtobarns.

(Eval trees: procedures)+≡

```

function parse_node_get_unit (pn) result (factor)
    real(default) :: factor
    real(default) :: unit
    type(parse_node_t), intent(in) :: pn
    type(parse_node_t), pointer :: pn_unit, pn_unit_power
    type(parse_node_t), pointer :: pn_frac, pn_num, pn_int, pn_div, pn_den
    integer :: num, den
    pn_unit => parse_node_get_sub_ptr (pn)
    select case (char (parse_node_get_key (pn_unit)))
    case ("TeV"); unit = 1.e3_default
    case ("GeV"); unit = 1
    case ("MeV"); unit = 1.e-3_default

```

```

case ("keV"); unit = 1.e-6_default
case ("eV"); unit = 1.e-9_default
case ("meV"); unit = 1.e-12_default
case ("nbarn"); unit = 1.e6_default
case ("pbarn"); unit = 1.e3_default
case ("fbarn"); unit = 1
case ("abarn"); unit = 1.e-3_default
case ("rad"); unit = 1
case ("mrad"); unit = 1.e-3_default
case ("degree"); unit = degree
case ("%"); unit = 1.e-2_default
case default
    call msg_bug (" Unit ' " // &
        char (parse_node_get_key (pn)) // "' is undefined.")
end select
pn_unit_power => parse_node_get_next_ptr (pn_unit)
if (associated (pn_unit_power)) then
    pn_frac => parse_node_get_sub_ptr (pn_unit_power, 2)
    pn_num => parse_node_get_sub_ptr (pn_frac)
    select case (char (parse_node_get_rule_key (pn_num)))
    case ("neg_int")
        pn_int => parse_node_get_sub_ptr (pn_num, 2)
        num = - parse_node_get_integer (pn_int)
    case ("pos_int")
        pn_int => parse_node_get_sub_ptr (pn_num, 2)
        num = parse_node_get_integer (pn_int)
    case ("integer_literal")
        num = parse_node_get_integer (pn_num)
    case default
        call parse_node_mismatch ("neg_int|pos_int|integer_literal", pn_num)
    end select
    pn_div => parse_node_get_next_ptr (pn_num)
    if (associated (pn_div)) then
        pn_den => parse_node_get_sub_ptr (pn_div, 2)
        den = parse_node_get_integer (pn_den)
    else
        den = 1
    end if
else
    num = 1
    den = 1
end if
factor = unit ** (real (num, default) / den)
end function parse_node_get_unit

```

There are only two predefined constants, but more can be added easily.

<Eval trees: procedures>+≡

```

subroutine eval_node_compile_constant (en, pn)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    if (debug_active (D_MODEL_F)) then
        print *, "read constant"; call parse_node_write (pn)
    end if
    allocate (en)

```

```

select case (char (parse_node_get_key (pn)))
case ("pi");      call eval_node_init_real (en, pi)
case ("I");       call eval_node_init_cmplx (en, imago)
case default
    call parse_node_mismatch ("pi or I", pn)
end select
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done constant"
end if
end subroutine eval_node_compile_constant

```

Compile a variable, with or without a specified type. Take the list of variables, look for the name and make a node with a pointer to the value. If no type is provided, the variable is numeric, and the stored value determines whether it is real or integer.

We explicitly demand that the variable is defined, so we do not accidentally point to variables that are declared only later in the script but have come into existence in a previous compilation pass.

Variables may actually be anonymous, these are expressions in disguise. In that case, the expression replaces the variable name in the parse tree, and we allocate an ordinary expression node in the eval tree.

Variables of type V.PDG (pdg-code array) are not treated here. They are handled by `eval_node_compile_cvariable`.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_variable (en, pn, var_list, var_type)
type(eval_node_t), pointer :: en
type(parse_node_t), intent(in), target :: pn
type(var_list_t), intent(in), target :: var_list
integer, intent(in), optional :: var_type
type(parse_node_t), pointer :: pn_name
type(string_t) :: var_name
logical, target, save :: no_lval
real(default), target, save :: no_rval
type(subvt_t), target, save :: no_pval
type(string_t), target, save :: no_sval
logical, target, save :: unknown = .false.
integer :: type
logical :: defined
logical, pointer :: known
logical, pointer :: lptr
integer, pointer :: iptr
real(default), pointer :: rptr
complex(default), pointer :: cptr
type(subvt_t), pointer :: pptr
type(string_t), pointer :: sptr
procedure(obs_unary_int), pointer :: obs1_iptr
procedure(obs_unary_real), pointer :: obs1_rptr
procedure(obs_binary_int), pointer :: obs2_iptr
procedure(obs_binary_real), pointer :: obs2_rptr
procedure(obs_sev_int), pointer :: obsev_iptr
procedure(obs_sev_real), pointer :: obsev_rptr
type(prt_t), pointer :: p1, p2

```

```

if (debug_active (D_MODEL_F)) then
  print *, "read variable"; call parse_node_write (pn)
end if
if (present (var_type)) then
  select case (var_type)
    case (V_REAL, V_OBS1_REAL, V_OBS2_REAL, V_INT, V_OBS1_INT, &
          V_OBS2_INT, V_CMPLX)
      pn_name => pn
    case default
      pn_name => parse_node_get_sub_ptr (pn, 2)
    end select
else
  pn_name => pn
end if
select case (char (parse_node_get_rule_key (pn_name)))
case ("expr")
  call eval_node_compile_expr (en, pn_name, var_list)
case ("lexpr")
  call eval_node_compile_lexpr (en, pn_name, var_list)
case ("sexpr")
  call eval_node_compile_sexpr (en, pn_name, var_list)
case ("pexpr")
  call eval_node_compile_pexpr (en, pn_name, var_list)
case ("variable")
  var_name = parse_node_get_string (pn_name)
  if (present (var_type)) then
    select case (var_type)
      case (V_LOG); var_name = "?" // var_name
      case (V_SEV); var_name = "@" // var_name
      case (V_STR); var_name = "$" // var_name ! $ sign
    end select
  end if
  call var_list%get_var_properties &
    (var_name, req_type=var_type, type=type, is_defined=defined)
  allocate (en)
  if (defined) then
    select case (type)
      case (V_LOG)
        call var_list%get_lptr (var_name, lptr, known)
        call eval_node_init_log_ptr (en, var_name, lptr, known)
      case (V_INT)
        call var_list%get_iptr (var_name, iptr, known)
        call eval_node_init_int_ptr (en, var_name, iptr, known)
      case (V_REAL)
        call var_list%get_rptr (var_name, rptr, known)
        call eval_node_init_real_ptr (en, var_name, rptr, known)
      case (V_CMPLX)
        call var_list%get_cptra (var_name, cptra, known)
        call eval_node_init_cmplx_ptr (en, var_name, cptra, known)
      case (V_SEV)
        call var_list%get_pptra (var_name, pptra, known)
        call eval_node_init_subevt_ptr (en, var_name, pptra, known)
      case (V_STR)
        call var_list%get_sptr (var_name, sptra, known)
    end select
  end if
end if

```

```

        call eval_node_init_string_ptr (en, var_name, sptr, known)
case (V_OBS1_INT)
    call var_list%get_obs1_iptr (var_name, obs1_iptr, p1)
    call eval_node_init_obs1_int_ptr (en, var_name, obs1_iptr, p1)
case (V_OBS2_INT)
    call var_list%get_obs2_iptr (var_name, obs2_iptr, p1, p2)
    call eval_node_init_obs2_int_ptr (en, var_name, obs2_iptr, p1, p2)
case (V_OBSEV_INT)
    call var_list%get_obsev_iptr (var_name, obsev_iptr, pptr)
    call eval_node_init_obsev_int_ptr (en, var_name, obsev_iptr, pptr)
case (V_OBS1_REAL)
    call var_list%get_obs1_rptr (var_name, obs1_rptr, p1)
    call eval_node_init_obs1_real_ptr (en, var_name, obs1_rptr, p1)
case (V_OBS2_REAL)
    call var_list%get_obs2_rptr (var_name, obs2_rptr, p1, p2)
    call eval_node_init_obs2_real_ptr (en, var_name, obs2_rptr, p1, p2)
case (V_OBSEV_REAL)
    call var_list%get_obsev_rptr (var_name, obsev_rptr, pptr)
    call eval_node_init_obsev_real_ptr (en, var_name, obsev_rptr, pptr)
case default
    call parse_node_write (pn)
    call msg_fatal ("Variable of this type " // &
        "is not allowed in the present context")
    if (present (var_type)) then
        select case (var_type)
        case (V_LOG)
            call eval_node_init_log_ptr (en, var_name, no_lval, unknown)
        case (V_SEV)
            call eval_node_init_subevt_ptr &
                (en, var_name, no_pval, unknown)
        case (V_STR)
            call eval_node_init_string_ptr &
                (en, var_name, no_sval, unknown)
        end select
    else
        call eval_node_init_real_ptr (en, var_name, no_rval, unknown)
    end if
end select
else
    call parse_node_write (pn)
    call msg_error ("This variable is undefined at this point")
    if (present (var_type)) then
        select case (var_type)
        case (V_LOG)
            call eval_node_init_log_ptr (en, var_name, no_lval, unknown)
        case (V_SEV)
            call eval_node_init_subevt_ptr &
                (en, var_name, no_pval, unknown)
        case (V_STR)
            call eval_node_init_string_ptr (en, var_name, no_sval, unknown)
        end select
    else
        call eval_node_init_real_ptr (en, var_name, no_rval, unknown)
    end if
end if

```



```

        end if
    end select
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done variable"
    end if
end subroutine eval_node_compile_variable

```

In a given context, a variable has to have a certain type.

(Eval trees: procedures)+≡

```

subroutine check_var_type (pn, ok, type_actual, type_requested)
    type(parse_node_t), intent(in) :: pn
    logical, intent(out) :: ok
    integer, intent(in) :: type_actual
    integer, intent(in), optional :: type_requested
    if (present (type_requested)) then
        select case (type_requested)
        case (V_LOG)
            select case (type_actual)
            case (V_LOG)
            case default
                call parse_node_write (pn)
                call msg_fatal ("Variable type is invalid (should be logical)")
                ok = .false.
            end select
        case (V_SEV)
            select case (type_actual)
            case (V_SEV)
            case default
                call parse_node_write (pn)
                call msg_fatal &
                    ("Variable type is invalid (should be particle set)")
                ok = .false.
            end select
        case (V_PDG)
            select case (type_actual)
            case (V_PDG)
            case default
                call parse_node_write (pn)
                call msg_fatal &
                    ("Variable type is invalid (should be PDG array)")
                ok = .false.
            end select
        case (V_STR)
            select case (type_actual)
            case (V_STR)
            case default
                call parse_node_write (pn)
                call msg_fatal &
                    ("Variable type is invalid (should be string)")
                ok = .false.
            end select
        case default
            call parse_node_write (pn)
    end if
end subroutine

```

```

        call msg_bug ("Variable type is unknown")
    end select
else
    select case (type_actual)
    case (V_REAL, V_OBS1_REAL, V_OBS2_REAL, V_INT, V_OBS1_INT, &
          V_OBS2_INT, V_CMPLX)
    case default
        call parse_node_write (pn)
        call msg_fatal ("Variable type is invalid (should be numeric)")
        ok = .false.
    end select
end if
ok = .true.
end subroutine check_var_type

```

Retrieve the result of an integration. If the requested process has been integrated, the results are available as special variables. (The variables cannot be accessed in the usual way since they contain brackets in their names.)

Since this compilation step may occur before the processes have been loaded, we have to initialize the required variables before they are used.

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_result (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in), target :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_key, pn_prc_id
    type(string_t) :: key, prc_id, var_name
    integer, pointer :: iptr
    real(default), pointer :: rptr
    logical, pointer :: known
    if (debug_active (D_MODEL_F)) then
        print *, "read result"; call parse_node_write (pn)
    end if
    pn_key => parse_node_get_sub_ptr (pn)
    pn_prc_id => parse_node_get_next_ptr (pn_key)
    key = parse_node_get_key (pn_key)
    prc_id = parse_node_get_string (pn_prc_id)
    var_name = key // "(" // prc_id // ")"
    if (var_list%contains (var_name)) then
        allocate (en)
        select case (char(key))
        case ("num_id", "n_calls")
            call var_list%get_iptr (var_name, iptr, known)
            call eval_node_init_int_ptr (en, var_name, iptr, known)
        case ("integral", "error")
            call var_list%get_rptr (var_name, rptr, known)
            call eval_node_init_real_ptr (en, var_name, rptr, known)
        end select
    else
        call msg_fatal ("Result variable '" // char (var_name) &
            // "' is undefined (call 'integrate' before use)")
    end if
    if (debug_active (D_MODEL_F)) then

```

```

        call eval_node_write (en)
        print *, "done result"
    end if
end subroutine eval_node_compile_result

```

Functions with a single argument. For non-constant arguments, watch for functions which convert their argument to a different type.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_unary_function (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_fname, pn_arg
    type(eval_node_t), pointer :: en1
    type(string_t) :: key
    integer :: t
    if (debug_active (D_MODEL_F)) then
        print *, "read unary function"; call parse_node_write (pn)
    end if
    pn_fname => parse_node_get_sub_ptr (pn)
    pn_arg => parse_node_get_next_ptr (pn_fname, tag="function_arg1")
    call eval_node_compile_expr &
        (en1, parse_node_get_sub_ptr (pn_arg, tag="expr"), var_list)
    t = en1%result_type
    allocate (en)
    key = parse_node_get_key (pn_fname)
    if (en1%type == EN_CONSTANT) then
        select case (char (key))
        case ("complex")
            select case (t)
            case (V_INT); call eval_node_init_cmplx (en, cmplx_i (en1))
            case (V_REAL); call eval_node_init_cmplx (en, cmplx_r (en1))
            case (V_CMPLX); deallocate (en); en => en1; en1 => null ()
            case default; call eval_type_error (pn, char (key), t)
            end select
        case ("real")
            select case (t)
            case (V_INT); call eval_node_init_real (en, real_i (en1))
            case (V_REAL); deallocate (en); en => en1; en1 => null ()
            case (V_CMPLX); call eval_node_init_real (en, real_c (en1))
            case default; call eval_type_error (pn, char (key), t)
            end select
        case ("int")
            select case (t)
            case (V_INT); deallocate (en); en => en1; en1 => null ()
            case (V_REAL); call eval_node_init_int (en, int_r (en1))
            case (V_CMPLX); call eval_node_init_int (en, int_c (en1))
            end select
        case ("nint")
            select case (t)
            case (V_INT); deallocate (en); en => en1; en1 => null ()
            case (V_REAL); call eval_node_init_int (en, nint_r (en1))
            case default; call eval_type_error (pn, char (key), t)

```

```

        end select
case ("floor")
    select case (t)
        case (V_INT); deallocate (en); en => en1; en1 => null ()
        case (V_REAL); call eval_node_init_int (en, floor_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("ceiling")
    select case (t)
        case (V_INT); deallocate (en); en => en1; en1 => null ()
        case (V_REAL); call eval_node_init_int (en, ceiling_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("abs")
    select case (t)
        case (V_INT); call eval_node_init_int (en, abs_i (en1))
        case (V_REAL); call eval_node_init_real (en, abs_r (en1))
        case (V_CMPLX); call eval_node_init_real (en, abs_c (en1))
    end select
case ("conj")
    select case (t)
        case (V_INT); call eval_node_init_int (en, conjg_i (en1))
        case (V_REAL); call eval_node_init_real (en, conjg_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, conjg_c (en1))
    end select
case ("sgn")
    select case (t)
        case (V_INT); call eval_node_init_int (en, sgn_i (en1))
        case (V_REAL); call eval_node_init_real (en, sgn_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("sqrt")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, sqrt_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, sqrt_c (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("exp")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, exp_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, exp_c (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("log")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, log_r (en1))
        case (V_CMPLX); call eval_node_init_cmplx (en, log_c (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("log10")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, log10_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select

```

```

case ("sin")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, sin_r (en1))
    case (V_CMPLX); call eval_node_init_cmplx (en, sin_c (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("cos")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, cos_r (en1))
    case (V_CMPLX); call eval_node_init_cmplx (en, cos_c (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("tan")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, tan_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("asin")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, asin_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("acos")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, acos_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("atan")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, atan_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("sinh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, sinh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("cosh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, cosh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("tanh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, tanh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("asinh")
  select case (t)
    case (V_REAL); call eval_node_init_real (en, asinh_r (en1))
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("acosh")
  select case (t)

```

```

        case (V_REAL); call eval_node_init_real (en, acosh_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case ("atanh")
    select case (t)
        case (V_REAL); call eval_node_init_real (en, atanh_r (en1))
        case default; call eval_type_error (pn, char (key), t)
    end select
case default
    call parse_node_mismatch ("function name", pn_fname)
end select
if (associated (en1)) then
    call eval_node_final_rec (en1)
    deallocate (en1)
end if
else
    select case (char (key))
        case ("complex")
            call eval_node_init_branch (en, key, V_CMPLX, en1)
        case ("real")
            call eval_node_init_branch (en, key, V_REAL, en1)
        case ("int", "nint", "floor", "ceiling")
            call eval_node_init_branch (en, key, V_INT, en1)
        case default
            call eval_node_init_branch (en, key, t, en1)
    end select
    select case (char (key))
        case ("complex")
            select case (t)
                case (V_INT); call eval_node_set_op1_cmplx (en, cmplx_i)
                case (V_REAL); call eval_node_set_op1_cmplx (en, cmplx_r)
                case (V_CMPLX); deallocate (en); en => en1
                case default; call eval_type_error (pn, char (key), t)
            end select
        case ("real")
            select case (t)
                case (V_INT); call eval_node_set_op1_real (en, real_i)
                case (V_REAL); deallocate (en); en => en1
                case (V_CMPLX); call eval_node_set_op1_real (en, real_c)
                case default; call eval_type_error (pn, char (key), t)
            end select
        case ("int")
            select case (t)
                case (V_INT); deallocate (en); en => en1
                case (V_REAL); call eval_node_set_op1_int (en, int_r)
                case (V_CMPLX); call eval_node_set_op1_int (en, int_c)
            end select
        case ("nint")
            select case (t)
                case (V_INT); deallocate (en); en => en1
                case (V_REAL); call eval_node_set_op1_int (en, nint_r)
                case default; call eval_type_error (pn, char (key), t)
            end select
        case ("floor")

```

```

        select case (t)
        case (V_INT); deallocate (en); en => en1
        case (V_REAL); call eval_node_set_op1_int (en, floor_r)
        case default; call eval_type_error (pn, char (key), t)
        end select
case ("ceiling")
    select case (t)
    case (V_INT); deallocate (en); en => en1
    case (V_REAL); call eval_node_set_op1_int (en, ceiling_r)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("abs")
    select case (t)
    case (V_INT); call eval_node_set_op1_int (en, abs_i)
    case (V_REAL); call eval_node_set_op1_real (en, abs_r)
    case (V_CMPLX);
        call eval_node_init_branch (en, key, V_REAL, en1)
        call eval_node_set_op1_real (en, abs_c)
    end select
case ("conj")
    select case (t)
    case (V_INT); call eval_node_set_op1_int (en, conjg_i)
    case (V_REAL); call eval_node_set_op1_real (en, conjg_r)
    case (V_CMPLX); call eval_node_set_op1_cmplx (en, conjg_c)
    end select
case ("sgn")
    select case (t)
    case (V_INT); call eval_node_set_op1_int (en, sgn_i)
    case (V_REAL); call eval_node_set_op1_real (en, sgn_r)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("sqrt")
    select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, sqrt_r)
    case (V_CMPLX); call eval_node_set_op1_cmplx (en, sqrt_c)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("exp")
    select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, exp_r)
    case (V_CMPLX); call eval_node_set_op1_cmplx (en, exp_c)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("log")
    select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, log_r)
    case (V_CMPLX); call eval_node_set_op1_cmplx (en, log_c)
    case default; call eval_type_error (pn, char (key), t)
    end select
case ("log10")
    select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, log10_r)
    case default; call eval_type_error (pn, char (key), t)
    end select

```

```

case ("sin")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, sin_r)
    case (V_CMPLX); call eval_node_set_op1_cmplx (en, sin_c)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("cos")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, cos_r)
    case (V_CMPLX); call eval_node_set_op1_cmplx (en, cos_c)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("tan")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, tan_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("asin")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, asin_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("acos")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, acos_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("atan")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, atan_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("sinh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, sinh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("cosh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, cosh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("tanh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, tanh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("asinh")
  select case (t)
    case (V_REAL); call eval_node_set_op1_real (en, asinh_r)
    case default; call eval_type_error (pn, char (key), t)
  end select
case ("acosh")
  select case (t)

```



```

        case (V_REAL); call eval_node_set_op1_real (en, acosh_r)
        case default; call eval_type_error (pn, char (key), t)
        end select
    case ("atanh")
        select case (t)
            case (V_REAL); call eval_node_set_op1_real (en, atanh_r)
            case default; call eval_type_error (pn, char (key), t)
            end select
        case default
            call parse_node_mismatch ("function name", pn_fname)
        end select
    end if
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done function"
    end if
end subroutine eval_node_compile_unary_function

```

Functions with two arguments.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_binary_function (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_fname, pn_arg, pn_arg1, pn_arg2
    type(eval_node_t), pointer :: en1, en2
    type(string_t) :: key
    integer :: t1, t2
    if (debug_active (D_MODEL_F)) then
        print *, "read binary function"; call parse_node_write (pn)
    end if
    pn_fname => parse_node_get_sub_ptr (pn)
    pn_arg => parse_node_get_next_ptr (pn_fname, tag="function_arg2")
    pn_arg1 => parse_node_get_sub_ptr (pn_arg, tag="expr")
    pn_arg2 => parse_node_get_next_ptr (pn_arg1, tag="expr")
    call eval_node_compile_expr (en1, pn_arg1, var_list)
    call eval_node_compile_expr (en2, pn_arg2, var_list)
    t1 = en1%result_type
    t2 = en2%result_type
    allocate (en)
    key = parse_node_get_key (pn_fname)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
        select case (char (key))
            case ("max")
                select case (t1)
                    case (V_INT)
                        select case (t2)
                            case (V_INT); call eval_node_init_int (en, max_ii (en1, en2))
                            case (V_REAL); call eval_node_init_real (en, max_ir (en1, en2))
                            case default; call eval_type_error (pn, char (key), t2)
                        end select
                    case (V_REAL)
                        select case (t2)
                            case (V_INT); call eval_node_init_real (en, max_ri (en1, en2))

```

```

        case (V_REAL); call eval_node_init_real (en, max_rr (en1, en2))
        case default;  call eval_type_error (pn, char (key), t2)
    end select
    case default;  call eval_type_error (pn, char (key), t1)
end select
case ("min")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_init_int  (en, min_ii (en1, en2))
        case (V_REAL); call eval_node_init_real (en, min_ir (en1, en2))
        case default; call eval_type_error (pn, char (key), t2)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_init_real (en, min_ri (en1, en2))
        case (V_REAL); call eval_node_init_real (en, min_rr (en1, en2))
        case default; call eval_type_error (pn, char (key), t2)
        end select
    case default;  call eval_type_error (pn, char (key), t1)
end select
case ("mod")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_init_int  (en, mod_ii (en1, en2))
        case (V_REAL); call eval_node_init_real (en, mod_ir (en1, en2))
        case default; call eval_type_error (pn, char (key), t2)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_init_real (en, mod_ri (en1, en2))
        case (V_REAL); call eval_node_init_real (en, mod_rr (en1, en2))
        case default; call eval_type_error (pn, char (key), t2)
        end select
    case default;  call eval_type_error (pn, char (key), t1)
end select
case ("modulo")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_init_int  (en, modulo_ii (en1, en2))
        case (V_REAL); call eval_node_init_real (en, modulo_ir (en1, en2))
        case default; call eval_type_error (pn, char (key), t2)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_init_real (en, modulo_ri (en1, en2))
        case (V_REAL); call eval_node_init_real (en, modulo_rr (en1, en2))
        case default; call eval_type_error (pn, char (key), t2)
        end select
    case default;  call eval_type_error (pn, char (key), t2)
end select
case default

```

```

        call parse_node_mismatch ("function name", pn_fname)
    end select
    call eval_node_final_rec (en1)
    deallocate (en1)
else
    call eval_node_init_branch (en, key, t1, en1, en2)
    select case (char (key))
    case ("max")
        select case (t1)
        case (V_INT)
            select case (t2)
            case (V_INT); call eval_node_set_op2_int (en, max_ii)
            case (V_REAL); call eval_node_set_op2_real (en, max_ir)
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case (V_REAL)
            select case (t2)
            case (V_INT); call eval_node_set_op2_real (en, max_ri)
            case (V_REAL); call eval_node_set_op2_real (en, max_rr)
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case default; call eval_type_error (pn, char (key), t2)
        end select
    case ("min")
        select case (t1)
        case (V_INT)
            select case (t2)
            case (V_INT); call eval_node_set_op2_int (en, min_ii)
            case (V_REAL); call eval_node_set_op2_real (en, min_ir)
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case (V_REAL)
            select case (t2)
            case (V_INT); call eval_node_set_op2_real (en, min_ri)
            case (V_REAL); call eval_node_set_op2_real (en, min_rr)
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case default; call eval_type_error (pn, char (key), t2)
        end select
    case ("mod")
        select case (t1)
        case (V_INT)
            select case (t2)
            case (V_INT); call eval_node_set_op2_int (en, mod_ii)
            case (V_REAL); call eval_node_set_op2_real (en, mod_ir)
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case (V_REAL)
            select case (t2)
            case (V_INT); call eval_node_set_op2_real (en, mod_ri)
            case (V_REAL); call eval_node_set_op2_real (en, mod_rr)
            case default; call eval_type_error (pn, char (key), t2)
            end select
        case default; call eval_type_error (pn, char (key), t2)
    end select
end select

```

```

end select
case ("modulo")
  select case (t1)
    case (V_INT)
      select case (t2)
        case (V_INT); call eval_node_set_op2_int (en, modulo_ii)
        case (V_REAL); call eval_node_set_op2_real (en, modulo_ir)
        case default; call eval_type_error (pn, char (key), t2)
      end select
    case (V_REAL)
      select case (t2)
        case (V_INT); call eval_node_set_op2_real (en, modulo_ri)
        case (V_REAL); call eval_node_set_op2_real (en, modulo_rr)
        case default; call eval_type_error (pn, char (key), t2)
      end select
      case default; call eval_type_error (pn, char (key), t2)
    end select
  case default
    call parse_node_mismatch ("function name", pn_fname)
  end select
end if
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done function"
end if
end subroutine eval_node_compile_binary_function

```

Variable definition

A block expression contains a variable definition (first argument) and an expression where the definition can be used (second argument). The `result_type` decides which type of expression is expected for the second argument. For numeric variables, if there is a mismatch between real and integer type, insert an extra node for type conversion.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_block_expr &
  (en, pn, var_list, result_type)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  integer, intent(in), optional :: result_type
  type(parse_node_t), pointer :: pn_var_spec, pn_var_subspec
  type(parse_node_t), pointer :: pn_var_type, pn_var_name, pn_var_expr
  type(parse_node_t), pointer :: pn_expr
  type(string_t) :: var_name
  type(eval_node_t), pointer :: en1, en2
  integer :: var_type
  logical :: new
  if (debug_active (D_MODEL_F)) then
    print *, "read block expr"; call parse_node_write (pn)
  end if
  new = .false.

```

```

pn_var_spec => parse_node_get_sub_ptr (pn, 2)
select case (char (parse_node_get_rule_key (pn_var_spec)))
case ("var_num");      var_type = V_NONE
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec)
case ("var_int");      var_type = V_INT
    new = .true.
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case ("var_real");     var_type = V_REAL
    new = .true.
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case ("var_cmplx");    var_type = V_CMPLX
    new = .true.
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case ("var_logical_new"); var_type = V_LOG
    new = .true.
    pn_var_subspec => parse_node_get_sub_ptr (pn_var_spec, 2)
    pn_var_name => parse_node_get_sub_ptr (pn_var_subspec, 2)
case ("var_logical_spec"); var_type = V_LOG
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case ("var_plist_new"); var_type = V_SEV
    new = .true.
    pn_var_subspec => parse_node_get_sub_ptr (pn_var_spec, 2)
    pn_var_name => parse_node_get_sub_ptr (pn_var_subspec, 2)
case ("var_plist_spec"); var_type = V_SEV
    new = .true.
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case ("var_alias");    var_type = V_PDG
    new = .true.
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case ("var_string_new"); var_type = V_STR
    new = .true.
    pn_var_subspec => parse_node_get_sub_ptr (pn_var_spec, 2)
    pn_var_name => parse_node_get_sub_ptr (pn_var_subspec, 2)
case ("var_string_spec"); var_type = V_STR
    pn_var_name => parse_node_get_sub_ptr (pn_var_spec, 2)
case default
    call parse_node_mismatch &
        ("logical|int|real|plist|alias", pn_var_type)
end select
pn_var_expr => parse_node_get_next_ptr (pn_var_name, 2)
pn_expr => parse_node_get_next_ptr (pn_var_spec, 2)
var_name = parse_node_get_string (pn_var_name)
select case (var_type)
case (V_LOG); var_name = "?" // var_name
case (V_SEV); var_name = "@" // var_name
case (V_STR); var_name = "$" // var_name    ! $ sign
end select
call var_list_check_user_var (var_list, var_name, var_type, new)
call eval_node_compile_genexpr (en1, pn_var_expr, var_list, var_type)
call insert_conversion_node (en1, var_type)
allocate (en)
call eval_node_init_block (en, var_name, var_type, en1, var_list)
call eval_node_compile_genexpr (en2, pn_expr, en%var_list, result_type)
call eval_node_set_expr (en, en2)

```

```

    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done block expr"
    end if
end subroutine eval_node_compile_block_expr

```

Insert a conversion node for integer/real/complex transformation if necessary.
 What shall we do for the complex to integer/real conversion?

(Eval trees: procedures)+≡

```

subroutine insert_conversion_node (en, result_type)
    type(eval_node_t), pointer :: en
    integer, intent(in) :: result_type
    type(eval_node_t), pointer :: en_conv
    select case (en%result_type)
    case (V_INT)
        select case (result_type)
        case (V_REAL)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("real"), V_REAL, en)
            call eval_node_set_op1_real (en_conv, real_i)
            en => en_conv
        case (V_CMPLX)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("complex"), V_CMPLX, en)
            call eval_node_set_op1_cmplx (en_conv, cmplx_i)
            en => en_conv
        end select
    case (V_REAL)
        select case (result_type)
        case (V_INT)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("int"), V_INT, en)
            call eval_node_set_op1_int (en_conv, int_r)
            en => en_conv
        case (V_CMPLX)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("complex"), V_CMPLX, en)
            call eval_node_set_op1_cmplx (en_conv, cmplx_r)
            en => en_conv
        end select
    case (V_CMPLX)
        select case (result_type)
        case (V_INT)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("int"), V_INT, en)
            call eval_node_set_op1_int (en_conv, int_c)
            en => en_conv
        case (V_REAL)
            allocate (en_conv)
            call eval_node_init_branch (en_conv, var_str ("real"), V_REAL, en)
            call eval_node_set_op1_real (en_conv, real_c)
            en => en_conv
        end select
    end select
end subroutine

```

```

        case default
        end select
    end subroutine insert_conversion_node

```

Conditionals

A conditional has the structure if lexpr then expr else expr. So we first evaluate the logical expression, then depending on the result the first or second expression. Note that the second expression is mandatory.

The `result_type`, if present, defines the requested type of the `then` and `else` clauses. Default is numeric (int/real). If there is a mismatch between real and integer result types, insert conversion nodes.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_conditional &
    (en, pn, var_list, result_type)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    integer, intent(in), optional :: result_type
    type(parse_node_t), pointer :: pn_condition, pn_expr
    type(parse_node_t), pointer :: pn_maybe_elseif, pn_elseif_branch
    type(parse_node_t), pointer :: pn_maybe_else, pn_else_branch, pn_else_expr
    type(eval_node_t), pointer :: en0, en1, en2
    integer :: restype
    if (debug_active (D_MODEL_F)) then
        print *, "read conditional"; call parse_node_write (pn)
    end if
    pn_condition => parse_node_get_sub_ptr (pn, 2, tag="lexpr")
    pn_expr => parse_node_get_next_ptr (pn_condition, 2)
    call eval_node_compile_lexpr (en0, pn_condition, var_list)
    call eval_node_compile_genexpr (en1, pn_expr, var_list, result_type)
    if (present (result_type)) then
        restype = major_result_type (result_type, en1%result_type)
    else
        restype = en1%result_type
    end if
    pn_maybe_elseif => parse_node_get_next_ptr (pn_expr)
    select case (char (parse_node_get_rule_key (pn_maybe_elseif)))
    case ("maybe_elseif_expr", &
        "maybe_elseif_lexpr", &
        "maybe_elseif_pexpr", &
        "maybe_elseif_cexpr", &
        "maybe_elseif_sexpr")
        pn_elseif_branch => parse_node_get_sub_ptr (pn_maybe_elseif)
        pn_maybe_else => parse_node_get_next_ptr (pn_maybe_elseif)
        select case (char (parse_node_get_rule_key (pn_maybe_else)))
        case ("maybe_else_expr", &
            "maybe_else_lexpr", &
            "maybe_else_pexpr", &
            "maybe_else_cexpr", &
            "maybe_else_sexpr")
            pn_else_branch => parse_node_get_sub_ptr (pn_maybe_else)

```

```

        pn_else_expr => parse_node_get_sub_ptr (pn_else_branch, 2)
    case default
        pn_else_expr => null ()
    end select
    call eval_node_compile_elseif &
        (en2, pn_elseif_branch, pn_else_expr, var_list, restype)
case ("maybe_else_expr", &
    "maybe_else_lexpr", &
    "maybe_else_pexpr", &
    "maybe_else_cexpr", &
    "maybe_else_sexpr")
    pn_maybe_else => pn_maybe_elseif
    pn_maybe_elseif => null ()
    pn_else_branch => parse_node_get_sub_ptr (pn_maybe_else)
    pn_else_expr => parse_node_get_sub_ptr (pn_else_branch, 2)
    call eval_node_compile_genexpr &
        (en2, pn_else_expr, var_list, restype)
case ("endif")
    call eval_node_compile_default_else (en2, restype)
case default
    call msg_bug ("Broken conditional: unexpected " &
        // char (parse_node_get_rule_key (pn_maybe_elseif)))
end select
call eval_node_create_conditional (en, en0, en1, en2, restype)
call conditional_insert_conversion_nodes (en, restype)
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done conditional"
end if
end subroutine eval_node_compile_conditional

```

This recursively generates 'elseif' conditionals as a chain of sub-nodes of the main conditional.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_elseif &
    (en, pn, pn_else_expr, var_list, result_type)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in), target :: pn
    type(parse_node_t), pointer :: pn_else_expr
    type(var_list_t), intent(in), target :: var_list
    integer, intent(inout) :: result_type
    type(parse_node_t), pointer :: pn_next, pn_condition, pn_expr
    type(eval_node_t), pointer :: en0, en1, en2
    pn_condition => parse_node_get_sub_ptr (pn, 2, tag="lexpr")
    pn_expr => parse_node_get_next_ptr (pn_condition, 2)
    call eval_node_compile_lexpr (en0, pn_condition, var_list)
    call eval_node_compile_genexpr (en1, pn_expr, var_list, result_type)
    result_type = major_result_type (result_type, en1%result_type)
    pn_next => parse_node_get_next_ptr (pn)
    if (associated (pn_next)) then
        call eval_node_compile_elseif &
            (en2, pn_next, pn_else_expr, var_list, result_type)
        result_type = major_result_type (result_type, en2%result_type)
    end if
end subroutine

```



```

else if (associated (pn_else_expr)) then
    call eval_node_compile_genexpr &
        (en2, pn_else_expr, var_list, result_type)
    result_type = major_result_type (result_type, en2%result_type)
else
    call eval_node_compile_default_else (en2, result_type)
end if
call eval_node_create_conditional (en, en0, en1, en2, result_type)
end subroutine eval_node_compile_elseif

```

This makes a default 'else' branch in case it was omitted. The default value just depends on the expected type.

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_default_else (en, result_type)
    type(eval_node_t), pointer :: en
    integer, intent(in) :: result_type
    type(subvt_t) :: pval_empty
    type(pdg_array_t) :: aval_undefined
    allocate (en)
    select case (result_type)
    case (V_LOG); call eval_node_init_log (en, .false.)
    case (V_INT); call eval_node_init_int (en, 0)
    case (V_REAL); call eval_node_init_real (en, 0._default)
    case (V_CMPLX)
        call eval_node_init_cmplx (en, (0._default, 0._default))
    case (V_SEV)
        call subvt_init (pval_empty)
        call eval_node_init_subvt (en, pval_empty)
    case (V_PDG)
        call eval_node_init_pdg_array (en, aval_undefined)
    case (V_STR)
        call eval_node_init_string (en, var_str (""))
    case default
        call msg_bug ("Undefined type for 'else' branch in conditional")
    end select
end subroutine eval_node_compile_default_else

```

If the logical expression is constant, we can simplify the conditional node by replacing it with the selected branch. Otherwise, we initialize a true branching.

(Eval trees: procedures)+≡

```

subroutine eval_node_create_conditional (en, en0, en1, en2, result_type)
    type(eval_node_t), pointer :: en, en0, en1, en2
    integer, intent(in) :: result_type
    if (en0%type == EN_CONSTANT) then
        if (en0%lval) then
            en => en1
            call eval_node_final_rec (en2)
            deallocate (en2)
        else
            en => en2
            call eval_node_final_rec (en1)
            deallocate (en1)
        end if
    end if

```

```

else
  allocate (en)
  call eval_node_init_conditional (en, result_type, en0, en1, en2)
end if
end subroutine eval_node_create_conditional

```

Return the numerical result type which should be used for the combination of the two result types.

<Eval trees: procedures>+≡

```

function major_result_type (t1, t2) result (t)
  integer :: t
  integer, intent(in) :: t1, t2
  select case (t1)
  case (V_INT)
    select case (t2)
    case (V_INT, V_REAL, V_CMPLX)
      t = t2
    case default
      call type_mismatch ()
    end select
  case (V_REAL)
    select case (t2)
    case (V_INT)
      t = t1
    case (V_REAL, V_CMPLX)
      t = t2
    case default
      call type_mismatch ()
    end select
  case (V_CMPLX)
    select case (t2)
    case (V_INT, V_REAL, V_CMPLX)
      t = t1
    case default
      call type_mismatch ()
    end select
  case default
    if (t1 == t2) then
      t = t1
    else
      call type_mismatch ()
    end if
  end select
contains
  subroutine type_mismatch ()
    call msg_bug ("Type mismatch in branches of a conditional expression")
  end subroutine type_mismatch
end function major_result_type

```

Recursively insert conversion nodes where necessary.

<Eval trees: procedures>+≡

```

recursive subroutine conditional_insert_conversion_nodes (en, result_type)
  type(eval_node_t), intent(inout), target :: en

```

```

integer, intent(in) :: result_type
select case (result_type)
case (V_INT, V_REAL, V_CMPLX)
    call insert_conversion_node (en%arg1, result_type)
    if (en%arg2%type == EN_CONDITIONAL) then
        call conditional_insert_conversion_nodes (en%arg2, result_type)
    else
        call insert_conversion_node (en%arg2, result_type)
    end if
end select
end subroutine conditional_insert_conversion_nodes

```

Logical expressions

A logical expression consists of one or more singlet logical expressions concatenated by ;. This is for allowing side-effects, only the last value is used.

(Eval trees: procedures) +=

```

recursive subroutine eval_node_compile_lexpr (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_term, pn_sequel, pn_arg
    type(eval_node_t), pointer :: en1, en2
    if (debug_active (D_MODEL_F)) then
        print *, "read lexpr"; call parse_node_write (pn)
    end if
    pn_term => parse_node_get_sub_ptr (pn, tag="lsinglet")
    call eval_node_compile_lsinglet (en, pn_term, var_list)
    pn_sequel => parse_node_get_next_ptr (pn_term, tag="lsequel")
    do while (associated (pn_sequel))
        pn_arg => parse_node_get_sub_ptr (pn_sequel, 2, tag="lsinglet")
        en1 => en
        call eval_node_compile_lsinglet (en2, pn_arg, var_list)
        allocate (en)
        if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
            call eval_node_init_log (en, ignore_first_ll (en1, en2))
            call eval_node_final_rec (en1)
            call eval_node_final_rec (en2)
            deallocate (en1, en2)
        else
            call eval_node_init_branch &
                (en, var_str ("lsequel"), V_LOG, en1, en2)
            call eval_node_set_op2_log (en, ignore_first_ll)
        end if
        pn_sequel => parse_node_get_next_ptr (pn_sequel)
    end do
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done lexpr"
    end if
end subroutine eval_node_compile_lexpr

```

A logical singlet expression consists of one or more logical terms concatenated by or.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_lsinglet (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_term, pn_alternative, pn_arg
  type(eval_node_t), pointer :: en1, en2
  if (debug_active (D_MODEL_F)) then
    print *, "read lsinglet"; call parse_node_write (pn)
  end if
  pn_term => parse_node_get_sub_ptr (pn, tag="lterm")
  call eval_node_compile_lterm (en, pn_term, var_list)
  pn_alternative => parse_node_get_next_ptr (pn_term, tag="alternative")
  do while (associated (pn_alternative))
    pn_arg => parse_node_get_sub_ptr (pn_alternative, 2, tag="lterm")
    en1 => en
    call eval_node_compile_lterm (en2, pn_arg, var_list)
    allocate (en)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
      call eval_node_init_log (en, or_ll (en1, en2))
      call eval_node_final_rec (en1)
      call eval_node_final_rec (en2)
      deallocate (en1, en2)
    else
      call eval_node_init_branch &
        (en, var_str ("alternative"), V_LOG, en1, en2)
      call eval_node_set_op2_log (en, or_ll)
    end if
    pn_alternative => parse_node_get_next_ptr (pn_alternative)
  end do
  if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done lsinglet"
  end if
end subroutine eval_node_compile_lsinglet

```

A logical term consists of one or more logical values concatenated by and.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_lterm (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_term, pn_coincidence, pn_arg
  type(eval_node_t), pointer :: en1, en2
  if (debug_active (D_MODEL_F)) then
    print *, "read lterm"; call parse_node_write (pn)
  end if
  pn_term => parse_node_get_sub_ptr (pn)
  call eval_node_compile_lvalue (en, pn_term, var_list)
  pn_coincidence => parse_node_get_next_ptr (pn_term, tag="coincidence")
  do while (associated (pn_coincidence))

```

```

pn_arg => parse_node_get_sub_ptr (pn_coincidence, 2)
en1 => en
call eval_node_compile_lvalue (en2, pn_arg, var_list)
allocate (en)
if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
    call eval_node_init_log (en, and_ll (en1, en2))
    call eval_node_final_rec (en1)
    call eval_node_final_rec (en2)
    deallocate (en1, en2)
else
    call eval_node_init_branch &
        (en, var_str ("coincidence"), V_LOG, en1, en2)
    call eval_node_set_op2_log (en, and_ll)
end if
pn_coincidence => parse_node_get_next_ptr (pn_coincidence)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done lterm"
end if
end subroutine eval_node_compile_lterm

```

Logical variables are disabled, because they are confused with the l.h.s. of compared expressions.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_lvalue (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    if (debug_active (D_MODEL_F)) then
        print *, "read lvalue"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("true")
        allocate (en)
        call eval_node_init_log (en, .true.)
    case ("false")
        allocate (en)
        call eval_node_init_log (en, .false.)
    case ("negation")
        call eval_node_compile_negation (en, pn, var_list)
    case ("lvariable")
        call eval_node_compile_variable (en, pn, var_list, V_LOG)
    case ("lexpr")
        call eval_node_compile_lexpr (en, pn, var_list)
    case ("block_lexpr")
        call eval_node_compile_block_expr (en, pn, var_list, V_LOG)
    case ("conditional_lexpr")
        call eval_node_compile_conditional (en, pn, var_list, V_LOG)
    case ("compared_expr")
        call eval_node_compile_compared_expr (en, pn, var_list, V_REAL)
    case ("compared_sexpr")
        call eval_node_compile_compared_expr (en, pn, var_list, V_STR)

```

```

case ("all_fun", "any_fun", "no_fun", "photon_isolation_fun")
    call eval_node_compile_log_function (en, pn, var_list)
case ("record_cmd")
    call eval_node_compile_record_cmd (en, pn, var_list)
case default
    call parse_node_mismatch &
        ("true|false|negation|lvariable|" // &
         "lexpr|block_lexpr|conditional_lexpr|" // &
         "compared_expr|compared_sexpr|logical_pexpr", pn)
end select
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done lvalue"
end if
end subroutine eval_node_compile_lvalue

```

A negation consists of the keyword `not` and a logical value.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_negation (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_arg
    type(eval_node_t), pointer :: en1
    if (debug_active (D_MODEL_F)) then
        print *, "read negation"; call parse_node_write (pn)
    end if
    pn_arg => parse_node_get_sub_ptr (pn, 2)
    call eval_node_compile_lvalue (en1, pn_arg, var_list)
    allocate (en)
    if (en1%type == EN_CONSTANT) then
        call eval_node_init_log (en, not_1 (en1))
        call eval_node_final_rec (en1)
        deallocate (en1)
    else
        call eval_node_init_branch (en, var_str ("not"), V_LOG, en1)
        call eval_node_set_op1_log (en, not_1)
    end if
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done negation"
    end if
end subroutine eval_node_compile_negation

```

Comparisons

Up to the loop, this is easy. There is always at least one comparison. This is evaluated, and the result is the logical node `en`. If it is constant, we keep its second sub-node as `en2`. (Thus, at the very end `en2` has to be deleted if `en` is (still) constant.)

If there is another comparison, we first check if the first comparison was constant. In that case, there are two possibilities: (i) it was true. Then, its

right-hand side is compared with the new right-hand side, and the result replaces the previous one which is deleted. (ii) it was false. In this case, the result of the whole comparison is false, and we can exit the loop without evaluating anything else.

Now assume that the first comparison results in a valid branch, its second sub-node kept as **en2**. We first need a copy of this, which becomes the new left-hand side. If **en2** is constant, we make an identical constant node **en1**. Otherwise, we make **en1** an appropriate pointer node. Next, the first branch is saved as **en0** and we evaluate the comparison between **en1** and the a right-hand side. If this turns out to be constant, there are again two possibilities: (i) true, then we revert to the previous result. (ii) false, then the wh

(Eval trees: procedures)+≡

```
recursive subroutine eval_node_compile_compared_expr (en, pn, var_list, type)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  integer, intent(in) :: type
  type(parse_node_t), pointer :: pn_comparison, pn_expr1
  type(eval_node_t), pointer :: en0, en1, en2
  if (debug_active (D_MODEL_F)) then
    print *, "read comparison"; call parse_node_write (pn)
  end if
  select case (type)
  case (V_INT, V_REAL)
    pn_expr1 => parse_node_get_sub_ptr (pn, tag="expr")
    call eval_node_compile_expr (en1, pn_expr1, var_list)
    pn_comparison => parse_node_get_next_ptr (pn_expr1, tag="comparison")
  case (V_STR)
    pn_expr1 => parse_node_get_sub_ptr (pn, tag="sexpr")
    call eval_node_compile_sexpr (en1, pn_expr1, var_list)
    pn_comparison => parse_node_get_next_ptr (pn_expr1, tag="str_comparison")
  end select
  call eval_node_compile_comparison &
    (en, en1, en2, pn_comparison, var_list, type)
  pn_comparison => parse_node_get_next_ptr (pn_comparison)
  SCAN_FURTHER: do while (associated (pn_comparison))
    if (en%type == EN_CONSTANT) then
      if (en%lval) then
        en1 => en2
        call eval_node_final_rec (en); deallocate (en)
        call eval_node_compile_comparison &
          (en, en1, en2, pn_comparison, var_list, type)
      else
        exit SCAN_FURTHER
      end if
    else
      allocate (en1)
      if (en2%type == EN_CONSTANT) then
        select case (en2%result_type)
        case (V_INT); call eval_node_init_int    (en1, en2%ival)
        case (V_REAL); call eval_node_init_real  (en1, en2%rval)
        case (V_STR); call eval_node_init_string (en1, en2%sval)
        end select
      end if
    end if
  end do
end
```

```

else
  select case (en2%result_type)
  case (V_INT); call eval_node_init_int_ptr &
    (en1, var_str ("(previous)"), en2%ival, en2%value_is_known)
  case (V_REAL); call eval_node_init_real_ptr &
    (en1, var_str ("(previous)"), en2%rval, en2%value_is_known)
  case (V_STR); call eval_node_init_string_ptr &
    (en1, var_str ("(previous)"), en2%sval, en2%value_is_known)
  end select
end if
en0 => en
call eval_node_compile_comparison &
  (en, en1, en2, pn_comparison, var_list, type)
if (en%type == EN_CONSTANT) then
  if (en%lval) then
    call eval_node_final_rec (en); deallocate (en)
    en => en0
  else
    call eval_node_final_rec (en0); deallocate (en0)
    exit SCAN_FURTHER
  end if
else
  en1 => en
  allocate (en)
  call eval_node_init_branch (en, var_str ("and"), V_LOG, en0, en1)
  call eval_node_set_op2_log (en, and_ll)
end if
end if
pn_comparison => parse_node_get_next_ptr (pn_comparison)
end do SCAN_FURTHER
if (en%type == EN_CONSTANT .and. associated (en2)) then
  call eval_node_final_rec (en2); deallocate (en2)
end if
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done compared_expr"
end if
end subroutine eval_node_compile_compared_expr

```

This takes two extra arguments: **en1**, the left-hand-side of the comparison, is already allocated and evaluated. **en2** (the right-hand side) and **en** (the result) are allocated by the routine. **pn** is the parse node which contains the operator and the right-hand side as subnodes.

If the result of the comparison is constant, **en1** is deleted but **en2** is kept, because it may be used in a subsequent comparison. **en** then becomes a constant. If the result is variable, **en** becomes a branch node which refers to **en1** and **en2**.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_comparison &
  (en, en1, en2, pn, var_list, type)
  type(eval_node_t), pointer :: en, en1, en2
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  integer, intent(in) :: type

```



```

type(parse_node_t), pointer :: pn_op, pn_arg
type(string_t) :: key
integer :: t1, t2
real(default), pointer :: tolerance_ptr
pn_op => parse_node_get_sub_ptr (pn)
key = parse_node_get_key (pn_op)
select case (type)
case (V_INT, V_REAL)
    pn_arg => parse_node_get_next_ptr (pn_op, tag="expr")
    call eval_node_compile_expr (en2, pn_arg, var_list)
case (V_STR)
    pn_arg => parse_node_get_next_ptr (pn_op, tag="sexpr")
    call eval_node_compile_sexpr (en2, pn_arg, var_list)
end select
t1 = en1%result_type
t2 = en2%result_type
allocate (en)
if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
    call var_list%get_rptr (var_str ("tolerance"), tolerance_ptr)
    en1%tolerance => tolerance_ptr
    select case (char (key))
    case ("<")
        select case (t1)
        case (V_INT)
            select case (t2)
            case (V_INT); call eval_node_init_log (en, comp_lt_ii (en1, en2))
            case (V_REAL); call eval_node_init_log (en, comp_ll_ir (en1, en2))
            end select
        case (V_REAL)
            select case (t2)
            case (V_INT); call eval_node_init_log (en, comp_ll_ri (en1, en2))
            case (V_REAL); call eval_node_init_log (en, comp_ll_rr (en1, en2))
            end select
        end select
    case (">")
        select case (t1)
        case (V_INT)
            select case (t2)
            case (V_INT); call eval_node_init_log (en, comp_gt_ii (en1, en2))
            case (V_REAL); call eval_node_init_log (en, comp_gg_ir (en1, en2))
            end select
        case (V_REAL)
            select case (t2)
            case (V_INT); call eval_node_init_log (en, comp_gg_ri (en1, en2))
            case (V_REAL); call eval_node_init_log (en, comp_gg_rr (en1, en2))
            end select
        end select
    case ("<=")
        select case (t1)
        case (V_INT)
            select case (t2)
            case (V_INT); call eval_node_init_log (en, comp_le_ii (en1, en2))
            case (V_REAL); call eval_node_init_log (en, comp_ls_ir (en1, en2))
            end select
        end select
    end select
end if

```

```

case (V_REAL)
  select case (t2)
    case (V_INT); call eval_node_init_log (en, comp_ls_ri (en1, en2))
    case (V_REAL); call eval_node_init_log (en, comp_ls_rr (en1, en2))
  end select
end select
case (">=")
  select case (t1)
    case (V_INT)
      select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_ge_ii (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_gs_ir (en1, en2))
      end select
    case (V_REAL)
      select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_gs_ri (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_gs_rr (en1, en2))
      end select
    end select
case ("==")
  select case (t1)
    case (V_INT)
      select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_eq_ii (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_se_ir (en1, en2))
      end select
    case (V_REAL)
      select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_se_ri (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_se_rr (en1, en2))
      end select
    case (V_STR)
      select case (t2)
        case (V_STR); call eval_node_init_log (en, comp_eq_ss (en1, en2))
      end select
    end select
case ("<>")
  select case (t1)
    case (V_INT)
      select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_ne_ii (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_ns_ir (en1, en2))
      end select
    case (V_REAL)
      select case (t2)
        case (V_INT); call eval_node_init_log (en, comp_ns_ri (en1, en2))
        case (V_REAL); call eval_node_init_log (en, comp_ns_rr (en1, en2))
      end select
    case (V_STR)
      select case (t2)
        case (V_STR); call eval_node_init_log (en, comp_ne_ss (en1, en2))
      end select
    end select
end select
end select

```

```

        call eval_node_final_rec (en1)
        deallocate (en1)
    else
        call eval_node_init_branch (en, key, V_LOG, en1, en2)
        select case (char (key))
        case ("<")
            select case (t1)
            case (V_INT)
                select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_lt_ii)
                case (V_REAL); call eval_node_set_op2_log (en, comp_ll_ir)
                end select
            case (V_REAL)
                select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_ll_ri)
                case (V_REAL); call eval_node_set_op2_log (en, comp_ll_rr)
                end select
            end select
        case (">")
            select case (t1)
            case (V_INT)
                select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_gt_ii)
                case (V_REAL); call eval_node_set_op2_log (en, comp_gg_ir)
                end select
            case (V_REAL)
                select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_gg_ri)
                case (V_REAL); call eval_node_set_op2_log (en, comp_gg_rr)
                end select
            end select
        case ("<=")
            select case (t1)
            case (V_INT)
                select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_le_ii)
                case (V_REAL); call eval_node_set_op2_log (en, comp_ls_ir)
                end select
            case (V_REAL)
                select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_ls_ri)
                case (V_REAL); call eval_node_set_op2_log (en, comp_ls_rr)
                end select
            end select
        case (">=")
            select case (t1)
            case (V_INT)
                select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_ge_ii)
                case (V_REAL); call eval_node_set_op2_log (en, comp_gs_ir)
                end select
            case (V_REAL)
                select case (t2)
                case (V_INT); call eval_node_set_op2_log (en, comp_gs_ri)

```

```

        case (V_REAL); call eval_node_set_op2_log (en, comp_gs_rr)
    end select
end select
case ("==")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_set_op2_log (en, comp_eq_ii)
        case (V_REAL); call eval_node_set_op2_log (en, comp_se_ir)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_set_op2_log (en, comp_se_ri)
        case (V_REAL); call eval_node_set_op2_log (en, comp_se_rr)
        end select
    case (V_STR)
        select case (t2)
        case (V_STR); call eval_node_set_op2_log (en, comp_eq_ss)
        end select
    end select
case ("<>")
    select case (t1)
    case (V_INT)
        select case (t2)
        case (V_INT); call eval_node_set_op2_log (en, comp_ne_ii)
        case (V_REAL); call eval_node_set_op2_log (en, comp_ns_ir)
        end select
    case (V_REAL)
        select case (t2)
        case (V_INT); call eval_node_set_op2_log (en, comp_ns_ri)
        case (V_REAL); call eval_node_set_op2_log (en, comp_ns_rr)
        end select
    case (V_STR)
        select case (t2)
        case (V_STR); call eval_node_set_op2_log (en, comp_ne_ss)
        end select
    end select
end select
call var_list%get_rptr (var_str ("tolerance"), tolerance_ptr)
en1%tolerance => tolerance_ptr
end if
end subroutine eval_node_compile_comparison

```

Recording analysis data

The **record** command is actually a logical expression which always evaluates true.

<Eval trees: procedures>+≡

```

recursive subroutine eval_node_compile_record_cmd (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list

```

```

type(parse_node_t), pointer :: pn_key, pn_tag, pn_arg
type(parse_node_t), pointer :: pn_arg1, pn_arg2, pn_arg3, pn_arg4
type(eval_node_t), pointer :: en0, en1, en2, en3, en4
real(default), pointer :: event_weight
if (debug_active (D_MODEL_F)) then
    print *, "read record_cmd"; call parse_node_write (pn)
end if
pn_key => parse_node_get_sub_ptr (pn)
pn_tag => parse_node_get_next_ptr (pn_key)
pn_arg => parse_node_get_next_ptr (pn_tag)
select case (char (parse_node_get_key (pn_key)))
case ("record")
    call var_list%get_rptr (var_str ("event_weight"), event_weight)
case ("record_unweighted")
    event_weight => null ()
case ("record_excess")
    call var_list%get_rptr (var_str ("event_excess"), event_weight)
end select
select case (char (parse_node_get_rule_key (pn_tag)))
case ("analysis_id")
    allocate (en0)
    call eval_node_init_string (en0, parse_node_get_string (pn_tag))
case default
    call eval_node_compile_sexpr (en0, pn_tag, var_list)
end select
allocate (en)
if (associated (pn_arg)) then
    pn_arg1 => parse_node_get_sub_ptr (pn_arg)
    call eval_node_compile_expr (en1, pn_arg1, var_list)
    if (en1%result_type == V_INT) &
        call insert_conversion_node (en1, V_REAL)
    pn_arg2 => parse_node_get_next_ptr (pn_arg1)
    if (associated (pn_arg2)) then
        call eval_node_compile_expr (en2, pn_arg2, var_list)
        if (en2%result_type == V_INT) &
            call insert_conversion_node (en2, V_REAL)
    pn_arg3 => parse_node_get_next_ptr (pn_arg2)
    if (associated (pn_arg3)) then
        call eval_node_compile_expr (en3, pn_arg3, var_list)
        if (en3%result_type == V_INT) &
            call insert_conversion_node (en3, V_REAL)
    pn_arg4 => parse_node_get_next_ptr (pn_arg3)
    if (associated (pn_arg4)) then
        call eval_node_compile_expr (en4, pn_arg4, var_list)
        if (en4%result_type == V_INT) &
            call insert_conversion_node (en4, V_REAL)
        call eval_node_init_record_cmd &
            (en, event_weight, en0, en1, en2, en3, en4)
    else
        call eval_node_init_record_cmd &
            (en, event_weight, en0, en1, en2, en3)
    end if
else
    call eval_node_init_record_cmd (en, event_weight, en0, en1, en2)

```

```

        end if
    else
        call eval_node_init_record_cmd (en, event_weight, en0, en1)
    end if
else
    call eval_node_init_record_cmd (en, event_weight, en0)
end if
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done record_cmd"
end if
end subroutine eval_node_compile_record_cmd

```

Particle-list expressions

A particle expression is a subevent or a concatenation of particle-list terms (using join).

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_pexpr (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_pterm, pn_concatenation, pn_op, pn_arg
    type(eval_node_t), pointer :: en1, en2
    type(subvt_t) :: subvt
    if (debug_active (D_MODEL_F)) then
        print *, "read pexpr"; call parse_node_write (pn)
    end if
    pn_pterm => parse_node_get_sub_ptr (pn)
    call eval_node_compile_pterm (en, pn_pterm, var_list)
    pn_concatenation => &
        parse_node_get_next_ptr (pn_pterm, tag="pconcatenation")
    do while (associated (pn_concatenation))
        pn_op => parse_node_get_sub_ptr (pn_concatenation)
        pn_arg => parse_node_get_next_ptr (pn_op)
        en1 => en
        call eval_node_compile_pterm (en2, pn_arg, var_list)
        allocate (en)
        if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
            call subvt_join (subvt, en1%pval, en2%pval)
            call eval_node_init_subvt (en, subvt)
            call eval_node_final_rec (en1)
            call eval_node_final_rec (en2)
            deallocate (en1, en2)
        else
            call eval_node_init_branch &
                (en, var_str ("join"), V_SEV, en1, en2)
            call eval_node_set_op2_sev (en, join_pp)
        end if
        pn_concatenation => parse_node_get_next_ptr (pn_concatenation)
    end do
    if (debug_active (D_MODEL_F)) then

```

```

        call eval_node_write (en)
        print *, "done pexpr"
    end if
end subroutine eval_node_compile_pexpr

```

A particle term is a subevent or a combination of particle-list values (using combine).

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_pterm (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_pvalue, pn_combination, pn_op, pn_arg
    type(eval_node_t), pointer :: en1, en2
    type(subvt_t) :: subvt
    if (debug_active (D_MODEL_F)) then
        print *, "read pterm"; call parse_node_write (pn)
    end if
    pn_pvalue => parse_node_get_sub_ptr (pn)
    call eval_node_compile_pvalue (en, pn_pvalue, var_list)
    pn_combination => &
        parse_node_get_next_ptr (pn_pvalue, tag="pcombination")
    do while (associated (pn_combination))
        pn_op => parse_node_get_sub_ptr (pn_combination)
        pn_arg => parse_node_get_next_ptr (pn_op)
        en1 => en
        call eval_node_compile_pvalue (en2, pn_arg, var_list)
        allocate (en)
        if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
            call subvt_combine (subvt, en1%pval, en2%pval)
            call eval_node_init_subvt (en, subvt)
            call eval_node_final_rec (en1)
            call eval_node_final_rec (en2)
            deallocate (en1, en2)
        else
            call eval_node_init_branch &
                (en, var_str ("combine"), V_SEV, en1, en2)
            call eval_node_set_op2_sev (en, combine_pp)
        end if
        pn_combination => parse_node_get_next_ptr (pn_combination)
    end do
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done pterm"
    end if
end subroutine eval_node_compile_pterm

```

A particle-list value is a PDG-code array, a particle identifier, a variable, a (grouped) pexpr, a block pexpr, a conditional, or a particle-list function.

The **cexpr** node is responsible for transforming a constant PDG-code array into a subevent. It takes the code array as its first argument, the event subevent as its second argument, and the requested particle type (incoming/outgoing) as its zero-th argument. The result is the list of particles in the event that match

the code array.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_pvalue (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_prefix_cexpr
  type(eval_node_t), pointer :: en1, en2, en0
  type(string_t) :: key
  type(subevt_t), pointer :: evt_ptr
  logical, pointer :: known
  if (debug_active (D_MODEL_F)) then
    print *, "read pvalue"; call parse_node_write (pn)
  end if
  select case (char (parse_node_get_rule_key (pn)))
  case ("pexpr_src")
    call eval_node_compile_prefix_cexpr (en1, pn, var_list)
    allocate (en2)
    if (var_list%contains (var_str ("@evt"))) then
      call var_list%get_pptr (var_str ("@evt"), evt_ptr, known)
      call eval_node_init_subevt_ptr (en2, var_str ("@evt"), evt_ptr, known)
      allocate (en)
      call eval_node_init_branch &
        (en, var_str ("prt_selection"), V_SEV, en1, en2)
      call eval_node_set_op2_sev (en, select_pdg_ca)
      allocate (en0)
      pn_prefix_cexpr => parse_node_get_sub_ptr (pn)
      key = parse_node_get_rule_key (pn_prefix_cexpr)
      select case (char (key))
      case ("beam_prt")
        call eval_node_init_int (en0, PRT_BEAM)
        en%arg0 => en0
      case ("incoming_prt")
        call eval_node_init_int (en0, PRT_INCOMING)
        en%arg0 => en0
      case ("outgoing_prt")
        call eval_node_init_int (en0, PRT_OUTGOING)
        en%arg0 => en0
      case ("unspecified_prt")
        call eval_node_init_int (en0, PRT_OUTGOING)
        en%arg0 => en0
      end select
    else
      call parse_node_write (pn)
      call msg_bug (" Missing event data while compiling pvalue")
    end if
  case ("pvariable")
    call eval_node_compile_variable (en, pn, var_list, V_SEV)
  case ("pexpr")
    call eval_node_compile_pexpr (en, pn, var_list)
  case ("block_pexpr")
    call eval_node_compile_block_expr (en, pn, var_list, V_SEV)
  case ("conditional_pexpr")
    call eval_node_compile_conditional (en, pn, var_list, V_SEV)

```



```

case ("join_fun", "combine_fun", "collect_fun", "cluster_fun", &
      "select_fun", "extract_fun", "sort_fun", "select_b_jet_fun", &
      "select_non_bjet_fun", "select_c_jet_fun", &
      "select_light_jet_fun", "photon_reco_fun")
  call eval_node_compile_prt_function (en, pn, var_list)
case default
  call parse_node_mismatch &
    ("prefix_cexpr|pvariable|" // &
     "grouped_pexpr|block_pexpr|conditional_pexpr|" // &
     "prt_function", pn)
end select
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done pvalue"
end if
end subroutine eval_node_compile_pvalue

```

Particle functions

This combines the treatment of 'join', 'combine', 'collect', 'cluster', 'select', and 'extract', as well as the functions for b , c and light jet selection and photon recombination which all have the same syntax. The one or two argument nodes are allocated. If there is a condition, the condition node is also allocated as a logical expression, for which the variable list is augmented by the appropriate (unary/binary) observables.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_prt_function (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_clause, pn_key, pn_cond, pn_args
  type(parse_node_t), pointer :: pn_arg0, pn_arg1, pn_arg2
  type(eval_node_t), pointer :: en0, en1, en2
  type(string_t) :: key
  if (debug_active (D_MODEL_F)) then
    print *, "read prt_function"; call parse_node_write (pn)
  end if
  pn_clause => parse_node_get_sub_ptr (pn)
  pn_key => parse_node_get_sub_ptr (pn_clause)
  pn_cond => parse_node_get_next_ptr (pn_key)
  if (associated (pn_cond)) &
    pn_arg0 => parse_node_get_sub_ptr (pn_cond, 2)
  pn_args => parse_node_get_next_ptr (pn_clause)
  pn_arg1 => parse_node_get_sub_ptr (pn_args)
  pn_arg2 => parse_node_get_next_ptr (pn_arg1)
  key = parse_node_get_key (pn_key)
  call eval_node_compile_pexpr (en1, pn_arg1, var_list)
  allocate (en)
  if (.not. associated (pn_arg2)) then
    select case (char (key))
    case ("collect")
      call eval_node_init_prt_fun_unary (en, en1, key, collect_p)

```

```

case ("cluster")
  if (fastjet_available ()) then
    call fastjet_init ()
  else
    call msg_fatal &
      (''cluster' function requires FastJet, which is not enabled")
  end if
  en1%var_list => var_list
  call eval_node_init_prt_fun_unary (en, en1, key, cluster_p)
  call var_list%get_iptr (var_str ("jet_algorithm"), en1%jet_algorithm)
  call var_list%get_rptr (var_str ("jet_r"), en1%jet_r)
  call var_list%get_rptr (var_str ("jet_p"), en1%jet_p)
  call var_list%get_rptr (var_str ("jet_ycut"), en1%jet_ycut)
  call var_list%get_rptr (var_str ("jet_dcut"), en1%jet_dcut)
case ("photon_recombination")
  en1%var_list => var_list
  call eval_node_init_prt_fun_unary &
    (en, en1, key, photon_recombination_p)
  call var_list%get_rptr (var_str ("photon_rec_r0"), en1%photon_rec_r0)
case ("select")
  call eval_node_init_prt_fun_unary (en, en1, key, select_p)
case ("extract")
  call eval_node_init_prt_fun_unary (en, en1, key, extract_p)
case ("sort")
  call eval_node_init_prt_fun_unary (en, en1, key, sort_p)
case ("select_b_jet")
  call eval_node_init_prt_fun_unary (en, en1, key, select_b_jet_p)
case ("select_non_b_jet")
  call eval_node_init_prt_fun_unary (en, en1, key, select_non_b_jet_p)
case ("select_c_jet")
  call eval_node_init_prt_fun_unary (en, en1, key, select_c_jet_p)
case ("select_light_jet")
  call eval_node_init_prt_fun_unary (en, en1, key, select_light_jet_p)
case default
  call msg_bug (" Unary particle function '" // char (key) // &
    "' undefined")
end select
else
  call eval_node_compile_pexpr (en2, pn_arg2, var_list)
  select case (char (key))
  case ("join")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, join_pp)
  case ("combine")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, combine_pp)
  case ("collect")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, collect_pp)
  case ("select")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, select_pp)
  case ("sort")
    call eval_node_init_prt_fun_binary (en, en1, en2, key, sort_pp)
  case default
    call msg_bug (" Binary particle function '" // char (key) // &
      "' undefined")
  end select
end select

```

```

end if
if (associated (pn_cond)) then
  call eval_node_set_observables (en, var_list)
  select case (char (key))
  case ("extract", "sort")
    call eval_node_compile_expr (en0, pn_arg0, en%var_list)
  case default
    call eval_node_compile_lexpr (en0, pn_arg0, en%var_list)
  end select
  en%arg0 => en0
end if
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done prt_function"
end if
end subroutine eval_node_compile_prt_function

```

The `eval` expression is similar, but here the expression `arg0` is mandatory, and the whole thing evaluates to a numeric value. To guarantee initialization of variables defined on subevents instead of a single (namely the first) particle of a subevent, we make sure that `en` points to the subevent stored in `en1`.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_eval_function (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_key, pn_arg0, pn_args, pn_arg1, pn_arg2
  type(eval_node_t), pointer :: en0, en1, en2
  type(string_t) :: key
  if (debug_active (D_MODEL_F)) then
    print *, "read eval_function"; call parse_node_write (pn)
  end if
  pn_key => parse_node_get_sub_ptr (pn)
  pn_arg0 => parse_node_get_next_ptr (pn_key)
  pn_args => parse_node_get_next_ptr (pn_arg0)
  pn_arg1 => parse_node_get_sub_ptr (pn_args)
  pn_arg2 => parse_node_get_next_ptr (pn_arg1)
  key = parse_node_get_key (pn_key)
  call eval_node_compile_pexpr (en1, pn_arg1, var_list)
  allocate (en)
  if (.not. associated (pn_arg2)) then
    call eval_node_init_eval_fun_unary (en, en1, key)
  else
    call eval_node_compile_pexpr (en2, pn_arg2, var_list)
    call eval_node_init_eval_fun_binary (en, en1, en2, key)
  end if
  en%pval => en1%pval
  call eval_node_set_observables (en, var_list)
  call eval_node_compile_expr (en0, pn_arg0, en%var_list)
  if (en0%result_type == V_INT) &
    call insert_conversion_node (en0, V_REAL)
  if (en0%result_type /= V_REAL) &
    call msg_fatal (" 'eval' function does not result in real value")

```

```

call eval_node_set_expr (en, en0)
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done eval_function"
end if
end subroutine eval_node_compile_eval_function

```

Logical functions of subevents. For `photon_isolation` there is a conditional selection expression instead of a mandatory logical expression, so in the case of the absence of the selection we have to create a logical `eval_node_t` with value `.true..`

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_log_function (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_clause, pn_key, pn_str, pn_cond
    type(parse_node_t), pointer :: pn_arg0, pn_args, pn_arg1, pn_arg2
    type(eval_node_t), pointer :: en0, en1, en2
    type(string_t) :: key
    if (debug_active (D_MODEL_F)) then
        print *, "read log_function"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("all_fun", "any_fun", "no_fun")
        pn_key => parse_node_get_sub_ptr (pn)
        pn_arg0 => parse_node_get_next_ptr (pn_key)
        pn_args => parse_node_get_next_ptr (pn_arg0)
    case ("photon_isolation_fun")
        pn_clause => parse_node_get_sub_ptr (pn)
        pn_key => parse_node_get_sub_ptr (pn_clause)
        pn_cond => parse_node_get_next_ptr (pn_key)
        if (associated (pn_cond)) then
            pn_arg0 => parse_node_get_sub_ptr (pn_cond, 2)
        else
            pn_arg0 => null ()
        end if
        pn_args => parse_node_get_next_ptr (pn_clause)
    case default
        call parse_node_mismatch ("all_fun|any_fun|" // &
            "no_fun|photon_isolation_fun", pn)
    end select
    pn_arg1 => parse_node_get_sub_ptr (pn_args)
    pn_arg2 => parse_node_get_next_ptr (pn_arg1)
    key = parse_node_get_key (pn_key)
    call eval_node_compile_pexpr (en1, pn_arg1, var_list)
    allocate (en)
    if (.not. associated (pn_arg2)) then
        select case (char (key))
        case ("all")
            call eval_node_init_log_fun_unary (en, en1, key, all_p)
        case ("any")
            call eval_node_init_log_fun_unary (en, en1, key, any_p)

```

```

        case ("no")
            call eval_node_init_log_fun_unary (en, en1, key, no_p)
        case default
            call msg_bug ("Unary logical particle function '" // char (key) // &
                "' undefined")
        end select
    else
        call eval_node_compile_pexpr (en2, pn_arg2, var_list)
        select case (char (key))
        case ("all")
            call eval_node_init_log_fun_binary (en, en1, en2, key, all_pp)
        case ("any")
            call eval_node_init_log_fun_binary (en, en1, en2, key, any_pp)
        case ("no")
            call eval_node_init_log_fun_binary (en, en1, en2, key, no_pp)
        case ("photon_isolation")
            en1%var_list => var_list
            call var_list%get_rptr (var_str ("photon_iso_eps"), en1%photon_iso_eps)
            call var_list%get_rptr (var_str ("photon_iso_n"), en1%photon_iso_n)
            call var_list%get_rptr (var_str ("photon_iso_r0"), en1%photon_iso_r0)
            call eval_node_init_log_fun_binary (en, en1, en2, key, photon_isolation_pp)
        case default
            call msg_bug ("Binary logical particle function '" // char (key) // &
                "' undefined")
        end select
    end if
    if (associated (pn_arg0)) then
        call eval_node_set_observables (en, var_list)
        select case (char (key))
        case ("all", "any", "no", "photon_isolation")
            call eval_node_compile_lexpr (en0, pn_arg0, en%var_list)
        case default
            call msg_bug ("Compiling logical particle function: missing mode")
        end select
        call eval_node_set_expr (en, en0, V_LOG)
    else
        select case (char (key))
        case ("photon_isolation")
            allocate (en0)
            call eval_node_init_log (en0, .true.)
            call eval_node_set_expr (en, en0, V_LOG)
        case default
            call msg_bug ("Only photon isolation can be called unconditionally")
        end select
    end if
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done log_function"
    end if
end subroutine eval_node_compile_log_function

```

Count function of subevents.

<Eval trees: procedures>+≡

```
recursive subroutine eval_node_compile_count_function (en, pn, var_list)
```

```

type(eval_node_t), pointer :: en
type(parse_node_t), intent(in) :: pn
type(var_list_t), intent(in), target :: var_list
type(parse_node_t), pointer :: pn_clause, pn_key, pn_cond, pn_args
type(parse_node_t), pointer :: pn_arg0, pn_arg1, pn_arg2
type(eval_node_t), pointer :: en0, en1, en2
type(string_t) :: key
if (debug_active (D_MODEL_F)) then
    print *, "read count_function"; call parse_node_write (pn)
end if
select case (char (parse_node_get_rule_key (pn)))
case ("count_fun")
    pn_clause => parse_node_get_sub_ptr (pn)
    pn_key => parse_node_get_sub_ptr (pn_clause)
    pn_cond => parse_node_get_next_ptr (pn_key)
    if (associated (pn_cond)) then
        pn_arg0 => parse_node_get_sub_ptr (pn_cond, 2)
    else
        pn_arg0 => null ()
    end if
    pn_args => parse_node_get_next_ptr (pn_clause)
end select
pn_arg1 => parse_node_get_sub_ptr (pn_args)
pn_arg2 => parse_node_get_next_ptr (pn_arg1)
key = parse_node_get_key (pn_key)
call eval_node_compile_pexpr (en1, pn_arg1, var_list)
allocate (en)
if (.not. associated (pn_arg2)) then
    select case (char (key))
    case ("count")
        call eval_node_init_int_fun_unary (en, en1, key, count_a)
    case default
        call msg_bug ("Unary subevent function '" // char (key) // &
            "' undefined")
    end select
else
    call eval_node_compile_pexpr (en2, pn_arg2, var_list)
    select case (char (key))
    case ("count")
        call eval_node_init_int_fun_binary (en, en1, en2, key, count_pp)
    case default
        call msg_bug ("Binary subevent function '" // char (key) // &
            "' undefined")
    end select
end if
if (associated (pn_arg0)) then
    call eval_node_set_observables (en, var_list)
    select case (char (key))
    case ("count")
        call eval_node_compile_lexpr (en0, pn_arg0, en%var_list)
        call eval_node_set_expr (en, en0, V_INT)
    end select
end if
if (debug_active (D_MODEL_F)) then

```

```

        call eval_node_write (en)
        print *, "done count_function"
    end if
end subroutine eval_node_compile_count_function

```

Numeric functions of subevents.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_numeric_function (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_key, pn_args
    type(parse_node_t), pointer :: pn_arg0, pn_arg1, pn_arg2
    type(eval_node_t), pointer :: en0, en1
    type(string_t) :: key
    type(var_entry_t), pointer :: var
    if (debug_active (D_MODEL_F)) then
        print *, "read numeric_function"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("sum_fun", "prod_fun")
        if (debug_active (D_MODEL_F)) then
            print *, "read sum_fun"; call parse_node_write (pn)
        end if
        pn_key => parse_node_get_sub_ptr (pn)
        pn_arg0 => parse_node_get_next_ptr (pn_key)
        pn_args => parse_node_get_next_ptr (pn_arg0)
    end select
    pn_arg1 => parse_node_get_sub_ptr (pn_args)
    pn_arg2 => parse_node_get_next_ptr (pn_arg1)
    key = parse_node_get_key (pn_key)
    call eval_node_compile_pexpr (en1, pn_arg1, var_list)
    if (associated (pn_arg2)) then
        call msg_fatal ("The " // char (key) // &
            " function can only be used for unary observables.")
    end if
    allocate (en)
    select case (char (key))
    case ("sum")
        call eval_node_init_real_fun_cum (en, en1, key, sum_a)
    case ("prod")
        call eval_node_init_real_fun_cum (en, en1, key, prod_a)
    case default
        call msg_bug ("Unary subevent function '" // char (key) // &
            "' undefined")
    end select
    call eval_node_set_observables (en, var_list)
    call eval_node_compile_expr (en0, pn_arg0, en%var_list)
    if (en0%result_type == V_INT) &
        call insert_conversion_node (en0, V_REAL)
    call eval_node_set_expr (en, en0, V_REAL)
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done numeric_function"
    end if
end subroutine eval_node_compile_numeric_function

```

```

end if
end subroutine eval_node_compile_numeric_function

```

PDG-code arrays

A PDG-code expression is (optionally) prefixed by `beam`, `incoming`, or `outgoing`, a block, or a conditional. In any case, it evaluates to a constant.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_prefix_cexpr (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_avalue, pn_prt
  type(string_t) :: key
  if (debug_active (D_MODEL_F)) then
    print *, "read prefix_cexpr"; call parse_node_write (pn)
  end if
  pn_avalue => parse_node_get_sub_ptr (pn)
  key = parse_node_get_rule_key (pn_avalue)
  select case (char (key))
  case ("beam_prt")
    pn_prt => parse_node_get_sub_ptr (pn_avalue, 2)
    call eval_node_compile_cexpr (en, pn_prt, var_list)
  case ("incoming_prt")
    pn_prt => parse_node_get_sub_ptr (pn_avalue, 2)
    call eval_node_compile_cexpr (en, pn_prt, var_list)
  case ("outgoing_prt")
    pn_prt => parse_node_get_sub_ptr (pn_avalue, 2)
    call eval_node_compile_cexpr (en, pn_prt, var_list)
  case ("unspecified_prt")
    pn_prt => parse_node_get_sub_ptr (pn_avalue, 1)
    call eval_node_compile_cexpr (en, pn_prt, var_list)
  case default
    call parse_node_mismatch &
      ("beam_prt|incoming_prt|outgoing_prt|unspecified_prt", &
        pn_avalue)
  end select
  if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done prefix_cexpr"
  end if
end subroutine eval_node_compile_prefix_cexpr

```

A PDG array is a string of PDG code definitions (or aliases), concatenated by `':'`. The code definitions may be variables which are not defined at compile time, so we have to allocate sub-nodes. This analogous to `eval_node_compile_term`.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_cexpr (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_prt, pn_concatenation

```



```

type(eval_node_t), pointer :: en1, en2
type(pdg_array_t) :: aval
if (debug_active (D_MODEL_F)) then
    print *, "read cexpr"; call parse_node_write (pn)
end if
pn_prt => parse_node_get_sub_ptr (pn)
call eval_node_compile_avalue (en, pn_prt, var_list)
pn_concatenation => parse_node_get_next_ptr (pn_prt)
do while (associated (pn_concatenation))
    pn_prt => parse_node_get_sub_ptr (pn_concatenation, 2)
    en1 => en
    call eval_node_compile_avalue (en2, pn_prt, var_list)
    allocate (en)
    if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
        call concat_cc (aval, en1, en2)
        call eval_node_init_pdg_array (en, aval)
        call eval_node_final_rec (en1)
        call eval_node_final_rec (en2)
        deallocate (en1, en2)
    else
        call eval_node_init_branch (en, var_str (":"), V_PDG, en1, en2)
        call eval_node_set_op2_pdg (en, concat_cc)
    end if
    pn_concatenation => parse_node_get_next_ptr (pn_concatenation)
end do
if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done cexpr"
end if
end subroutine eval_node_compile_cexpr

```

Compile a PDG-code type value. It may be either an integer expression or a variable of type PDG array, optionally quoted.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_avalue (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    if (debug_active (D_MODEL_F)) then
        print *, "read avalue"; call parse_node_write (pn)
    end if
    select case (char (parse_node_get_rule_key (pn)))
    case ("pdg_code")
        call eval_node_compile_pdg_code (en, pn, var_list)
    case ("cvariable", "variable", "prt_name")
        call eval_node_compile_cvariable (en, pn, var_list)
    case ("cexpr")
        call eval_node_compile_cexpr (en, pn, var_list)
    case ("block_cexpr")
        call eval_node_compile_block_expr (en, pn, var_list, V_PDG)
    case ("conditional_cexpr")
        call eval_node_compile_conditional (en, pn, var_list, V_PDG)
    case default

```

```

        call parse_node_mismatch &
            ("grouped_cexpr|block_cexpr|conditional_cexpr|" // &
             "pdg_code|cvariable|prt_name", pn)
    end select
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done avalue"
    end if
end subroutine eval_node_compile_avalue

```

Compile a PDG-code expression, which is the key PDG with an integer expression as argument. The procedure is analogous to `eval_node_compile_unary_function`.

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_pdg_code (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in), target :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_arg
    type(eval_node_t), pointer :: en1
    type(string_t) :: key
    type(pdg_array_t) :: aval
    integer :: t
    if (debug_active (D_MODEL_F)) then
        print *, "read PDG code"; call parse_node_write (pn)
    end if
    pn_arg => parse_node_get_sub_ptr (pn, 2)
    call eval_node_compile_expr &
        (en1, parse_node_get_sub_ptr (pn_arg, tag="expr"), var_list)
    t = en1%result_type
    allocate (en)
    key = "PDG"
    if (en1%type == EN_CONSTANT) then
        select case (t)
            case (V_INT)
                call pdg_i (aval, en1)
                call eval_node_init_pdg_array (en, aval)
            case default; call eval_type_error (pn, char (key), t)
        end select
        call eval_node_final_rec (en1)
        deallocate (en1)
    else
        select case (t)
            case (V_INT); call eval_node_set_op1_pdg (en, pdg_i)
            case default; call eval_type_error (pn, char (key), t)
        end select
    end if
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done function"
    end if
end subroutine eval_node_compile_pdg_code

```

This is entirely analogous to `eval_node_compile_variable`. However, PDG-

array variables occur in different contexts.

To avoid name clashes between PDG-array variables and ordinary variables, we prepend a character (*). This is not visible to the user.

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_cvariable (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in), target :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_name
  type(string_t) :: var_name
  type(pdg_array_t), pointer :: aptr
  type(pdg_array_t), target, save :: no_aval
  logical, pointer :: known
  logical, target, save :: unknown = .false.
  if (debug_active (D_MODEL_F)) then
    print *, "read cvariable"; call parse_node_write (pn)
  end if
  pn_name => pn
  var_name = parse_node_get_string (pn_name)
  allocate (en)
  if (var_list%contains (var_name)) then
    call var_list%get_aptr (var_name, aptr, known)
    call eval_node_init_pdg_array_ptr (en, var_name, aptr, known)
  else
    call parse_node_write (pn)
    call msg_error ("This PDG-array variable is undefined at this point")
    call eval_node_init_pdg_array_ptr (en, var_name, no_aval, unknown)
  end if
  if (debug_active (D_MODEL_F)) then
    call eval_node_write (en)
    print *, "done cvariable"
  end if
end subroutine eval_node_compile_cvariable

```

String expressions

A string expression is either a string value or a concatenation of string values.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_sexpr (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_svalue, pn_concatenation, pn_op, pn_arg
  type(eval_node_t), pointer :: en1, en2
  type(string_t) :: string
  if (debug_active (D_MODEL_F)) then
    print *, "read sexpr"; call parse_node_write (pn)
  end if
  pn_svalue => parse_node_get_sub_ptr (pn)
  call eval_node_compile_svalue (en, pn_svalue, var_list)
  pn_concatenation => &
    parse_node_get_next_ptr (pn_svalue, tag="str_concatenation")

```

```

do while (associated (pn_concatenation))
  pn_op => parse_node_get_sub_ptr (pn_concatenation)
  pn_arg => parse_node_get_next_ptr (pn_op)
  en1 => en
  call eval_node_compile_svalue (en2, pn_arg, var_list)
  allocate (en)
  if (en1%type == EN_CONSTANT .and. en2%type == EN_CONSTANT) then
    call concat_ss (string, en1, en2)
    call eval_node_init_string (en, string)
    call eval_node_final_rec (en1)
    call eval_node_final_rec (en2)
    deallocate (en1, en2)
  else
    call eval_node_init_branch &
      (en, var_str ("concat"), V_STR, en1, en2)
    call eval_node_set_op2_str (en, concat_ss)
  end if
  pn_concatenation => parse_node_get_next_ptr (pn_concatenation)
end do
if (debug_active (D_MODEL_F)) then
  call eval_node_write (en)
  print *, "done sexpr"
end if
end subroutine eval_node_compile_sexpr

```

A string value is a string literal, a variable, a (grouped) sexpr, a block sexpr, or a conditional.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_svalue (en, pn, var_list)
  type(eval_node_t), pointer :: en
  type(parse_node_t), intent(in) :: pn
  type(var_list_t), intent(in), target :: var_list
  if (debug_active (D_MODEL_F)) then
    print *, "read svalue"; call parse_node_write (pn)
  end if
  select case (char (parse_node_get_rule_key (pn)))
  case ("svariable")
    call eval_node_compile_variable (en, pn, var_list, V_STR)
  case ("sexpr")
    call eval_node_compile_sexpr (en, pn, var_list)
  case ("block_sexpr")
    call eval_node_compile_block_expr (en, pn, var_list, V_STR)
  case ("conditional_sexpr")
    call eval_node_compile_conditional (en, pn, var_list, V_STR)
  case ("sprintf_fun")
    call eval_node_compile_sprintf (en, pn, var_list)
  case ("string_literal")
    allocate (en)
    call eval_node_init_string (en, parse_node_get_string (pn))
  case default
    call parse_node_mismatch &
      ("svariable|" // &
       "grouped_sexpr|block_sexpr|conditional_sexpr|" // &

```

```

        "string_function|string_literal", pn)
    end select
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done svalue"
    end if
end subroutine eval_node_compile_svalue

```

There is currently one string function, `sprintf`. For `sprintf`, the first argument (no brackets) is the format string, the optional arguments in brackets are the expressions or variables to be formatted.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_compile_sprintf (en, pn, var_list)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    type(parse_node_t), pointer :: pn_clause, pn_key, pn_args
    type(parse_node_t), pointer :: pn_arg0
    type(eval_node_t), pointer :: en0, en1
    integer :: n_args
    type(string_t) :: key
    if (debug_active (D_MODEL_F)) then
        print *, "read sprintf_fun"; call parse_node_write (pn)
    end if
    pn_clause => parse_node_get_sub_ptr (pn)
    pn_key    => parse_node_get_sub_ptr (pn_clause)
    pn_arg0   => parse_node_get_next_ptr (pn_key)
    pn_args   => parse_node_get_next_ptr (pn_clause)
    call eval_node_compile_sexpr (en0, pn_arg0, var_list)
    if (associated (pn_args)) then
        call eval_node_compile_sprintf_args (en1, pn_args, var_list, n_args)
    else
        n_args = 0
        en1 => null ()
    end if
    allocate (en)
    key = parse_node_get_key (pn_key)
    call eval_node_init_format_string (en, en0, en1, key, n_args)
    if (debug_active (D_MODEL_F)) then
        call eval_node_write (en)
        print *, "done sprintf_fun"
    end if
end subroutine eval_node_compile_sprintf

```

(Eval trees: procedures)+≡

```

subroutine eval_node_compile_sprintf_args (en, pn, var_list, n_args)
    type(eval_node_t), pointer :: en
    type(parse_node_t), intent(in) :: pn
    type(var_list_t), intent(in), target :: var_list
    integer, intent(out) :: n_args
    type(parse_node_t), pointer :: pn_arg
    integer :: i
    type(eval_node_t), pointer :: en1, en2

```

```

n_args = parse_node_get_n_sub (pn)
en => null ()
do i = n_args, 1, -1
  pn_arg => parse_node_get_sub_ptr (pn, i)
  select case (char (parse_node_get_rule_key (pn_arg)))
    case ("lvariable")
      call eval_node_compile_variable (en1, pn_arg, var_list, V_LOG)
    case ("svariable")
      call eval_node_compile_variable (en1, pn_arg, var_list, V_STR)
    case ("expr")
      call eval_node_compile_expr (en1, pn_arg, var_list)
    case default
      call parse_node_mismatch ("variable|svariable|lvariable|expr", pn_arg)
  end select
  if (associated (en)) then
    en2 => en
    allocate (en)
    call eval_node_init_branch &
      (en, var_str ("sprintf_arg"), V_NONE, en1, en2)
  else
    allocate (en)
    call eval_node_init_branch &
      (en, var_str ("sprintf_arg"), V_NONE, en1)
  end if
end do
end subroutine eval_node_compile_sprintf_args

```

Evaluation. We allocate the argument list and apply the Fortran wrapper for the `sprintf` function.

(Eval trees: procedures)+≡

```

subroutine evaluate_sprintf (string, n_args, en_fmt, en_arg)
  type(string_t), intent(out) :: string
  integer, intent(in) :: n_args
  type(eval_node_t), pointer :: en_fmt
  type(eval_node_t), intent(in), optional, target :: en_arg
  type(eval_node_t), pointer :: en_branch, en_var
  type(sprintf_arg_t), dimension(:), allocatable :: arg
  type(string_t) :: fmt
  logical :: autoformat
  integer :: i, j, sprintf_argc
  autoformat = .not. associated (en_fmt)
  if (autoformat) fmt = ""
  if (present (en_arg)) then
    sprintf_argc = 0
    en_branch => en_arg
    do i = 1, n_args
      select case (en_branch%arg1%result_type)
        case (V_CMPLX); sprintf_argc = sprintf_argc + 2
        case default ; sprintf_argc = sprintf_argc + 1
      end select
      en_branch => en_branch%arg2
    end do
    allocate (arg (sprintf_argc))
  end if
end subroutine evaluate_sprintf

```

```

j = 1
en_branch => en_arg
do i = 1, n_args
  en_var => en_branch%arg1
  select case (en_var%result_type)
  case (V_LOG)
    call sprintf_arg_init (arg(j), en_var%lval)
    if (autoformat) fmt = fmt // "%s "
  case (V_INT);
    call sprintf_arg_init (arg(j), en_var%ival)
    if (autoformat) fmt = fmt // "%i "
  case (V_REAL);
    call sprintf_arg_init (arg(j), en_var%rval)
    if (autoformat) fmt = fmt // "%g "
  case (V_STR)
    call sprintf_arg_init (arg(j), en_var%sval)
    if (autoformat) fmt = fmt // "%s "
  case (V_CMPLX)
    call sprintf_arg_init (arg(j), real (en_var%cval, default))
    j = j + 1
    call sprintf_arg_init (arg(j), aimag (en_var%cval))
    if (autoformat) fmt = fmt // "(%g + %g * I) "
  case default
    call eval_node_write (en_var)
    call msg_error ("sprintf is implemented " &
      // "for logical, integer, real, and string values only")
  end select
  j = j + 1
  en_branch => en_branch%arg2
end do
else
  allocate (arg(0))
end if
if (autoformat) then
  string = sprintf (trim (fmt), arg)
else
  string = sprintf (en_fmt%sval, arg)
end if
end subroutine evaluate_sprintf

```

28.3.5 Auxiliary functions for the compiler

Issue an error that the current node could not be compiled because of type mismatch:

```

<Eval trees: procedures>+≡
subroutine eval_type_error (pn, string, t)
  type(parse_node_t), intent(in) :: pn
  character(*), intent(in) :: string
  integer, intent(in) :: t
  type(string_t) :: type
  select case (t)
  case (V_NONE); type = "(none)"

```

```

case (V_LOG); type = "'logical'"
case (V_INT); type = "'integer'"
case (V_REAL); type = "'real'"
case (V_CMPLX); type = "'complex'"
case default; type = "(unknown)"
end select
call parse_node_write (pn)
call msg_fatal (" The " // string // &
               " operation is not defined for the given argument type " // &
               char (type))
end subroutine eval_type_error

```

If two numerics are combined, the result is integer if both arguments are integer, if one is integer and the other real or both are real, than its argument is real, otherwise complex.

(Eval trees: procedures)+≡

```

function numeric_result_type (t1, t2) result (t)
  integer, intent(in) :: t1, t2
  integer :: t
  if (t1 == V_INT .and. t2 == V_INT) then
    t = V_INT
  else if (t1 == V_INT .and. t2 == V_REAL) then
    t = V_REAL
  else if (t1 == V_REAL .and. t2 == V_INT) then
    t = V_REAL
  else if (t1 == V_REAL .and. t2 == V_REAL) then
    t = V_REAL
  else
    t = V_CMPLX
  end if
end function numeric_result_type

```

28.3.6 Evaluation

Evaluation is done recursively. For leaf nodes nothing is to be done.

Evaluating particle-list functions: First, we evaluate the particle lists. If a condition is present, we assign the particle pointers of the condition node to the allocated particle entries in the parent node, keeping in mind that the observables in the variable stack used for the evaluation of the condition also contain pointers to these entries. Then, the assigned procedure is evaluated, which sets the subevent in the parent node. If required, the procedure evaluates the condition node once for each (pair of) particles to determine the result.

(Eval trees: procedures)+≡

```

recursive subroutine eval_node_evaluate (en)
  type(eval_node_t), intent(inout) :: en
  logical :: exist
  select case (en%type)
  case (EN_UNARY)
    if (associated (en%arg1)) then
      call eval_node_evaluate (en%arg1)
      en%value_is_known = en%arg1%value_is_known
    end if
  end select
end subroutine eval_node_evaluate

```



```

else
    en%value_is_known = .false.
end if
if (en%value_is_known) then
    select case (en%result_type)
    case (V_LOG); en%lval = en%op1_log (en%arg1)
    case (V_INT); en%ival = en%op1_int (en%arg1)
    case (V_REAL); en%rval = en%op1_real (en%arg1)
    case (V_CMPLX); en%cval = en%op1_cmplx (en%arg1)
    case (V_PDG);
        call en%op1_pdg (en%aval, en%arg1)
    case (V_SEV)
        if (associated (en%arg0)) then
            call en%op1_sev (en%pval, en%arg1, en%arg0)
        else
            call en%op1_sev (en%pval, en%arg1)
        end if
    case (V_STR)
        call en%op1_str (en%sval, en%arg1)
    end select
end if
case (EN_BINARY)
    if (associated (en%arg1) .and. associated (en%arg2)) then
        call eval_node_evaluate (en%arg1)
        call eval_node_evaluate (en%arg2)
        en%value_is_known = &
            en%arg1%value_is_known .and. en%arg2%value_is_known
    else
        en%value_is_known = .false.
    end if
    if (en%value_is_known) then
        select case (en%result_type)
        case (V_LOG); en%lval = en%op2_log (en%arg1, en%arg2)
        case (V_INT); en%ival = en%op2_int (en%arg1, en%arg2)
        case (V_REAL); en%rval = en%op2_real (en%arg1, en%arg2)
        case (V_CMPLX); en%cval = en%op2_cmplx (en%arg1, en%arg2)
        case (V_PDG)
            call en%op2_pdg (en%aval, en%arg1, en%arg2)
        case (V_SEV)
            if (associated (en%arg0)) then
                call en%op2_sev (en%pval, en%arg1, en%arg2, en%arg0)
            else
                call en%op2_sev (en%pval, en%arg1, en%arg2)
            end if
        case (V_STR)
            call en%op2_str (en%sval, en%arg1, en%arg2)
        end select
    end if
case (EN_BLOCK)
    if (associated (en%arg1) .and. associated (en%arg0)) then
        call eval_node_evaluate (en%arg1)
        call eval_node_evaluate (en%arg0)
        en%value_is_known = en%arg0%value_is_known
    else

```

```

        en%value_is_known = .false.
    end if
    if (en%value_is_known) then
        select case (en%result_type)
            case (V_LOG); en%lval = en%arg0%lval
            case (V_INT); en%ival = en%arg0%ival
            case (V_REAL); en%rval = en%arg0%rval
            case (V_CMPLX); en%cval = en%arg0%cval
            case (V_PDG); en%aval = en%arg0%aval
            case (V_SEV); en%pval = en%arg0%pval
            case (V_STR); en%sval = en%arg0%sval
        end select
    end if
    case (EN_CONDITIONAL)
        if (associated(en%arg0)) then
            call eval_node_evaluate(en%arg0)
            en%value_is_known = en%arg0%value_is_known
        else
            en%value_is_known = .false.
        end if
        if (en%arg0%value_is_known) then
            if (en%arg0%lval) then
                call eval_node_evaluate(en%arg1)
                en%value_is_known = en%arg1%value_is_known
                if (en%value_is_known) then
                    select case (en%result_type)
                        case (V_LOG); en%lval = en%arg1%lval
                        case (V_INT); en%ival = en%arg1%ival
                        case (V_REAL); en%rval = en%arg1%rval
                        case (V_CMPLX); en%cval = en%arg1%cval
                        case (V_PDG); en%aval = en%arg1%aval
                        case (V_SEV); en%pval = en%arg1%pval
                        case (V_STR); en%sval = en%arg1%sval
                    end select
                end if
            else
                call eval_node_evaluate(en%arg2)
                en%value_is_known = en%arg2%value_is_known
                if (en%value_is_known) then
                    select case (en%result_type)
                        case (V_LOG); en%lval = en%arg2%lval
                        case (V_INT); en%ival = en%arg2%ival
                        case (V_REAL); en%rval = en%arg2%rval
                        case (V_CMPLX); en%cval = en%arg2%cval
                        case (V_PDG); en%aval = en%arg2%aval
                        case (V_SEV); en%pval = en%arg2%pval
                        case (V_STR); en%sval = en%arg2%sval
                    end select
                end if
            end if
        end if
    case (EN_RECORD_CMD)
        exist = .true.
        en%lval = .false.

```

```

call eval_node_evaluate (en%arg0)
if (en%arg0%value_is_known) then
  if (associated (en%arg1)) then
    call eval_node_evaluate (en%arg1)
    if (en%arg1%value_is_known) then
      if (associated (en%arg2)) then
        call eval_node_evaluate (en%arg2)
        if (en%arg2%value_is_known) then
          if (associated (en%arg3)) then
            call eval_node_evaluate (en%arg3)
            if (en%arg3%value_is_known) then
              if (associated (en%arg4)) then
                call eval_node_evaluate (en%arg4)
                if (en%arg4%value_is_known) then
                  if (associated (en%rval)) then
                    call analysis_record_data (en%arg0%sval, &
                      en%arg1%rval, en%arg2%rval, &
                      en%arg3%rval, en%arg4%rval, &
                      weight=en%rval, exist=exist, &
                      success=en%lval)
                  else
                    call analysis_record_data (en%arg0%sval, &
                      en%arg1%rval, en%arg2%rval, &
                      en%arg3%rval, en%arg4%rval, &
                      exist=exist, success=en%lval)
                  end if
                end if
              end if
            end if
          end if
        end if
      end if
    end if
  else
    if (associated (en%rval)) then
      call analysis_record_data (en%arg0%sval, &
        en%arg1%rval, en%arg2%rval, &
        en%arg3%rval, &
        weight=en%rval, exist=exist, &
        success=en%lval)
    else
      call analysis_record_data (en%arg0%sval, &
        en%arg1%rval, en%arg2%rval, &
        en%arg3%rval, &
        exist=exist, success=en%lval)
    end if
  end if
end if
else
  if (associated (en%rval)) then
    call analysis_record_data (en%arg0%sval, &
      en%arg1%rval, en%arg2%rval, &
      weight=en%rval, exist=exist, &
      success=en%lval)
  else
    call analysis_record_data (en%arg0%sval, &
      en%arg1%rval, en%arg2%rval, &
      exist=exist, success=en%lval)
  end if
end if
end if

```

```

        end if
    else
        if (associated (en%rval)) then
            call analysis_record_data (en%arg0%sval, &
                en%arg1%rval, &
                weight=en%rval, exist=exist, success=en%lval)
        else
            call analysis_record_data (en%arg0%sval, &
                en%arg1%rval, &
                exist=exist, success=en%lval)
        end if
    end if
end if
else
    if (associated (en%rval)) then
        call analysis_record_data (en%arg0%sval, 1._default, &
            weight=en%rval, exist=exist, success=en%lval)
    else
        call analysis_record_data (en%arg0%sval, 1._default, &
            exist=exist, success=en%lval)
    end if
end if
if (.not. exist) then
    call msg_error ("Analysis object '" // char (en%arg0%sval) &
        // "' is undefined")
    en%arg0%value_is_known = .false.
end if
end if
case (EN_OBS1_INT)
    en%ival = en%obs1_int (en%prt1)
    en%value_is_known = .true.
case (EN_OBS2_INT)
    en%ival = en%obs2_int (en%prt1, en%prt2)
    en%value_is_known = .true.
case (EN_OBSEV_INT)
    en%ival = en%obsev_int (en%pval)
    en%value_is_known = .true.
case (EN_OBS1_REAL)
    en%rval = en%obs1_real (en%prt1)
    en%value_is_known = .true.
case (EN_OBS2_REAL)
    en%rval = en%obs2_real (en%prt1, en%prt2)
    en%value_is_known = .true.
case (EN_OBSEV_REAL)
    en%rval = en%obsev_real (en%pval)
    en%value_is_known = .true.
case (EN_PRT_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = en%arg1%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            call en%op1_sev (en%pval, en%arg1, en%arg0)
        end if
    end if
end if

```

```

        else
            call en%op1_sev (en%pval, en%arg1)
        end if
    end if
case (EN_PRT_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = &
        en%arg1%value_is_known .and. en%arg2%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            en%arg0%prt2 => en%prt2
            call en%op2_sev (en%pval, en%arg1, en%arg2, en%arg0)
        else
            call en%op2_sev (en%pval, en%arg1, en%arg2)
        end if
    end if
case (EN_EVAL_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = subevt_is_nonempty (en%arg1%pval)
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%index = 1
        en%arg0%prt1 => en%prt1
        en%prt1 = subevt_get_prt (en%arg1%pval, 1)
        call eval_node_evaluate (en%arg0)
        en%rval = en%arg0%rval
    end if
case (EN_EVAL_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = &
        subevt_is_nonempty (en%arg1%pval) .and. &
        subevt_is_nonempty (en%arg2%pval)
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%arg0%prt1 => en%prt1
        en%arg0%prt2 => en%prt2
        en%index = 1
        call eval_pp (en%arg1, en%arg2, en%arg0, en%rval, en%value_is_known)
    end if
case (EN_LOG_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = .true.
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%arg0%prt1 => en%prt1
        en%lval = en%op1_cut (en%arg1, en%arg0)
    end if
case (EN_LOG_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)

```

```

    en%value_is_known = .true.
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%arg0%prt1 => en%prt1
        en%arg0%prt2 => en%prt2
        en%lval = en%op2_cut (en%arg1, en%arg2, en%arg0)
    end if
case (EN_INT_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = en%arg1%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            call en%op1_evi (en%ival, en%arg1, en%arg0)
        else
            call en%op1_evi (en%ival, en%arg1)
        end if
    end if
case (EN_INT_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = &
        en%arg1%value_is_known .and. &
        en%arg2%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            en%arg0%prt2 => en%prt2
            call en%op2_evi (en%ival, en%arg1, en%arg2, en%arg0)
        else
            call en%op2_evi (en%ival, en%arg1, en%arg2)
        end if
    end if
case (EN_REAL_FUN_UNARY)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = en%arg1%value_is_known
    if (en%value_is_known) then
        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            call en%op1_evr (en%rval, en%arg1, en%arg0)
        else
            call en%op1_evr (en%rval, en%arg1)
        end if
    end if
case (EN_REAL_FUN_BINARY)
    call eval_node_evaluate (en%arg1)
    call eval_node_evaluate (en%arg2)
    en%value_is_known = &
        en%arg1%value_is_known .and. &
        en%arg2%value_is_known
    if (en%value_is_known) then

```

```

        if (associated (en%arg0)) then
            en%arg0%index => en%index
            en%arg0%prt1 => en%prt1
            en%arg0%prt2 => en%prt2
            call en%op2_evr (en%rval, en%arg1, en%arg2, en%arg0)
        else
            call en%op2_evr (en%rval, en%arg1, en%arg2)
        end if
    end if
case (EN_REAL_FUN_CUM)
    call eval_node_evaluate (en%arg1)
    en%value_is_known = .true.
    if (en%value_is_known) then
        en%arg0%index => en%index
        en%arg0%prt1 => en%prt1
        en%rval = en%opcum_evr (en%arg1, en%arg0)
    end if
case (EN_FORMAT_STR)
    if (associated (en%arg0)) then
        call eval_node_evaluate (en%arg0)
        en%value_is_known = en%arg0%value_is_known
    else
        en%value_is_known = .true.
    end if
    if (associated (en%arg1)) then
        call eval_node_evaluate (en%arg1)
        en%value_is_known = &
            en%value_is_known .and. en%arg1%value_is_known
        if (en%value_is_known) then
            call evaluate_sprintf (en%sval, en%ival, en%arg0, en%arg1)
        end if
    else
        if (en%value_is_known) then
            call evaluate_sprintf (en%sval, en%ival, en%arg0)
        end if
    end if
end select
if (debug2_active (D_MODEL_F)) then
    print *, "eval_node_evaluate"
    call eval_node_write (en)
end if
end subroutine eval_node_evaluate

```

Test method

This is called from a unit test: initialize a particular observable.

<Eval trees: eval node: TBP>+≡

```
procedure :: test_obs => eval_node_test_obs
```

<Eval trees: procedures>+≡

```

subroutine eval_node_test_obs (node, var_list, var_name)
    class(eval_node_t), intent(inout) :: node
    type(var_list_t), intent(in) :: var_list

```

```

    type(string_t), intent(in) :: var_name
    procedure(obs_unary_int), pointer :: obs1_iptr
    type(prt_t), pointer :: p1
    call var_list%get_obs1_iptr (var_name, obs1_iptr, p1)
    call eval_node_init_obs1_int_ptr (node, var_name, obs1_iptr, p1)
end subroutine eval_node_test_obs

```

28.3.7 Evaluation syntax

We have two different flavors of the syntax: with and without particles.

<Eval trees: public>+≡

```

    public :: syntax_expr
    public :: syntax_pexpr

```

<Eval trees: variables>≡

```

    type(syntax_t), target, save :: syntax_expr
    type(syntax_t), target, save :: syntax_pexpr

```

These are for testing only and may be removed:

<Eval trees: public>+≡

```

    public :: syntax_expr_init
    public :: syntax_pexpr_init

```

<Eval trees: procedures>+≡

```

    subroutine syntax_expr_init ()
        type(ifile_t) :: ifile
        call define_expr_syntax (ifile, particles=.false., analysis=.false.)
        call syntax_init (syntax_expr, ifile)
        call ifile_final (ifile)
    end subroutine syntax_expr_init

```

```

    subroutine syntax_pexpr_init ()
        type(ifile_t) :: ifile
        call define_expr_syntax (ifile, particles=.true., analysis=.false.)
        call syntax_init (syntax_pexpr, ifile)
        call ifile_final (ifile)
    end subroutine syntax_pexpr_init

```

<Eval trees: public>+≡

```

    public :: syntax_expr_final
    public :: syntax_pexpr_final

```

<Eval trees: procedures>+≡

```

    subroutine syntax_expr_final ()
        call syntax_final (syntax_expr)
    end subroutine syntax_expr_final

```

```

    subroutine syntax_pexpr_final ()
        call syntax_final (syntax_pexpr)
    end subroutine syntax_pexpr_final

```

<Eval trees: public>+≡

```

    public :: syntax_pexpr_write

```


<Eval trees: procedures>+≡

```
subroutine syntax_pexpr_write (unit)
  integer, intent(in), optional :: unit
  call syntax_write (syntax_pexpr, unit)
end subroutine syntax_pexpr_write
```

<Eval trees: public>+≡

```
public :: define_expr_syntax
```

Numeric expressions.

<Eval trees: procedures>+≡

```
subroutine define_expr_syntax (ifile, particles, analysis)
  type(ifile_t), intent(inout) :: ifile
  logical, intent(in) :: particles, analysis
  type(string_t) :: numeric_pexpr
  type(string_t) :: var_plist, var_alias
  if (particles) then
    numeric_pexpr = " | numeric_pexpr"
    var_plist = " | var_plist"
    var_alias = " | var_alias"
  else
    numeric_pexpr = ""
    var_plist = ""
    var_alias = ""
  end if
  call ifile_append (ifile, "SEQ expr = subexpr addition*")
  call ifile_append (ifile, "ALT subexpr = addition | term")
  call ifile_append (ifile, "SEQ addition = plus_or_minus term")
  call ifile_append (ifile, "SEQ term = factor multiplication*")
  call ifile_append (ifile, "SEQ multiplication = times_or_over factor")
  call ifile_append (ifile, "SEQ factor = value exponentiation?")
  call ifile_append (ifile, "SEQ exponentiation = to_the value")
  call ifile_append (ifile, "ALT plus_or_minus = '+' | '-'")
  call ifile_append (ifile, "ALT times_or_over = '*' | '/'")
  call ifile_append (ifile, "ALT to_the = '^' | '**")
  call ifile_append (ifile, "KEY '+'")
  call ifile_append (ifile, "KEY '-'")
  call ifile_append (ifile, "KEY '*'")
  call ifile_append (ifile, "KEY '/'")
  call ifile_append (ifile, "KEY '^'")
  call ifile_append (ifile, "KEY '**")
  call ifile_append (ifile, "ALT value = signed_value | unsigned_value")
  call ifile_append (ifile, "SEQ signed_value = '-' unsigned_value")
  call ifile_append (ifile, "ALT unsigned_value = " // &
    "numeric_value | constant | variable | " // &
    "result | " // &
    "grouped_expr | block_expr | conditional_expr | " // &
    "unary_function | binary_function" // &
    numeric_pexpr)
  call ifile_append (ifile, "ALT numeric_value = integer_value | " &
    "// "real_value | complex_value")
  call ifile_append (ifile, "SEQ integer_value = integer_literal unit_expr?")
  call ifile_append (ifile, "SEQ real_value = real_literal unit_expr?")
  call ifile_append (ifile, "SEQ complex_value = complex_literal unit_expr?")
```

```

call ifile_append (ifile, "INT integer_literal")
call ifile_append (ifile, "REA real_literal")
call ifile_append (ifile, "COM complex_literal")
call ifile_append (ifile, "SEQ unit_expr = unit unit_power?")
call ifile_append (ifile, "ALT unit = " // &
    "TeV | GeV | MeV | keV | eV | meV | " // &
    "nbarn | pbarn | fbarn | abarn | " // &
    "rad | mrad | degree | '%'"")
call ifile_append (ifile, "KEY TeV")
call ifile_append (ifile, "KEY GeV")
call ifile_append (ifile, "KEY MeV")
call ifile_append (ifile, "KEY keV")
call ifile_append (ifile, "KEY eV")
call ifile_append (ifile, "KEY meV")
call ifile_append (ifile, "KEY nbarn")
call ifile_append (ifile, "KEY pbarn")
call ifile_append (ifile, "KEY fbarn")
call ifile_append (ifile, "KEY abarn")
call ifile_append (ifile, "KEY rad")
call ifile_append (ifile, "KEY mrad")
call ifile_append (ifile, "KEY degree")
call ifile_append (ifile, "KEY '%'"")
call ifile_append (ifile, "SEQ unit_power = '^' frac_expr")
call ifile_append (ifile, "ALT frac_expr = frac | grouped_frac")
call ifile_append (ifile, "GRO grouped_frac = ( frac_expr )")
call ifile_append (ifile, "SEQ frac = signed_int div?")
call ifile_append (ifile, "ALT signed_int = " &
    // "neg_int | pos_int | integer_literal")
call ifile_append (ifile, "SEQ neg_int = '-' integer_literal")
call ifile_append (ifile, "SEQ pos_int = '+' integer_literal")
call ifile_append (ifile, "SEQ div = '/' integer_literal")
call ifile_append (ifile, "ALT constant = pi | I")
call ifile_append (ifile, "KEY pi")
call ifile_append (ifile, "KEY I")
call ifile_append (ifile, "IDE variable")
call ifile_append (ifile, "SEQ result = result_key result_arg")
call ifile_append (ifile, "ALT result_key = " // &
    "num_id | integral | error")
call ifile_append (ifile, "KEY num_id")
call ifile_append (ifile, "KEY integral")
call ifile_append (ifile, "KEY error")
call ifile_append (ifile, "GRO result_arg = ( process_id )")
call ifile_append (ifile, "IDE process_id")
call ifile_append (ifile, "SEQ unary_function = fun_unary function_arg1")
call ifile_append (ifile, "SEQ binary_function = fun_binary function_arg2")
call ifile_append (ifile, "ALT fun_unary = " // &
    "complex | real | int | nint | floor | ceiling | abs | conjg | sgn | " // &
    "sqrt | exp | log | log10 | " // &
    "sin | cos | tan | asin | acos | atan | " // &
    "sinh | cosh | tanh | asinh | acosh | atanh")
call ifile_append (ifile, "KEY complex")
call ifile_append (ifile, "KEY real")
call ifile_append (ifile, "KEY int")
call ifile_append (ifile, "KEY nint")

```

```

call ifile_append (ifile, "KEY floor")
call ifile_append (ifile, "KEY ceiling")
call ifile_append (ifile, "KEY abs")
call ifile_append (ifile, "KEY conjg")
call ifile_append (ifile, "KEY sgn")
call ifile_append (ifile, "KEY sqrt")
call ifile_append (ifile, "KEY exp")
call ifile_append (ifile, "KEY log")
call ifile_append (ifile, "KEY log10")
call ifile_append (ifile, "KEY sin")
call ifile_append (ifile, "KEY cos")
call ifile_append (ifile, "KEY tan")
call ifile_append (ifile, "KEY asin")
call ifile_append (ifile, "KEY acos")
call ifile_append (ifile, "KEY atan")
call ifile_append (ifile, "KEY sinh")
call ifile_append (ifile, "KEY cosh")
call ifile_append (ifile, "KEY tanh")
call ifile_append (ifile, "KEY asinh")
call ifile_append (ifile, "KEY acosh")
call ifile_append (ifile, "KEY atanh")
call ifile_append (ifile, "ALT fun_binary = max | min | mod | modulo")
call ifile_append (ifile, "KEY max")
call ifile_append (ifile, "KEY min")
call ifile_append (ifile, "KEY mod")
call ifile_append (ifile, "KEY modulo")
call ifile_append (ifile, "ARG function_arg1 = ( expr )")
call ifile_append (ifile, "ARG function_arg2 = ( expr, expr )")
call ifile_append (ifile, "GRO grouped_expr = ( expr )")
call ifile_append (ifile, "SEQ block_expr = let var_spec in expr")
call ifile_append (ifile, "KEY let")
call ifile_append (ifile, "ALT var_spec = " // &
    "var_num | var_int | var_real | var_complex | " // &
    "var_logical" // var_plist // var_alias // " | var_string")
call ifile_append (ifile, "SEQ var_num = var_name '=' expr")
call ifile_append (ifile, "SEQ var_int = int var_name '=' expr")
call ifile_append (ifile, "SEQ var_real = real var_name '=' expr")
call ifile_append (ifile, "SEQ var_complex = complex var_name '=' complex_expr")
call ifile_append (ifile, "ALT complex_expr = " // &
    "cexpr_real | cexpr_complex")
call ifile_append (ifile, "ARG cexpr_complex = ( expr, expr )")
call ifile_append (ifile, "SEQ cexpr_real = expr")
call ifile_append (ifile, "IDE var_name")
call ifile_append (ifile, "KEY '='")
call ifile_append (ifile, "KEY in")
call ifile_append (ifile, "SEQ conditional_expr = " // &
    "if lexpr then expr maybe_elseif_expr maybe_else_expr endif")
call ifile_append (ifile, "SEQ maybe_elseif_expr = elseif_expr*")
call ifile_append (ifile, "SEQ maybe_else_expr = else_expr?")
call ifile_append (ifile, "SEQ elseif_expr = elseif lexpr then expr")
call ifile_append (ifile, "SEQ else_expr = else expr")
call ifile_append (ifile, "KEY if")
call ifile_append (ifile, "KEY then")
call ifile_append (ifile, "KEY elseif")

```

```

call ifile_append (ifile, "KEY else")
call ifile_append (ifile, "KEY endif")
call define_lexpr_syntax (ifile, particles, analysis)
call define_sexpr_syntax (ifile)
if (particles) then
    call define_pexpr_syntax (ifile)
    call define_cexpr_syntax (ifile)
    call define_var_plist_syntax (ifile)
    call define_var_alias_syntax (ifile)
    call define_numeric_pexpr_syntax (ifile)
    call define_logical_pexpr_syntax (ifile)
end if

end subroutine define_expr_syntax

```

Logical expressions.

<Eval trees: procedures>+≡

```

subroutine define_lexpr_syntax (ifile, particles, analysis)
    type(ifile_t), intent(inout) :: ifile
    logical, intent(in) :: particles, analysis
    type(string_t) :: logical_pexpr, record_cmd
    if (particles) then
        logical_pexpr = " | logical_pexpr"
    else
        logical_pexpr = ""
    end if
    if (analysis) then
        record_cmd = " | record_cmd"
    else
        record_cmd = ""
    end if
    call ifile_append (ifile, "SEQ lexpr = lsinglet lsequel*")
    call ifile_append (ifile, "SEQ lsequel = ';' lsinglet")
    call ifile_append (ifile, "SEQ lsinglet = lterm alternative*")
    call ifile_append (ifile, "SEQ alternative = or lterm")
    call ifile_append (ifile, "SEQ lterm = lvalue coincidence*")
    call ifile_append (ifile, "SEQ coincidence = and lvalue")
    call ifile_append (ifile, "KEY ';'")
    call ifile_append (ifile, "KEY or")
    call ifile_append (ifile, "KEY and")
    call ifile_append (ifile, "ALT lvalue = " // &
        "true | false | lvariable | negation | " // &
        "grouped_lexpr | block_lexpr | conditional_lexpr | " // &
        "compared_expr | compared_sexpr" // &
        logical_pexpr // record_cmd)
    call ifile_append (ifile, "KEY true")
    call ifile_append (ifile, "KEY false")
    call ifile_append (ifile, "SEQ lvariable = '?' alt_lvariable")
    call ifile_append (ifile, "KEY '?'")
    call ifile_append (ifile, "ALT alt_lvariable = variable | grouped_lexpr")
    call ifile_append (ifile, "SEQ negation = not lvalue")
    call ifile_append (ifile, "KEY not")
    call ifile_append (ifile, "GRO grouped_lexpr = ( lexpr )")
    call ifile_append (ifile, "SEQ block_lexpr = let var_spec in lexpr")

```

```

call ifile_append (ifile, "ALT var_logical = " // &
    "var_logical_new | var_logical_spec")
call ifile_append (ifile, "SEQ var_logical_new = logical var_logical_spec")
call ifile_append (ifile, "KEY logical")
call ifile_append (ifile, "SEQ var_logical_spec = '?' var_name = lexpr")
call ifile_append (ifile, "SEQ conditional_lexpr = " // &
    "if lexpr then lexpr maybe_elseif_lexpr maybe_else_lexpr endif")
call ifile_append (ifile, "SEQ maybe_elseif_lexpr = elseif_lexpr*")
call ifile_append (ifile, "SEQ maybe_else_lexpr = else_lexpr?")
call ifile_append (ifile, "SEQ elseif_lexpr = elseif lexpr then lexpr")
call ifile_append (ifile, "SEQ else_lexpr = else lexpr")
call ifile_append (ifile, "SEQ compared_expr = expr comparison+")
call ifile_append (ifile, "SEQ comparison = compare expr")
call ifile_append (ifile, "ALT compare = " // &
    "'<' | '>' | '<=' | '>=' | '==' | '<>'")
call ifile_append (ifile, "KEY '<'"")
call ifile_append (ifile, "KEY '>'"")
call ifile_append (ifile, "KEY '<='")
call ifile_append (ifile, "KEY '>='")
call ifile_append (ifile, "KEY '=='")
call ifile_append (ifile, "KEY '<>'")
call ifile_append (ifile, "SEQ compared_sexpr = sexpr str_comparison+")
call ifile_append (ifile, "SEQ str_comparison = str_compare sexpr")
call ifile_append (ifile, "ALT str_compare = '==' | '<>'")
if (analysis) then
    call ifile_append (ifile, "SEQ record_cmd = " // &
        "record_key analysis_tag record_arg?")
    call ifile_append (ifile, "ALT record_key = " // &
        "record | record_unweighted | record_excess")
    call ifile_append (ifile, "KEY record")
    call ifile_append (ifile, "KEY record_unweighted")
    call ifile_append (ifile, "KEY record_excess")
    call ifile_append (ifile, "ALT analysis_tag = analysis_id | sexpr")
    call ifile_append (ifile, "IDE analysis_id")
    call ifile_append (ifile, "ARG record_arg = ( expr+ )")
end if
end subroutine define_lexpr_syntax

```

String expressions.

(Eval trees: procedures)+≡

```

subroutine define_sexpr_syntax (ifile)
    type(ifile_t), intent(inout) :: ifile
    call ifile_append (ifile, "SEQ sexpr = svalue str_concatenation*")
    call ifile_append (ifile, "SEQ str_concatenation = '&' svalue")
    call ifile_append (ifile, "KEY '&'")
    call ifile_append (ifile, "ALT svalue = " // &
        "grouped_sexpr | block_sexpr | conditional_sexpr | " // &
        "svariable | string_function | string_literal")
    call ifile_append (ifile, "GRO grouped_sexpr = ( sexpr )")
    call ifile_append (ifile, "SEQ block_sexpr = let var_spec in sexpr")
    call ifile_append (ifile, "SEQ conditional_sexpr = " // &
        "if lexpr then sexpr maybe_elseif_sexpr maybe_else_sexpr endif")
    call ifile_append (ifile, "SEQ maybe_elseif_sexpr = elseif_sexpr*")
    call ifile_append (ifile, "SEQ maybe_else_sexpr = else_sexpr?")

```

```

call ifile_append (ifile, "SEQ elsif_sexpr = elsif lexpr then sexpr")
call ifile_append (ifile, "SEQ else_sexpr = else sexpr")
call ifile_append (ifile, "SEQ svariable = '$' alt_svariable")
call ifile_append (ifile, "KEY '$'")
call ifile_append (ifile, "ALT alt_svariable = variable | grouped_sexpr")
call ifile_append (ifile, "ALT var_string = " // &
    "var_string_new | var_string_spec")
call ifile_append (ifile, "SEQ var_string_new = string var_string_spec")
call ifile_append (ifile, "KEY string")
call ifile_append (ifile, "SEQ var_string_spec = '$' var_name = sexpr") ! $
call ifile_append (ifile, "ALT string_function = sprintf_fun")
call ifile_append (ifile, "SEQ sprintf_fun = sprintf_clause sprintf_args?")
call ifile_append (ifile, "SEQ sprintf_clause = sprintf sexpr")
call ifile_append (ifile, "KEY sprintf")
call ifile_append (ifile, "ARG sprintf_args = ( sprintf_arg* )")
call ifile_append (ifile, "ALT sprintf_arg = " &
    // "lvariable | svariable | expr")
call ifile_append (ifile, "QUO string_literal = '""'...'""')
end subroutine define_sexpr_syntax

```

Eval trees that evaluate to subevents.

(*Eval trees: procedures*)+≡

```

subroutine define_pexpr_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "SEQ pexpr = pterm pconcatenation*")
  call ifile_append (ifile, "SEQ pconcatenation = '&' pterm")
  ! call ifile_append (ifile, "KEY '&'") !!! (Key exists already)
  call ifile_append (ifile, "SEQ pterm = pvalue pcombination*")
  call ifile_append (ifile, "SEQ pcombination = '+' pvalue")
  ! call ifile_append (ifile, "KEY '+'") !!! (Key exists already)
  call ifile_append (ifile, "ALT pvalue = " // &
    "pexpr_src | pvariable | " // &
    "grouped_pexpr | block_pexpr | conditional_pexpr | " // &
    "prt_function")
  call ifile_append (ifile, "SEQ pexpr_src = prefix_cexpr")
  call ifile_append (ifile, "ALT prefix_cexpr = " // &
    "beam_prt | incoming_prt | outgoing_prt | unspecified_prt")
  call ifile_append (ifile, "SEQ beam_prt = beam cexpr")
  call ifile_append (ifile, "KEY beam")
  call ifile_append (ifile, "SEQ incoming_prt = incoming cexpr")
  call ifile_append (ifile, "KEY incoming")
  call ifile_append (ifile, "SEQ outgoing_prt = outgoing cexpr")
  call ifile_append (ifile, "KEY outgoing")
  call ifile_append (ifile, "SEQ unspecified_prt = cexpr")
  call ifile_append (ifile, "SEQ pvariable = '@' alt_pvariable")
  call ifile_append (ifile, "KEY '@'")
  call ifile_append (ifile, "ALT alt_pvariable = variable | grouped_pexpr")
  call ifile_append (ifile, "GRO grouped_pexpr = '[' pexpr ']')")
  call ifile_append (ifile, "SEQ block_pexpr = let var_spec in pexpr")
  call ifile_append (ifile, "SEQ conditional_pexpr = " // &
    "if lexpr then pexpr maybe_elseif_pexpr maybe_else_pexpr endif")
  call ifile_append (ifile, "SEQ maybe_elseif_pexpr = elsif_pexpr*")
  call ifile_append (ifile, "SEQ maybe_else_pexpr = else_pexpr?")
  call ifile_append (ifile, "SEQ elsif_pexpr = elsif lexpr then pexpr")

```

```

call ifile_append (ifile, "SEQ else_pexpr = else pexpr")
call ifile_append (ifile, "ALT prt_function = " // &
    "join_fun | combine_fun | collect_fun | cluster_fun | " // &
    "photon_reco_fun | " // &
    "select_fun | extract_fun | sort_fun | " // &
    "select_b_jet_fun | select_non_b_jet_fun | " // &
    "select_c_jet_fun | select_light_jet_fun")
call ifile_append (ifile, "SEQ join_fun = join_clause pargs2")
call ifile_append (ifile, "SEQ combine_fun = combine_clause pargs2")
call ifile_append (ifile, "SEQ collect_fun = collect_clause pargs1")
call ifile_append (ifile, "SEQ cluster_fun = cluster_clause pargs1")
call ifile_append (ifile, "SEQ photon_reco_fun = photon_reco_clause pargs1")
call ifile_append (ifile, "SEQ select_fun = select_clause pargs1")
call ifile_append (ifile, "SEQ extract_fun = extract_clause pargs1")
call ifile_append (ifile, "SEQ sort_fun = sort_clause pargs1")
call ifile_append (ifile, "SEQ select_b_jet_fun = " // &
    "select_b_jet_clause pargs1")
call ifile_append (ifile, "SEQ select_non_b_jet_fun = " // &
    "select_non_b_jet_clause pargs1")
call ifile_append (ifile, "SEQ select_c_jet_fun = " // &
    "select_c_jet_clause pargs1")
call ifile_append (ifile, "SEQ select_light_jet_fun = " // &
    "select_light_jet_clause pargs1")
call ifile_append (ifile, "SEQ join_clause = join condition?")
call ifile_append (ifile, "SEQ combine_clause = combine condition?")
call ifile_append (ifile, "SEQ collect_clause = collect condition?")
call ifile_append (ifile, "SEQ cluster_clause = cluster condition?")
call ifile_append (ifile, "SEQ photon_reco_clause = photon_recombination condition?")
call ifile_append (ifile, "SEQ select_clause = select condition?")
call ifile_append (ifile, "SEQ extract_clause = extract position?")
call ifile_append (ifile, "SEQ sort_clause = sort criterion?")
call ifile_append (ifile, "SEQ select_b_jet_clause = " // &
    "select_b_jet condition?")
call ifile_append (ifile, "SEQ select_non_b_jet_clause = " // &
    "select_non_b_jet condition?")
call ifile_append (ifile, "SEQ select_c_jet_clause = " // &
    "select_c_jet condition?")
call ifile_append (ifile, "SEQ select_light_jet_clause = " // &
    "select_light_jet condition?")
call ifile_append (ifile, "KEY join")
call ifile_append (ifile, "KEY combine")
call ifile_append (ifile, "KEY collect")
call ifile_append (ifile, "KEY cluster")
call ifile_append (ifile, "KEY photon_recombination")
call ifile_append (ifile, "KEY select")
call ifile_append (ifile, "SEQ condition = if lexpr")
call ifile_append (ifile, "KEY extract")
call ifile_append (ifile, "SEQ position = index expr")
call ifile_append (ifile, "KEY sort")
call ifile_append (ifile, "KEY select_b_jet")
call ifile_append (ifile, "KEY select_non_b_jet")
call ifile_append (ifile, "KEY select_c_jet")
call ifile_append (ifile, "KEY select_light_jet")
call ifile_append (ifile, "SEQ criterion = by expr")

```

```

call ifile_append (ifile, "KEY index")
call ifile_append (ifile, "KEY by")
call ifile_append (ifile, "ARG pargs2 = '[' pexpr, pexpr ']'")
call ifile_append (ifile, "ARG pargs1 = '[' pexpr, pexpr? ']'")
end subroutine define_pexpr_syntax

```

Eval trees that evaluate to PDG-code arrays.

(Eval trees: procedures)+≡

```

subroutine define_cexpr_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "SEQ cexpr = avalue concatenation*")
  call ifile_append (ifile, "SEQ concatenation = ':' avalue")
  call ifile_append (ifile, "KEY ':'")
  call ifile_append (ifile, "ALT avalue = " // &
    "grouped_cexpr | block_cexpr | conditional_cexpr | " // &
    "variable | pdg_code | prt_name")
  call ifile_append (ifile, "GRO grouped_cexpr = ( cexpr )")
  call ifile_append (ifile, "SEQ block_cexpr = let var_spec in cexpr")
  call ifile_append (ifile, "SEQ conditional_cexpr = " // &
    "if lexpr then cexpr maybe_elseif_cexpr maybe_else_cexpr endif")
  call ifile_append (ifile, "SEQ maybe_elseif_cexpr = elseif_cexpr*")
  call ifile_append (ifile, "SEQ maybe_else_cexpr = else_cexpr?")
  call ifile_append (ifile, "SEQ elseif_cexpr = elseif lexpr then cexpr")
  call ifile_append (ifile, "SEQ else_cexpr = else cexpr")
  call ifile_append (ifile, "SEQ pdg_code = pdg pdg_arg")
  call ifile_append (ifile, "KEY pdg")
  call ifile_append (ifile, "ARG pdg_arg = ( expr )")
  call ifile_append (ifile, "QUO prt_name = '""'...'""'")
end subroutine define_cexpr_syntax

```

Extra variable types.

(Eval trees: procedures)+≡

```

subroutine define_var_plist_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "ALT var_plist = var_plist_new | var_plist_spec")
  call ifile_append (ifile, "SEQ var_plist_new = subevt var_plist_spec")
  call ifile_append (ifile, "KEY subevt")
  call ifile_append (ifile, "SEQ var_plist_spec = '@' var_name '=' pexpr")
end subroutine define_var_plist_syntax

subroutine define_var_alias_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "SEQ var_alias = alias var_name '=' cexpr")
  call ifile_append (ifile, "KEY alias")
end subroutine define_var_alias_syntax

```

Particle-list expressions that evaluate to numeric values

(Eval trees: procedures)+≡

```

subroutine define_numeric_pexpr_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "ALT numeric_pexpr = " &
    // "eval_fun | count_fun | sum_fun | " &

```



```

        // "prod_fun")
    call ifile_append (ifile, "SEQ eval_fun = eval expr pargs1")
    call ifile_append (ifile, "SEQ count_fun = count_clause pargs1")
    call ifile_append (ifile, "SEQ count_clause = count condition?")
    call ifile_append (ifile, "SEQ sum_fun = sum expr pargs1")
    call ifile_append (ifile, "SEQ prod_fun = prod expr pargs1")
    call ifile_append (ifile, "KEY eval")
    call ifile_append (ifile, "KEY count")
    call ifile_append (ifile, "KEY sum")
    call ifile_append (ifile, "KEY prod")
end subroutine define_numeric_pexpr_syntax

```

Particle-list functions that evaluate to logical values.

(Eval trees: procedures)+≡

```

subroutine define_logical_pexpr_syntax (ifile)
    type(ifile_t), intent(inout) :: ifile
    call ifile_append (ifile, "ALT logical_pexpr = " // &
        "all_fun | any_fun | no_fun | " // &
        "photon_isolation_fun")
    call ifile_append (ifile, "SEQ all_fun = all lexpr pargs1")
    call ifile_append (ifile, "SEQ any_fun = any lexpr pargs1")
    call ifile_append (ifile, "SEQ no_fun = no lexpr pargs1")
    call ifile_append (ifile, "SEQ photon_isolation_fun = " // &
        "photon_isolation_clause pargs2")
    call ifile_append (ifile, "SEQ photon_isolation_clause = " // &
        "photon_isolation condition?")
    call ifile_append (ifile, "KEY all")
    call ifile_append (ifile, "KEY any")
    call ifile_append (ifile, "KEY no")
    call ifile_append (ifile, "KEY photon_isolation")
end subroutine define_logical_pexpr_syntax

```

All characters that can occur in expressions (apart from alphanumeric).

(Eval trees: procedures)+≡

```

subroutine lexer_init_eval_tree (lexer, particles)
    type(lexer_t), intent(out) :: lexer
    logical, intent(in) :: particles
    type(keyword_list_t), pointer :: keyword_list
    if (particles) then
        keyword_list => syntax_get_keyword_list_ptr (syntax_pexpr)
    else
        keyword_list => syntax_get_keyword_list_ptr (syntax_expr)
    end if
    call lexer_init (lexer, &
        comment_chars = "#!", &
        quote_chars = "'", &
        quote_match = "'", &
        single_chars = "()[];:&%?@$@", &
        special_class = [ "+-*/^", "<>=~ " ], &
        keyword_list = keyword_list)
end subroutine lexer_init_eval_tree

```

28.3.8 Set up appropriate parse trees

Parse an input stream as a specific flavor of expression. The appropriate expression syntax has to be available.

<Eval trees: public>+≡

```
public :: parse_tree_init_expr
public :: parse_tree_init_lexpr
public :: parse_tree_init_pexpr
public :: parse_tree_init_cexpr
public :: parse_tree_init_sexpr
```

<Eval trees: procedures>+≡

```
subroutine parse_tree_init_expr (parse_tree, stream, particles)
  type(parse_tree_t), intent(out) :: parse_tree
  type(stream_t), intent(inout), target :: stream
  logical, intent(in) :: particles
  type(lexer_t) :: lexer
  call lexer_init_eval_tree (lexer, particles)
  call lexer_assign_stream (lexer, stream)
  if (particles) then
    call parse_tree_init &
      (parse_tree, syntax_pexpr, lexer, var_str ("expr"))
  else
    call parse_tree_init &
      (parse_tree, syntax_expr, lexer, var_str ("expr"))
  end if
  call lexer_final (lexer)
end subroutine parse_tree_init_expr
```

```
subroutine parse_tree_init_lexpr (parse_tree, stream, particles)
  type(parse_tree_t), intent(out) :: parse_tree
  type(stream_t), intent(inout), target :: stream
  logical, intent(in) :: particles
  type(lexer_t) :: lexer
  call lexer_init_eval_tree (lexer, particles)
  call lexer_assign_stream (lexer, stream)
  if (particles) then
    call parse_tree_init &
      (parse_tree, syntax_pexpr, lexer, var_str ("lexpr"))
  else
    call parse_tree_init &
      (parse_tree, syntax_expr, lexer, var_str ("lexpr"))
  end if
  call lexer_final (lexer)
end subroutine parse_tree_init_lexpr
```

```
subroutine parse_tree_init_pexpr (parse_tree, stream)
  type(parse_tree_t), intent(out) :: parse_tree
  type(stream_t), intent(inout), target :: stream
  type(lexer_t) :: lexer
  call lexer_init_eval_tree (lexer, .true.)
  call lexer_assign_stream (lexer, stream)
  call parse_tree_init &
    (parse_tree, syntax_pexpr, lexer, var_str ("pexpr"))
  call lexer_final (lexer)
```

```

end subroutine parse_tree_init_pexpr

subroutine parse_tree_init_cexpr (parse_tree, stream)
  type(parse_tree_t), intent(out) :: parse_tree
  type(stream_t), intent(inout), target :: stream
  type(lexer_t) :: lexer
  call lexer_init_eval_tree (lexer, .true.)
  call lexer_assign_stream (lexer, stream)
  call parse_tree_init &
    (parse_tree, syntax_pexpr, lexer, var_str ("cexpr"))
  call lexer_final (lexer)
end subroutine parse_tree_init_cexpr

subroutine parse_tree_init_sexpr (parse_tree, stream, particles)
  type(parse_tree_t), intent(out) :: parse_tree
  type(stream_t), intent(inout), target :: stream
  logical, intent(in) :: particles
  type(lexer_t) :: lexer
  call lexer_init_eval_tree (lexer, particles)
  call lexer_assign_stream (lexer, stream)
  if (particles) then
    call parse_tree_init &
      (parse_tree, syntax_pexpr, lexer, var_str ("sepr"))
  else
    call parse_tree_init &
      (parse_tree, syntax_expr, lexer, var_str ("sepr"))
  end if
  call lexer_final (lexer)
end subroutine parse_tree_init_sexpr

```

28.3.9 The evaluation tree

The evaluation tree contains the initial variable list and the root node.

```

<Eval trees: public>+≡
  public :: eval_tree_t

<Eval trees: types>+≡
  type, extends (expr_t) :: eval_tree_t
  private
    type(parse_node_t), pointer :: pn => null ()
    type(var_list_t) :: var_list
    type(eval_node_t), pointer :: root => null ()
  contains
    <Eval trees: eval tree: TBP>
  end type eval_tree_t

```

Init from stream, using a temporary parse tree.

```

<Eval trees: eval tree: TBP>≡
  procedure :: init_stream => eval_tree_init_stream

<Eval trees: procedures>+≡
  subroutine eval_tree_init_stream &
    (eval_tree, stream, var_list, subvt, result_type)

```

```

class(eval_tree_t), intent(out), target :: eval_tree
type(stream_t), intent(inout), target :: stream
type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), target, optional :: subevt
integer, intent(in), optional :: result_type
type(parse_tree_t) :: parse_tree
type(parse_node_t), pointer :: nd_root
integer :: type
type = V_REAL; if (present (result_type)) type = result_type
select case (type)
case (V_INT, V_REAL, V_CMPLX)
    call parse_tree_init_expr (parse_tree, stream, present (subevt))
case (V_LOG)
    call parse_tree_init_lexpr (parse_tree, stream, present (subevt))
case (V_SEV)
    call parse_tree_init_pexpr (parse_tree, stream)
case (V_PDG)
    call parse_tree_init_cexpr (parse_tree, stream)
case (V_STR)
    call parse_tree_init_sexpr (parse_tree, stream, present (subevt))
end select
nd_root => parse_tree%get_root_ptr ()
if (associated (nd_root)) then
    select case (type)
    case (V_INT, V_REAL, V_CMPLX)
        call eval_tree_init_expr (eval_tree, nd_root, var_list, subevt)
    case (V_LOG)
        call eval_tree_init_lexpr (eval_tree, nd_root, var_list, subevt)
    case (V_SEV)
        call eval_tree_init_pexpr (eval_tree, nd_root, var_list, subevt)
    case (V_PDG)
        call eval_tree_init_cexpr (eval_tree, nd_root, var_list, subevt)
    case (V_STR)
        call eval_tree_init_sexpr (eval_tree, nd_root, var_list, subevt)
    end select
end if
call parse_tree_final (parse_tree)
end subroutine eval_tree_init_stream

```

API (to be superseded by the methods below): Init from a given parse-tree node. If we evaluate an expression that contains particle-list references, the original subevent has to be supplied. The initial variable list is optional.

(Eval trees: eval tree: TBP)+≡

```

procedure :: init_expr  => eval_tree_init_expr
procedure :: init_lexpr => eval_tree_init_lexpr
procedure :: init_pexpr => eval_tree_init_pexpr
procedure :: init_cexpr => eval_tree_init_cexpr
procedure :: init_sexpr => eval_tree_init_sexpr

```

(Eval trees: procedures)+≡

```

subroutine eval_tree_init_expr &
    (expr, parse_node, var_list, subevt)
class(eval_tree_t), intent(out), target :: expr
type(parse_node_t), intent(in), target :: parse_node

```

```

type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), optional, target :: subevt
call eval_tree_link_var_list (expr, var_list)
if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
call eval_node_compile_expr &
    (expr%root, parse_node, expr%var_list)
end subroutine eval_tree_init_expr

subroutine eval_tree_init_lexpr &
    (expr, parse_node, var_list, subevt)
class(eval_tree_t), intent(out), target :: expr
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), optional, target :: subevt
call eval_tree_link_var_list (expr, var_list)
if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
call eval_node_compile_lexpr &
    (expr%root, parse_node, expr%var_list)
end subroutine eval_tree_init_lexpr

subroutine eval_tree_init_pexpr &
    (expr, parse_node, var_list, subevt)
class(eval_tree_t), intent(out), target :: expr
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), optional, target :: subevt
call eval_tree_link_var_list (expr, var_list)
if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
call eval_node_compile_pexpr &
    (expr%root, parse_node, expr%var_list)
end subroutine eval_tree_init_pexpr

subroutine eval_tree_init_cexpr &
    (expr, parse_node, var_list, subevt)
class(eval_tree_t), intent(out), target :: expr
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), optional, target :: subevt
call eval_tree_link_var_list (expr, var_list)
if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
call eval_node_compile_cexpr &
    (expr%root, parse_node, expr%var_list)
end subroutine eval_tree_init_cexpr

subroutine eval_tree_init_sexpr &
    (expr, parse_node, var_list, subevt)
class(eval_tree_t), intent(out), target :: expr
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), optional, target :: subevt
call eval_tree_link_var_list (expr, var_list)
if (present (subevt)) call eval_tree_set_subevt (expr, subevt)
call eval_node_compile_sexpr &
    (expr%root, parse_node, expr%var_list)

```

```
end subroutine eval_tree_init_sexpr
```

Alternative: set up the expression using the parse node that has already been stored. We assume that the `subevt` or any other variable that may be referred to has already been added to the local variable list.

<Eval trees: eval tree: TBP>+≡

```
procedure :: setup_expr  => eval_tree_setup_expr
procedure :: setup_lexpr => eval_tree_setup_lexpr
procedure :: setup_pexpr => eval_tree_setup_pexpr
procedure :: setup_cexpr => eval_tree_setup_cexpr
procedure :: setup_sexpr => eval_tree_setup_sexpr
```

<Eval trees: procedures>+≡

```
subroutine eval_tree_setup_expr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
  call eval_tree_link_var_list (expr, vars)
  call eval_node_compile_expr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_expr

subroutine eval_tree_setup_lexpr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
  call eval_tree_link_var_list (expr, vars)
  call eval_node_compile_lexpr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_lexpr

subroutine eval_tree_setup_pexpr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
  call eval_tree_link_var_list (expr, vars)
  call eval_node_compile_pexpr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_pexpr

subroutine eval_tree_setup_cexpr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
  call eval_tree_link_var_list (expr, vars)
  call eval_node_compile_cexpr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_cexpr

subroutine eval_tree_setup_sexpr (expr, vars)
  class(eval_tree_t), intent(inout), target :: expr
  class(vars_t), intent(in), target :: vars
  call eval_tree_link_var_list (expr, vars)
  call eval_node_compile_sexpr (expr%root, expr%pn, expr%var_list)
end subroutine eval_tree_setup_sexpr
```

This extra API function handles numerical constant expressions only. The only nontrivial part is the optional unit.

<Eval trees: eval tree: TBP>+≡

```
procedure :: init_numeric_value => eval_tree_init_numeric_value
```

```

<Eval trees: procedures>+≡
  subroutine eval_tree_init_numeric_value (eval_tree, parse_node)
    class(eval_tree_t), intent(out), target :: eval_tree
    type(parse_node_t), intent(in), target :: parse_node
    call eval_node_compile_numeric_value (eval_tree%root, parse_node)
  end subroutine eval_tree_init_numeric_value

```

Initialize the variable list, linking it to a context variable list.

```

<Eval trees: procedures>+≡
  subroutine eval_tree_link_var_list (eval_tree, vars)
    type(eval_tree_t), intent(inout), target :: eval_tree
    class(vars_t), intent(in), target :: vars
    call eval_tree%var_list%link (vars)
  end subroutine eval_tree_link_var_list

```

Include a subevent object in the initialization. We add a pointer to this as variable @evt in the local variable list.

```

<Eval trees: procedures>+≡
  subroutine eval_tree_set_subevt (eval_tree, subevt)
    type(eval_tree_t), intent(inout), target :: eval_tree
    type(subevt_t), intent(in), target :: subevt
    logical, save, target :: known = .true.
    call var_list_append_subevt_ptr &
      (eval_tree%var_list, var_str ("@evt"), subevt, known, &
        intrinsic=.true.)
  end subroutine eval_tree_set_subevt

```

Finalizer.

```

<Eval trees: eval tree: TBP>+≡
  procedure :: final => eval_tree_final

```

```

<Eval trees: procedures>+≡
  subroutine eval_tree_final (expr)
    class(eval_tree_t), intent(inout) :: expr
    call expr%var_list%final ()
    if (associated (expr%root)) then
      call eval_node_final_rec (expr%root)
      deallocate (expr%root)
    end if
  end subroutine eval_tree_final

```

```

<Eval trees: eval tree: TBP>+≡
  procedure :: evaluate => eval_tree_evaluate

```

```

<Eval trees: procedures>+≡
  subroutine eval_tree_evaluate (expr)
    class(eval_tree_t), intent(inout) :: expr
    if (associated (expr%root)) then
      call eval_node_evaluate (expr%root)
    end if
  end subroutine eval_tree_evaluate

```

Check if the eval tree is allocated.

```

<Eval trees: procedures>+≡
function eval_tree_is_defined (eval_tree) result (flag)
  logical :: flag
  type(eval_tree_t), intent(in) :: eval_tree
  flag = associated (eval_tree%root)
end function eval_tree_is_defined

```

Check if the eval tree result is constant.

```

<Eval trees: procedures>+≡
function eval_tree_is_constant (eval_tree) result (flag)
  logical :: flag
  type(eval_tree_t), intent(in) :: eval_tree
  if (associated (eval_tree%root)) then
    flag = eval_tree%root%type == EN_CONSTANT
  else
    flag = .false.
  end if
end function eval_tree_is_constant

```

Insert a conversion node at the root, if necessary (only for real/int conversion)

```

<Eval trees: procedures>+≡
subroutine eval_tree_convert_result (eval_tree, result_type)
  type(eval_tree_t), intent(inout) :: eval_tree
  integer, intent(in) :: result_type
  if (associated (eval_tree%root)) then
    call insert_conversion_node (eval_tree%root, result_type)
  end if
end subroutine eval_tree_convert_result

```

Return the value of the top node, after evaluation. If the tree is empty, return the type of V_NONE. When extracting the value, no check for existence is done. For numeric values, the functions are safe against real/integer mismatch.

```

<Eval trees: eval tree: TBP>+≡
procedure :: is_known => eval_tree_result_is_known
procedure :: get_log => eval_tree_get_log
procedure :: get_int => eval_tree_get_int
procedure :: get_real => eval_tree_get_real
procedure :: get_cmplx => eval_tree_get_cmplx
procedure :: get_pdg_array => eval_tree_get_pdg_array
procedure :: get_subevt => eval_tree_get_subevt
procedure :: get_string => eval_tree_get_string

<Eval trees: procedures>+≡
function eval_tree_get_result_type (expr) result (type)
  integer :: type
  class(eval_tree_t), intent(in) :: expr
  if (associated (expr%root)) then
    type = expr%root%result_type
  else
    type = V_NONE
  end if
end function

```



```

end function eval_tree_get_result_type

function eval_tree_result_is_known (expr) result (flag)
    logical :: flag
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        select case (expr%root%result_type)
            case (V_LOG, V_INT, V_REAL)
                flag = expr%root%value_is_known
            case default
                flag = .true.
        end select
    else
        flag = .false.
    end if
end function eval_tree_result_is_known

function eval_tree_result_is_known_ptr (expr) result (ptr)
    logical, pointer :: ptr
    class(eval_tree_t), intent(in) :: expr
    logical, target, save :: known = .true.
    if (associated (expr%root)) then
        select case (expr%root%result_type)
            case (V_LOG, V_INT, V_REAL)
                ptr => expr%root%value_is_known
            case default
                ptr => known
        end select
    else
        ptr => null ()
    end if
end function eval_tree_result_is_known_ptr

function eval_tree_get_log (expr) result (lval)
    logical :: lval
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) lval = expr%root%lval
end function eval_tree_get_log

function eval_tree_get_int (expr) result (ival)
    integer :: ival
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        select case (expr%root%result_type)
            case (V_INT); ival = expr%root%ival
            case (V_REAL); ival = expr%root%rval
            case (V_CMPLX); ival = expr%root%cval
        end select
    end if
end function eval_tree_get_int

function eval_tree_get_real (expr) result (rval)
    real(default) :: rval
    class(eval_tree_t), intent(in) :: expr

```

```

    if (associated (expr%root)) then
        select case (expr%root%result_type)
            case (V_REAL); rval = expr%root%rval
            case (V_INT);  rval = expr%root%ival
            case (V_CMPLX); rval = expr%root%cval
        end select
    end if
end function eval_tree_get_real

function eval_tree_get_cmplx (expr) result (cval)
    complex(default) :: cval
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        select case (expr%root%result_type)
            case (V_CMPLX); cval = expr%root%cval
            case (V_REAL);  cval = expr%root%rval
            case (V_INT);   cval = expr%root%ival
        end select
    end if
end function eval_tree_get_cmplx

function eval_tree_get_pdg_array (expr) result (aval)
    type(pdg_array_t) :: aval
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        aval = expr%root%aval
    end if
end function eval_tree_get_pdg_array

function eval_tree_get_subevt (expr) result (pval)
    type(subevt_t) :: pval
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        pval = expr%root%pval
    end if
end function eval_tree_get_subevt

function eval_tree_get_string (expr) result (sval)
    type(string_t) :: sval
    class(eval_tree_t), intent(in) :: expr
    if (associated (expr%root)) then
        sval = expr%root%sval
    end if
end function eval_tree_get_string

```

Return a pointer to the value of the top node.

(Eval trees: procedures)+≡

```

function eval_tree_get_log_ptr (eval_tree) result (lval)
    logical, pointer :: lval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        lval => eval_tree%root%lval
    else

```

```

        lval => null ()
    end if
end function eval_tree_get_log_ptr

function eval_tree_get_int_ptr (eval_tree) result (ival)
    integer, pointer :: ival
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        ival => eval_tree%root%ival
    else
        ival => null ()
    end if
end function eval_tree_get_int_ptr

function eval_tree_get_real_ptr (eval_tree) result (rval)
    real(default), pointer :: rval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        rval => eval_tree%root%rval
    else
        rval => null ()
    end if
end function eval_tree_get_real_ptr

function eval_tree_get_cmplx_ptr (eval_tree) result (cval)
    complex(default), pointer :: cval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        cval => eval_tree%root%cval
    else
        cval => null ()
    end if
end function eval_tree_get_cmplx_ptr

function eval_tree_get_subevt_ptr (eval_tree) result (pval)
    type(subevt_t), pointer :: pval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        pval => eval_tree%root%pval
    else
        pval => null ()
    end if
end function eval_tree_get_subevt_ptr

function eval_tree_get_pdg_array_ptr (eval_tree) result (aval)
    type(pdg_array_t), pointer :: aval
    type(eval_tree_t), intent(in) :: eval_tree
    if (associated (eval_tree%root)) then
        aval => eval_tree%root%aval
    else
        aval => null ()
    end if
end function eval_tree_get_pdg_array_ptr

```

```

function eval_tree_get_string_ptr (eval_tree) result (sval)
  type(string_t), pointer :: sval
  type(eval_tree_t), intent(in) :: eval_tree
  if (associated (eval_tree%root)) then
    sval => eval_tree%root%sval
  else
    sval => null ()
  end if
end function eval_tree_get_string_ptr

```

<Eval trees: eval tree: TBP>+≡

```

procedure :: write => eval_tree_write

```

<Eval trees: procedures>+≡

```

subroutine eval_tree_write (expr, unit, write_vars)
  class(eval_tree_t), intent(in) :: expr
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: write_vars
  integer :: u
  logical :: vl
  u = given_output_unit (unit); if (u < 0) return
  vl = .false.; if (present (write_vars)) vl = write_vars
  write (u, "(1x,A)") "Evaluation tree:"
  if (associated (expr%root)) then
    call eval_node_write_rec (expr%root, unit)
  else
    write (u, "(3x,A)") "[empty]"
  end if
  if (vl) call var_list_write (expr%var_list, unit)
end subroutine eval_tree_write

```

Use the written representation for generating an MD5 sum:

<Eval trees: procedures>+≡

```

function eval_tree_get_md5sum (eval_tree) result (md5sum_et)
  character(32) :: md5sum_et
  type(eval_tree_t), intent(in) :: eval_tree
  integer :: u
  u = free_unit ()
  open (unit = u, status = "scratch", action = "readwrite")
  call eval_tree_write (eval_tree, unit=u)
  rewind (u)
  md5sum_et = md5sum (u)
  close (u)
end function eval_tree_get_md5sum

```

28.3.10 Direct evaluation

These procedures create an eval tree and evaluate it on-the-fly, returning only the final value. The evaluation must yield a well-defined value, unless the `is_known` flag is present, which will be set accordingly.

<Eval trees: public>+≡

```

public :: eval_log

```

```

public :: eval_int
public :: eval_real
public :: eval_cmplx
public :: eval_subevt
public :: eval_pdg_array
public :: eval_string

<Eval trees: procedures>+≡
function eval_log &
    (parse_node, var_list, subevt, is_known) result (lval)
    logical :: lval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
    type(eval_tree_t), target :: eval_tree
    call eval_tree_init_lexpr &
        (eval_tree, parse_node, var_list, subevt)
    call eval_tree_evaluate (eval_tree)
    if (eval_tree_result_is_known (eval_tree)) then
        if (present (is_known)) is_known = .true.
        lval = eval_tree_get_log (eval_tree)
    else if (present (is_known)) then
        is_known = .false.
    else
        call eval_tree_unknown (eval_tree, parse_node)
        lval = .false.
    end if
    call eval_tree_final (eval_tree)
end function eval_log

function eval_int &
    (parse_node, var_list, subevt, is_known) result (ival)
    integer :: ival
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
    type(eval_tree_t), target :: eval_tree
    call eval_tree_init_expr &
        (eval_tree, parse_node, var_list, subevt)
    call eval_tree_evaluate (eval_tree)
    if (eval_tree_result_is_known (eval_tree)) then
        if (present (is_known)) is_known = .true.
        ival = eval_tree_get_int (eval_tree)
    else if (present (is_known)) then
        is_known = .false.
    else
        call eval_tree_unknown (eval_tree, parse_node)
        ival = 0
    end if
    call eval_tree_final (eval_tree)
end function eval_int

function eval_real &

```

```

        (parse_node, var_list, subevt, is_known) result (rval)
real(default) :: rval
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), optional, target :: subevt
logical, intent(out), optional :: is_known
type(eval_tree_t), target :: eval_tree
call eval_tree_init_expr &
    (eval_tree, parse_node, var_list, subevt)
call eval_tree_evaluate (eval_tree)
if (eval_tree_result_is_known (eval_tree)) then
    if (present (is_known)) is_known = .true.
    rval = eval_tree_get_real (eval_tree)
else if (present (is_known)) then
    is_known = .false.
else
    call eval_tree_unknown (eval_tree, parse_node)
    rval = 0
end if
call eval_tree_final (eval_tree)
end function eval_real

function eval_cmplx &
    (parse_node, var_list, subevt, is_known) result (cval)
complex(default) :: cval
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), optional, target :: subevt
logical, intent(out), optional :: is_known
type(eval_tree_t), target :: eval_tree
call eval_tree_init_expr &
    (eval_tree, parse_node, var_list, subevt)
call eval_tree_evaluate (eval_tree)
if (eval_tree_result_is_known (eval_tree)) then
    if (present (is_known)) is_known = .true.
    cval = eval_tree_get_cmplx (eval_tree)
else if (present (is_known)) then
    is_known = .false.
else
    call eval_tree_unknown (eval_tree, parse_node)
    cval = 0
end if
call eval_tree_final (eval_tree)
end function eval_cmplx

function eval_subevt &
    (parse_node, var_list, subevt, is_known) result (pval)
type(subevt_t) :: pval
type(parse_node_t), intent(in), target :: parse_node
type(var_list_t), intent(in), target :: var_list
type(subevt_t), intent(in), optional, target :: subevt
logical, intent(out), optional :: is_known
type(eval_tree_t), target :: eval_tree
call eval_tree_init_pexpr &

```

```

        (eval_tree, parse_node, var_list, subevt)
    call eval_tree_evaluate (eval_tree)
    if (eval_tree_result_is_known (eval_tree)) then
        if (present (is_known)) is_known = .true.
        pval = eval_tree_get_subevt (eval_tree)
    else if (present (is_known)) then
        is_known = .false.
    else
        call eval_tree_unknown (eval_tree, parse_node)
    end if
    call eval_tree_final (eval_tree)
end function eval_subevt

function eval_pdg_array &
    (parse_node, var_list, subevt, is_known) result (aval)
    type(pdg_array_t) :: aval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
    type(eval_tree_t), target :: eval_tree
    call eval_tree_init_cexpr &
        (eval_tree, parse_node, var_list, subevt)
    call eval_tree_evaluate (eval_tree)
    if (eval_tree_result_is_known (eval_tree)) then
        if (present (is_known)) is_known = .true.
        aval = eval_tree_get_pdg_array (eval_tree)
    else if (present (is_known)) then
        is_known = .false.
    else
        call eval_tree_unknown (eval_tree, parse_node)
    end if
    call eval_tree_final (eval_tree)
end function eval_pdg_array

function eval_string &
    (parse_node, var_list, subevt, is_known) result (sval)
    type(string_t) :: sval
    type(parse_node_t), intent(in), target :: parse_node
    type(var_list_t), intent(in), target :: var_list
    type(subevt_t), intent(in), optional, target :: subevt
    logical, intent(out), optional :: is_known
    type(eval_tree_t), target :: eval_tree
    call eval_tree_init_sexpr &
        (eval_tree, parse_node, var_list, subevt)
    call eval_tree_evaluate (eval_tree)
    if (eval_tree_result_is_known (eval_tree)) then
        if (present (is_known)) is_known = .true.
        sval = eval_tree_get_string (eval_tree)
    else if (present (is_known)) then
        is_known = .false.
    else
        call eval_tree_unknown (eval_tree, parse_node)
        sval = ""
    end if
end function eval_string

```

```

    end if
    call eval_tree_final (eval_tree)
end function eval_string

```

Here is a variant that returns numeric values of all possible kinds, the appropriate kind to be selected later:

```

<Eval trees: public>+≡
    public :: eval_numeric

<Eval trees: procedures>+≡
    subroutine eval_numeric &
        (parse_node, var_list, subevt, ival, rval, cval, &
         is_known, result_type)
        type(parse_node_t), intent(in), target :: parse_node
        type(var_list_t), intent(in), target :: var_list
        type(subevt_t), intent(in), optional, target :: subevt
        integer, intent(out), optional :: ival
        real(default), intent(out), optional :: rval
        complex(default), intent(out), optional :: cval
        logical, intent(out), optional :: is_known
        integer, intent(out), optional :: result_type
        type(eval_tree_t), target :: eval_tree
        call eval_tree_init_expr &
            (eval_tree, parse_node, var_list, subevt)
        call eval_tree_evaluate (eval_tree)
        if (eval_tree_result_is_known (eval_tree)) then
            if (present (ival)) ival = eval_tree_get_int (eval_tree)
            if (present (rval)) rval = eval_tree_get_real (eval_tree)
            if (present (cval)) cval = eval_tree_get_cmplx (eval_tree)
            if (present (is_known)) is_known = .true.
        else
            call eval_tree_unknown (eval_tree, parse_node)
            if (present (ival)) ival = 0
            if (present (rval)) rval = 0
            if (present (cval)) cval = 0
            if (present (is_known)) is_known = .false.
        end if
        if (present (result_type)) &
            result_type = eval_tree_get_result_type (eval_tree)
        call eval_tree_final (eval_tree)
    end subroutine eval_numeric

```

Error message with debugging info:

```

<Eval trees: procedures>+≡
    subroutine eval_tree_unknown (eval_tree, parse_node)
        type(eval_tree_t), intent(in) :: eval_tree
        type(parse_node_t), intent(in) :: parse_node
        call parse_node_write_rec (parse_node)
        call eval_tree_write (eval_tree)
        call msg_error ("Evaluation yields an undefined result, inserting default")
    end subroutine eval_tree_unknown

```


28.3.11 Factory Type

Since `eval_tree_t` is an implementation of `expr_t`, we also need a matching factory type and build method.

```
<Eval trees: public>+≡
    public :: eval_tree_factory_t

<Eval trees: types>+≡
    type, extends (expr_factory_t) :: eval_tree_factory_t
    private
        type(parse_node_t), pointer :: pn => null ()
    contains
    <Eval trees: eval tree factory: TBP>
    end type eval_tree_factory_t
```

Output: delegate to the output of the embedded parse node.

```
<Eval trees: eval tree factory: TBP>≡
    procedure :: write => eval_tree_factory_write

<Eval trees: procedures>+≡
    subroutine eval_tree_factory_write (expr_factory, unit)
        class(eval_tree_factory_t), intent(in) :: expr_factory
        integer, intent(in), optional :: unit
        if (associated (expr_factory%pn)) then
            call parse_node_write_rec (expr_factory%pn, unit)
        end if
    end subroutine eval_tree_factory_write
```

Initializer: take a parse node and hide it thus from the environment.

```
<Eval trees: eval tree factory: TBP>+≡
    procedure :: init => eval_tree_factory_init

<Eval trees: procedures>+≡
    subroutine eval_tree_factory_init (expr_factory, pn)
        class(eval_tree_factory_t), intent(out) :: expr_factory
        type(parse_node_t), intent(in), pointer :: pn
        expr_factory%pn => pn
    end subroutine eval_tree_factory_init
```

Factory method: allocate expression with correct eval tree type. If the stored parse node is not associate, don't allocate.

```
<Eval trees: eval tree factory: TBP>+≡
    procedure :: build => eval_tree_factory_build

<Eval trees: procedures>+≡
    subroutine eval_tree_factory_build (expr_factory, expr)
        class(eval_tree_factory_t), intent(in) :: expr_factory
        class(expr_t), intent(out), allocatable :: expr
        if (associated (expr_factory%pn)) then
            allocate (eval_tree_t :: expr)
            select type (expr)
            type is (eval_tree_t)
                expr%pn => expr_factory%pn
            end select
```

```

        end if
    end subroutine eval_tree_factory_build

```

28.3.12 Unit tests

Test module, followed by the corresponding implementation module.

```

<eval_trees_ut.f90>≡
  <File header>

  module eval_trees_ut
    use unit_tests
    use eval_trees_uti

    <Standard module head>

    <Eval trees: public test>

    contains

    <Eval trees: test driver>

  end module eval_trees_ut

<eval_trees_uti.f90>≡
  <File header>

  module eval_trees_uti

    <Use kinds>
    <Use strings>

    use ifiles
    use lexers
    use lorentz
    use syntax_rules, only: syntax_write
    use pdg_arrays
    use subevents
    use variables
    use observables

    use eval_trees

    <Standard module head>

    <Eval trees: test declarations>

    contains

    <Eval trees: tests>

  end module eval_trees_uti

```

API: driver for the unit tests below.

```
<Eval trees: public test>≡
  public :: expressions_test

<Eval trees: test driver>≡
  subroutine expressions_test (u, results)
    integer, intent(in) :: u
    type (test_results_t), intent(inout) :: results
  <Eval trees: execute tests>
  end subroutine expressions_test
```

Testing the routines of the expressions module. First a simple unary observable and the node evaluation.

```
<Eval trees: execute tests>≡
  call test (expressions_1, "expressions_1", &
    "check simple observable", &
    u, results)

<Eval trees: test declarations>≡
  public :: expressions_1

<Eval trees: tests>≡
  subroutine expressions_1 (u)
    integer, intent(in) :: u
    type(var_list_t), pointer :: var_list => null ()
    type(eval_node_t), pointer :: node => null ()
    type(prt_t), pointer :: prt => null ()
    type(string_t) :: var_name

    write (u, "(A)")  "* Test output: Expressions"
    write (u, "(A)")  "* Purpose: test simple observable and node evaluation"
    write (u, "(A)")

    write (u, "(A)")  "* Setting a unary observable:"
    write (u, "(A)")

    allocate (var_list)
    allocate (prt)
    call var_list_set_observables_unary (var_list, prt)
    call var_list%write (u)

    write (u, "(A)")  "* Evaluating the observable node:"
    write (u, "(A)")

    var_name = "PDG"

    allocate (node)
    call node%test_obs (var_list, var_name)
    call node%write (u)

    write (u, "(A)")  "* Cleanup"
    write (u, "(A)")

    call node%final_rec ()
    deallocate (node)
```

```

!!! Workaround for NAGFOR 6.2
! call var_list%final ()
deallocate (var_list)
deallocate (prt)

write (u, "(A)")
write (u, "(A)")  "* Test output end: expressions_1"

end subroutine expressions_1

```

Parse a complicated expression, transfer it to a parse tree and evaluate.

```

<Eval trees: execute tests>+≡
  call test (expressions_2, "expressions_2", &
    "check expression transfer to parse tree", &
    u, results)

<Eval trees: test declarations>+≡
  public :: expressions_2

<Eval trees: tests>+≡
  subroutine expressions_2 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(eval_tree_t) :: eval_tree
    type(string_t) :: expr_text
    type(var_list_t), pointer :: var_list => null ()

    write (u, "(A)")  "* Test output: Expressions"
    write (u, "(A)")  "* Purpose: test parse routines"
    write (u, "(A)")

    call syntax_expr_init ()
    call syntax_write (syntax_expr, u)
    allocate (var_list)
    call var_list_append_real (var_list, var_str ("tolerance"), 0._default)
    call var_list_append_real (var_list, var_str ("x"), -5._default)
    call var_list_append_int (var_list, var_str ("foo"), -27)
    call var_list_append_real (var_list, var_str ("mb"), 4._default)
    expr_text = &
      "let real twopi = 2 * pi in" // &
      " twopi * sqrt (25.d0 - mb^2)" // &
      " / (let int mb_or_0 = max (mb, 0) in" // &
      " 1 + (if -1 TeV <= x < mb_or_0 then abs(x) else x endif))"
    call ifile_append (ifile, expr_text)
    call stream_init (stream, ifile)
    call var_list%write (u)
    call eval_tree%init_stream (stream, var_list=var_list)
    call eval_tree%evaluate ()
    call eval_tree%write (u)

    write (u, "(A)")  "* Input string:"
    write (u, "(A,A)")  " ", char (expr_text)
    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"
  end subroutine expressions_2

```

```

call stream_final (stream)
call ifile_final (ifile)
call eval_tree%final ()
call var_list%final ()
deallocate (var_list)
call syntax_expr_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: expressions_2"

end subroutine expressions_2

```

Test a subevent expression.

```

<Eval trees: execute tests>+≡
call test (expressions_3, "expressions_3", &
  "check subevent expressions", &
  u, results)

<Eval trees: test declarations>+≡
public :: expressions_3

<Eval trees: tests>+≡
subroutine expressions_3 (u)
  integer, intent(in) :: u
  type(subvt_t) :: subvt

  write (u, "(A)")  "* Test output: Expressions"
  write (u, "(A)")  "* Purpose: test subevent expressions"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize subevent:"
  write (u, "(A)")

  call subvt_init (subvt)
  call subvt_reset (subvt, 1)
  call subvt_set_incoming (subvt, 1, &
    22, vector4_moving (1.e3_default, 1.e3_default, 1), &
    0._default, [2])
  call subvt_write (subvt, u)
  call subvt_reset (subvt, 4)
  call subvt_reset (subvt, 3)
  call subvt_set_incoming (subvt, 1, &
    21, vector4_moving (1.e3_default, 1.e3_default, 3), &
    0._default, [1])
  call subvt_polarize (subvt, 1, -1)
  call subvt_set_outgoing (subvt, 2, &
    1, vector4_moving (0._default, 1.e3_default, 3), &
    -1.e6_default, [7])
  call subvt_set_composite (subvt, 3, &
    vector4_moving (-1.e3_default, 0._default, 3), &
    [2, 7])
  call subvt_write (subvt, u)

  write (u, "(A)")

```

```

write (u, "(A)")  "* Test output end: expressions_3"

end subroutine expressions_3

```

Test expressions from a PDG array.

```

<Eval trees: execute tests>+=
  call test (expressions_4, "expressions_4", &
    "check pdg array expressions", &
    u, results)

<Eval trees: test declarations>+=
  public :: expressions_4

<Eval trees: tests>+=
  subroutine expressions_4 (u)
    integer, intent(in) :: u
    type(subvt_t), target :: subvt
    type(string_t) :: expr_text
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(eval_tree_t) :: eval_tree
    type(var_list_t), pointer :: var_list => null ()
    type(pdg_array_t) :: aval

    write (u, "(A)")  "* Test output: Expressions"
    write (u, "(A)")  "* Purpose: test pdg array expressions"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization:"
    write (u, "(A)")

    call syntax_pexpr_init ()
    call syntax_write (syntax_pexpr, u)
    allocate (var_list)
    call var_list_append_real (var_list, var_str ("tolerance"), 0._default)
    aval = 0
    call var_list_append_pdg_array (var_list, var_str ("particle"), aval)
    aval = [11,-11]
    call var_list_append_pdg_array (var_list, var_str ("lepton"), aval)
    aval = 22
    call var_list_append_pdg_array (var_list, var_str ("photon"), aval)
    aval = 1
    call var_list_append_pdg_array (var_list, var_str ("u"), aval)
    call subvt_init (subvt)
    call subvt_reset (subvt, 6)
    call subvt_set_incoming (subvt, 1, &
      1, vector4_moving (1._default, 1._default, 1), 0._default)
    call subvt_set_incoming (subvt, 2, &
      -1, vector4_moving (2._default, 2._default, 1), 0._default)
    call subvt_set_outgoing (subvt, 3, &
      22, vector4_moving (3._default, 3._default, 1), 0._default)
    call subvt_set_outgoing (subvt, 4, &
      22, vector4_moving (4._default, 4._default, 1), 0._default)
    call subvt_set_outgoing (subvt, 5, &
      11, vector4_moving (5._default, 5._default, 1), 0._default)

```

```

call subevt_set_outgoing (subevt, 6, &
-11, vector4_moving (6._default, 6._default, 1), 0._default)
write (u, "(A)")
write (u, "(A)")  "* Expression:"
expr_text = &
"let alias quark = pdg(1):pdg(2):pdg(3) in" // &
"  any E > 3 GeV " // &
"    [sort by - Pt " // &
"      [select if Index < 6 " // &
"        [photon:pdg(-11):pdg(3):quark " // &
"          & incoming particle]]]" // &
"  and" // &
"    eval Theta [extract index -1 [photon]] > 45 degree" // &
"  and" // &
"    count [incoming photon] * 3 > 0"
write (u, "(A,A)")  " ", char (expr_text)
write (u, "(A)")

write (u, "(A)")
write (u, "(A)")  "* Extract the evaluation tree:"
write (u, "(A)")

call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call eval_tree%init_stream (stream, var_list, subevt, V_LOG)
call eval_tree%write (u)
call eval_tree%evaluate ()

write (u, "(A)")
write (u, "(A)")  "* Evaluate the tree:"
write (u, "(A)")

call eval_tree%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call stream_final (stream)
call ifile_final (ifile)
call eval_tree%final ()
call var_list%final ()
deallocate (var_list)
call syntax_pexpr_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: expressions_4"

end subroutine expressions_4

```

28.4 Physics Models

A model object represents a physics model. It contains a table of particle data, a list of parameters, and a vertex table. The list of parameters is a variable list which includes the real parameters (which are pointers to the particle data table) and PDG array variables for the particles themselves. The vertex list is used for phase-space generation, not for calculating the matrix element.

The actual numeric model data are in the base type `model_data_t`, as part of the `qft` section. We implement the `model_t` as an extension of this, for convenient direct access to the base-type methods via inheritance. (Alternatively, we could delegate these calls explicitly.) The extension contains administrative additions, such as the methods for recalculating derived data and keeping the parameter set consistent. It thus acts as a proxy of the actual model-data object towards the WHIZARD package. There are further proxy objects, such as the `parameter_t` array which provides the interface to the actual numeric parameters.

Model definitions are read from model files. Therefore, this module contains a parser for model files. The parameter definitions (derived parameters) are Sindarin expressions.

The models, as read from file, are stored in a model library which is a simple list of model definitions. For setting up a process object we should make a copy (an instance) of a model, which gets the current parameter values from the global variable list.

28.4.1 Module

```
<models.f90>≡  
<File header>  
  
module models  
  
    use, intrinsic :: iso_c_binding !NODEP!  
  
    <Use kinds>  
    use kinds, only: c_default_float  
    <Use strings>  
    use io_units  
    use diagnostics  
    use md5  
    use os_interface  
    use physics_defs, only: UNDEFINED  
    use model_data  
  
    use ifiles  
    use syntax_rules  
    use lexers  
    use parser  
    use pdg_arrays  
    use variables  
    use expr_base  
    use eval_trees
```



```

    use ttv_formfactors, only: init_parameters

    <Standard module head>

    <Models: public>

    <Models: parameters>

    <Models: types>

    <Models: interfaces>

    <Models: variables>

contains

    <Models: procedures>

end module models

```

28.4.2 Physics Parameters

A parameter has a name, a value. Derived parameters also have a definition in terms of other parameters, which is stored as an `eval_tree`. External parameters are set by an external program.

This parameter object should be considered as a proxy object. The parameter name and value are stored in a corresponding `modelpar_data_t` object which is located in a `model_data_t` object. The latter is a component of the `model_t` handler. Methods of `parameter_t` can be delegated to the `par_data_t` component.

The `block_name` and `block_index` values, if nonempty, indicate the possibility of reading this parameter from a SLHA-type input file. (Within the `parameter_t` object, this info is just used for I/O, the actual block register is located in the parent `model_t` object.)

The `pn` component is a pointer to the parameter definition inside the model parse tree. It allows us to recreate the `eval_tree` when making copies (instances) of the parameter object.

```

<Models: parameters>≡
    integer, parameter :: PAR_NONE = 0, PAR_UNUSED = -1
    integer, parameter :: PAR_INDEPENDENT = 1, PAR_DERIVED = 2
    integer, parameter :: PAR_EXTERNAL = 3

<Models: types>≡
    type :: parameter_t
    private
    integer :: type = PAR_NONE
    class(modelpar_data_t), pointer :: data => null ()
    type(string_t) :: block_name
    integer, dimension(:), allocatable :: block_index
    type(parse_node_t), pointer :: pn => null ()
    class(expr_t), allocatable :: expr
contains

```

```

    <Models: parameter: TBP>
end type parameter_t

```

Initialization depends on parameter type. Independent parameters are initialized by a constant value or a constant numerical expression (which may contain a unit). Derived parameters are initialized by an arbitrary numerical expression, which makes use of the current variable list. The expression is evaluated by the function `parameter_reset`.

This implementation supports only real parameters and real values.

```

<Models: parameter: TBP>≡
  procedure :: init_independent_value => parameter_init_independent_value
  procedure :: init_independent => parameter_init_independent
  procedure :: init_derived => parameter_init_derived
  procedure :: init_external => parameter_init_external
  procedure :: init_unused => parameter_init_unused

<Models: procedures>≡
  subroutine parameter_init_independent_value (par, par_data, name, value)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
    par%type = PAR_INDEPENDENT
    par%data => par_data
    call par%data%init (name, value)
  end subroutine parameter_init_independent_value

  subroutine parameter_init_independent (par, par_data, name, pn)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    type(parse_node_t), intent(in), target :: pn
    par%type = PAR_INDEPENDENT
    par%pn => pn
    allocate (eval_tree_t :: par%expr)
    select type (expr => par%expr)
    type is (eval_tree_t)
      call expr%init_numeric_value (pn)
    end select
    par%data => par_data
    call par%data%init (name, par%expr%get_real ())
  end subroutine parameter_init_independent

  subroutine parameter_init_derived (par, par_data, name, pn, var_list)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    type(parse_node_t), intent(in), target :: pn
    type(var_list_t), intent(in), target :: var_list
    par%type = PAR_DERIVED
    par%pn => pn
    allocate (eval_tree_t :: par%expr)
    select type (expr => par%expr)
    type is (eval_tree_t)

```

```

        call expr%init_expr (pn, var_list=var_list)
    end select
    par%data => par_data
!    call par%expr%evaluate ()
    call par%data%init (name, 0._default)
end subroutine parameter_init_derived

subroutine parameter_init_external (par, par_data, name)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    par%type = PAR_EXTERNAL
    par%data => par_data
    call par%data%init (name, 0._default)
end subroutine parameter_init_external

subroutine parameter_init_unused (par, par_data, name)
    class(parameter_t), intent(out) :: par
    class(modelpar_data_t), intent(in), target :: par_data
    type(string_t), intent(in) :: name
    par%type = PAR_UNUSED
    par%data => par_data
    call par%data%init (name, 0._default)
end subroutine parameter_init_unused

```

The finalizer is needed for the evaluation tree in the definition.

```

<Models: parameter: TBP>+≡
    procedure :: final => parameter_final

<Models: procedures>+≡
    subroutine parameter_final (par)
        class(parameter_t), intent(inout) :: par
        if (allocated (par%expr)) then
            call par%expr%final ()
        end if
    end subroutine parameter_final

```

All derived parameters should be recalculated if some independent parameters have changed:

```

<Models: parameter: TBP>+≡
    procedure :: reset_derived => parameter_reset_derived

<Models: procedures>+≡
    subroutine parameter_reset_derived (par)
        class(parameter_t), intent(inout) :: par
        select case (par%type)
        case (PAR_DERIVED)
            call par%expr%evaluate ()
            par%data = par%expr%get_real ()
        end select
    end subroutine parameter_reset_derived

```

Output. [We should have a formula format for the eval tree, suitable for input and output!]

```

<Models: parameter: TBP>+≡
  procedure :: write => parameter_write

<Models: procedures>+≡
  subroutine parameter_write (par, unit, write_defs)
    class(parameter_t), intent(in) :: par
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: write_defs
    logical :: defs
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    defs = .false.; if (present (write_defs)) defs = write_defs
    select case (par%type)
    case (PAR_INDEPENDENT)
      write (u, "(3x,A)", advance="no") "parameter"
      call par%data%write (u)
    case (PAR_DERIVED)
      write (u, "(3x,A)", advance="no") "derived"
      call par%data%write (u)
    case (PAR_EXTERNAL)
      write (u, "(3x,A)", advance="no") "external"
      call par%data%write (u)
    case (PAR_UNUSED)
      write (u, "(3x,A)", advance="no") "unused"
      write (u, "(1x,A)", advance="no") char (par%data%get_name ())
    end select
    select case (par%type)
    case (PAR_INDEPENDENT)
      if (allocated (par%block_index)) then
        write (u, "(1x,A,1x,A,*(1x,I0))" &
          "slha_entry", char (par%block_name), par%block_index)
      else
        write (u, "(A)")
      end if
    case (PAR_DERIVED)
      if (defs) then
        call par%expr%write (unit)
      else
        write (u, "(A)")
      end if
    case default
      write (u, "(A)")
    end select
  end subroutine parameter_write

```

Screen output variant. Restrict output to the given parameter type.

```

<Models: parameter: TBP>+≡
  procedure :: show => parameter_show

<Models: procedures>+≡
  subroutine parameter_show (par, l, u, partype)
    class(parameter_t), intent(in) :: par

```

```

integer, intent(in) :: l, u
integer, intent(in) :: partype
if (par%type == partype) then
    call par%data%show (l, u)
end if
end subroutine parameter_show

```

28.4.3 SLHA block register

For the optional SLHA interface, the model record contains a register of SLHA-type block names together with index values, which point to a particular parameter. These are private types:

```

⟨Models: types⟩ +=
    type :: slha_entry_t
        integer, dimension(:), allocatable :: block_index
        integer :: i_par = 0
    end type slha_entry_t

⟨Models: types⟩ +=
    type :: slha_block_t
        type(string_t) :: name
        integer :: n_entry = 0
        type(slha_entry_t), dimension(:), allocatable :: entry
    end type slha_block_t

```

28.4.4 Model Object

A model object holds all information about parameters, particles, and vertices. For models that require an external program for parameter calculation, there is the pointer to a function that does this calculation, given the set of independent and derived parameters.

As explained above, the type inherits from `model_data_t`, which is the actual storage for the model data.

When reading a model, we create a parse tree. Parameter definitions are available via parse nodes. Since we may need those later when making model instances, we keep the whole parse tree in the model definition (but not in the instances).

```

⟨Models: public⟩ =
    public :: model_t

⟨Models: types⟩ +=
    type, extends (model_data_t) :: model_t
        private
        character(32) :: md5sum = ""
        logical :: ufo_model = .false.
        type(string_t) :: ufo_path
        type(string_t), dimension(:), allocatable :: schemes
        type(string_t), allocatable :: selected_scheme
        type(parameter_t), dimension(:), allocatable :: par

```

```

integer :: n_slha_block = 0
type(slha_block_t), dimension(:), allocatable :: slha_block
integer :: max_par_name_length = 0
integer :: max_field_name_length = 0
type(var_list_t) :: var_list
type(string_t) :: dlname
procedure(model_init_external_parameters), nopass, pointer :: &
    init_external_parameters => null ()
type(dlaccess_t) :: dlaccess
type(parse_tree_t) :: parse_tree
contains
  <Models: model: TBP>
end type model_t

```

This is the interface for a procedure that initializes the calculation of external parameters, given the array of all parameters.

```

<Models: interfaces>≡
  abstract interface
    subroutine model_init_external_parameters (par) bind (C)
      import
      real(c_default_float), dimension(*), intent(inout) :: par
    end subroutine model_init_external_parameters
  end interface

```

Initialization: Specify the number of parameters, particles, vertices and allocate memory. If an associated DL library is specified, load this library.

The model may already carry scheme information, so we have to save and restore the scheme number when actually initializing the `model_data_t` base.

```

<Models: model: TBP>≡
  generic :: init => model_init
  procedure, private :: model_init

<Models: procedures>+≡
  subroutine model_init &
    (model, name, libname, os_data, n_par, n_prt, n_vtx, ufo)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in) :: name, libname
    type(os_data_t), intent(in) :: os_data
    integer, intent(in) :: n_par, n_prt, n_vtx
    logical, intent(in), optional :: ufo
    type(c_funptr) :: c_funptr
    type(string_t) :: libpath
    integer :: scheme_num
    scheme_num = model%get_scheme_num ()
    call model%basic_init (name, n_par, n_prt, n_vtx)
    if (present (ufo)) model%ufo_model = ufo
    call model%set_scheme_num (scheme_num)
    if (libname /= "") then
      if (.not. os_data%use_testfiles) then
        libpath = os_data%whizard_models_libpath_local
        model%dlname = os_get_dlname ( &
          libpath // "/" // libname, os_data, ignore=.true.)
      end if
    end if
  end subroutine

```

```

        if (model%dlname == "") then
            libpath = os_data%whizard_models_libpath
            model%dlname = os_get_dlname (libpath // "/" // libname, os_data)
        end if
    else
        model%dlname = ""
    end if
    if (model%dlname /= "") then
        if (.not. dlaccess_is_open (model%dlaccess)) then
            if (logging) &
                call msg_message ("Loading model auxiliary library '" &
                    // char (libpath) // "/" // char (model%dlname) // "'")
            call dlaccess_init (model%dlaccess, os_data%whizard_models_libpath, &
                model%dlname, os_data)
            if (dlaccess_has_error (model%dlaccess)) then
                call msg_message (char (dlaccess_get_error (model%dlaccess)))
                call msg_fatal ("Loading model auxiliary library '" &
                    // char (model%dlname) // "' failed")
                return
            end if
            c_fptr = dlaccess_get_c_funptr (model%dlaccess, &
                var_str ("init_external_parameters"))
            if (dlaccess_has_error (model%dlaccess)) then
                call msg_message (char (dlaccess_get_error (model%dlaccess)))
                call msg_fatal ("Loading function from auxiliary library '" &
                    // char (model%dlname) // "' failed")
                return
            end if
            call c_f_procpointer (c_fptr, model% init_external_parameters)
        end if
    end if
end subroutine model_init

```

For a model instance, we do not attempt to load a DL library. This is the core of the full initializer above.

```

<Models: model: TBP>+≡
    procedure, private :: basic_init => model_basic_init

<Models: procedures>+≡
    subroutine model_basic_init (model, name, n_par, n_prt, n_vtx)
        class(model_t), intent(inout) :: model
        type(string_t), intent(in) :: name
        integer, intent(in) :: n_par, n_prt, n_vtx
        allocate (model%par (n_par))
        call model%model_data_t%init (name, n_par, 0, n_prt, n_vtx)
    end subroutine model_basic_init

```

Finalization: The variable list contains allocated pointers, also the parse tree. We also close the DL access object, if any, that enables external parameter calculation.

```

<Models: model: TBP>+≡
    procedure :: final => model_final

```

```

<Models: procedures>+≡
subroutine model_final (model)
  class(model_t), intent(inout) :: model
  integer :: i
  if (allocated (model%par)) then
    do i = 1, size (model%par)
      call model%par(i)%final ()
    end do
  end if
  call model%var_list%final (follow_link=.false.)
  if (model%dlname /= "") call dlaccess_final (model%dlaccess)
  call parse_tree_final (model%parse_tree)
  call model%model_data_t%final ()
end subroutine model_final

```

Output. By default, the output is in the form of an input file. If `verbose` is true, for each derived parameter the definition (eval tree) is displayed, and the vertex hash table is shown.

```

<Models: model: TBP>+≡
  procedure :: write => model_write

<Models: procedures>+≡
subroutine model_write (model, unit, verbose, &
  show_md5sum, show_variables, show_parameters, &
  show_particles, show_vertices, show_scheme)
  class(model_t), intent(in) :: model
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  logical, intent(in), optional :: show_md5sum
  logical, intent(in), optional :: show_variables
  logical, intent(in), optional :: show_parameters
  logical, intent(in), optional :: show_particles
  logical, intent(in), optional :: show_vertices
  logical, intent(in), optional :: show_scheme
  logical :: verb, show_md5, show_par, show_var
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  verb = .false.; if (present (verbose)) verb = verbose
  show_md5 = .true.; if (present (show_md5sum)) &
    show_md5 = show_md5sum
  show_par = .true.; if (present (show_parameters)) &
    show_par = show_parameters
  show_var = verb; if (present (show_variables)) &
    show_var = show_variables
  write (u, "(A,A,A)") 'model ', char (model%get_name ()), ' '
  if (show_md5 .and. model%md5sum /= "") &
    write (u, "(1x,A,A,A)") "! md5sum = '", model%md5sum, "' "
  if (model%is_ufo_model ()) then
    write (u, "(1x,A)") "! model derived from UFO source"
  else if (model%has_schemes ()) then
    write (u, "(1x,A)", advance="no") "! schemes ="
    do i = 1, size (model%schemes)
      if (i > 1) write (u, "(',')", advance="no")
      write (u, "(1x,A,A,A)", advance="no") &

```



```

        "'", char (model%schemes(i)), ""
    end do
    write (u, *)
    if (allocated (model%selected_scheme)) then
        write (u, "(1x,A,A,A,I0,A)") &
            "! selected scheme = '", char (model%get_scheme ()), &
            "' (" , model%get_scheme_num (), ")"
    end if
end if
if (show_par) then
    write (u, "(A)")
    do i = 1, size (model%par)
        call model%par(i)%write (u, write_defs=verbose)
    end do
end if
call model%model_data_t%write (unit, verbose, &
    show_md5sum, show_variables, &
    show_parameters=.false., &
    show_particles=show_particles, &
    show_vertices=show_vertices, &
    show_scheme=show_scheme)
if (show_var) then
    write (u, "(A)")
    call var_list_write (model%var_list, unit, follow_link=.false.)
end if
end subroutine model_write

```

Screen output, condensed form.

<Models: model: TBP>+≡

```

    procedure :: show => model_show

```

<Models: procedures>+≡

```

subroutine model_show (model, unit)
    class(model_t), intent(in) :: model
    integer, intent(in), optional :: unit
    integer :: i, u, l
    u = given_output_unit (unit)
    write (u, "(A,1x,A)") "Model:", char (model%get_name ())
    if (model%has_schemes ()) then
        write (u, "(2x,A,A,A,I0,A)") "Scheme: '", &
            char (model%get_scheme ()), "' (" , model%get_scheme_num (), ")"
    end if
    l = model%max_field_name_length
    call model%show_fields (l, u)
    l = model%max_par_name_length
    if (any (model%par%type == PAR_INDEPENDENT)) then
        write (u, "(2x,A)") "Independent parameters:"
        do i = 1, size (model%par)
            call model%par(i)%show (l, u, PAR_INDEPENDENT)
        end do
    end if
    if (any (model%par%type == PAR_DERIVED)) then
        write (u, "(2x,A)") "Derived parameters:"
        do i = 1, size (model%par)

```

```

        call model%par(i)%show (1, u, PAR_DERIVED)
    end do
end if
if (any (model%par%type == PAR_EXTERNAL)) then
    write (u, "(2x,A)") "External parameters:"
    do i = 1, size (model%par)
        call model%par(i)%show (1, u, PAR_EXTERNAL)
    end do
end if
if (any (model%par%type == PAR_UNUSED)) then
    write (u, "(2x,A)") "Unused parameters:"
    do i = 1, size (model%par)
        call model%par(i)%show (1, u, PAR_UNUSED)
    end do
end if
end subroutine model_show

```

Show all fields/particles.

```

<Models: model: TBP>+≡
    procedure :: show_fields => model_show_fields

<Models: procedures>+≡
    subroutine model_show_fields (model, l, unit)
        class(model_t), intent(in), target :: model
        integer, intent(in) :: l
        integer, intent(in), optional :: unit
        type(field_data_t), pointer :: field
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(2x,A)") "Particles:"
        do i = 1, model%get_n_field ()
            field => model%get_field_ptr_by_index (i)
            call field%show (1, u)
        end do
    end subroutine model_show_fields

```

Show the list of stable, unstable, polarized, or unpolarized particles, respectively.

```

<Models: model: TBP>+≡
    procedure :: show_stable => model_show_stable
    procedure :: show_unstable => model_show_unstable
    procedure :: show_polarized => model_show_polarized
    procedure :: show_unpolarized => model_show_unpolarized

<Models: procedures>+≡
    subroutine model_show_stable (model, unit)
        class(model_t), intent(in), target :: model
        integer, intent(in), optional :: unit
        type(field_data_t), pointer :: field
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(A,1x)", advance="no") "Stable particles:"
        do i = 1, model%get_n_field ()
            field => model%get_field_ptr_by_index (i)
            if (field%is_stable (.false.)) then

```

```

        write (u, "(1x,A)", advance="no") char (field%get_name (.false.))
    end if
    if (field%has_antiparticle ()) then
        if (field%is_stable (.true.)) then
            write (u, "(1x,A)", advance="no") char (field%get_name (.true.))
        end if
    end if
end do
write (u, *)
end subroutine model_show_stable

subroutine model_show_unstable (model, unit)
    class(model_t), intent(in), target :: model
    integer, intent(in), optional :: unit
    type(field_data_t), pointer :: field
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(A,1x)", advance="no") "Unstable particles:"
    do i = 1, model%get_n_field ()
        field => model%get_field_ptr_by_index (i)
        if (.not. field%is_stable (.false.)) then
            write (u, "(1x,A)", advance="no") char (field%get_name (.false.))
        end if
        if (field%has_antiparticle ()) then
            if (.not. field%is_stable (.true.)) then
                write (u, "(1x,A)", advance="no") char (field%get_name (.true.))
            end if
        end if
    end do
    write (u, *)
end subroutine model_show_unstable

subroutine model_show_polarized (model, unit)
    class(model_t), intent(in), target :: model
    integer, intent(in), optional :: unit
    type(field_data_t), pointer :: field
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(A,1x)", advance="no") "Polarized particles:"
    do i = 1, model%get_n_field ()
        field => model%get_field_ptr_by_index (i)
        if (field%is_polarized (.false.)) then
            write (u, "(1x,A)", advance="no") char (field%get_name (.false.))
        end if
        if (field%has_antiparticle ()) then
            if (field%is_polarized (.true.)) then
                write (u, "(1x,A)", advance="no") char (field%get_name (.true.))
            end if
        end if
    end do
    write (u, *)
end subroutine model_show_polarized

subroutine model_show_unpolarized (model, unit)

```

```

class(model_t), intent(in), target :: model
integer, intent(in), optional :: unit
type(field_data_t), pointer :: field
integer :: u, i
u = given_output_unit (unit)
write (u, "(A,1x)", advance="no") "Unpolarized particles:"
do i = 1, model%get_n_field ()
  field => model%get_field_ptr_by_index (i)
  if (.not. field%is_polarized (.false.)) then
    write (u, "(1x,A)", advance="no") &
      char (field%get_name (.false.))
  end if
  if (field%has_antiparticle ()) then
    if (.not. field%is_polarized (.true.)) then
      write (u, "(1x,A)", advance="no") char (field%get_name (.true.))
    end if
  end if
end do
write (u, *)
end subroutine model_show_unpolarized

```

Retrieve the MD5 sum of a model (actually, of the model file).

```

<Models: model: TBP>+≡
  procedure :: get_md5sum => model_get_md5sum

<Models: procedures>+≡
  function model_get_md5sum (model) result (md5sum)
    character(32) :: md5sum
    class(model_t), intent(in) :: model
    md5sum = model%md5sum
  end function model_get_md5sum

```

Parameters are defined by an expression which may be constant or arbitrary.

```

<Models: model: TBP>+≡
  procedure :: &
    set_parameter_constant => model_set_parameter_constant
  procedure, private :: &
    set_parameter_parse_node => model_set_parameter_parse_node
  procedure :: &
    set_parameter_external => model_set_parameter_external
  procedure :: &
    set_parameter_unused => model_set_parameter_unused

<Models: procedures>+≡
  subroutine model_set_parameter_constant (model, i, name, value)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    real(default), intent(in) :: value
    logical, save, target :: known = .true.
    class(modelpar_data_t), pointer :: par_data
    real(default), pointer :: value_ptr
    par_data => model%get_par_real_ptr (i)
    call model%par(i)%init_independent_value (par_data, name, value)
  end subroutine model_set_parameter_constant

```

```

value_ptr => par_data%get_real_ptr ()
call var_list_append_real_ptr (model%var_list, &
    name, value_ptr, &
    is_known=known, intrinsic=.true.)
model%max_par_name_length = max (model%max_par_name_length, len (name))
end subroutine model_set_parameter_constant

subroutine model_set_parameter_parse_node (model, i, name, pn, constant)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    type(parse_node_t), intent(in), target :: pn
    logical, intent(in) :: constant
    logical, save, target :: known = .true.
    class(modelpar_data_t), pointer :: par_data
    real(default), pointer :: value_ptr
    par_data => model%get_par_real_ptr (i)
    if (constant) then
        call model%par(i)%init_independent (par_data, name, pn)
    else
        call model%par(i)%init_derived (par_data, name, pn, model%var_list)
    end if
    value_ptr => par_data%get_real_ptr ()
    call var_list_append_real_ptr (model%var_list, &
        name, value_ptr, &
        is_known=known, locked=.not.constant, intrinsic=.true.)
    model%max_par_name_length = max (model%max_par_name_length, len (name))
end subroutine model_set_parameter_parse_node

subroutine model_set_parameter_external (model, i, name)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    logical, save, target :: known = .true.
    class(modelpar_data_t), pointer :: par_data
    real(default), pointer :: value_ptr
    par_data => model%get_par_real_ptr (i)
    call model%par(i)%init_external (par_data, name)
    value_ptr => par_data%get_real_ptr ()
    call var_list_append_real_ptr (model%var_list, &
        name, value_ptr, &
        is_known=known, locked=.true., intrinsic=.true.)
    model%max_par_name_length = max (model%max_par_name_length, len (name))
end subroutine model_set_parameter_external

subroutine model_set_parameter_unused (model, i, name)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name
    class(modelpar_data_t), pointer :: par_data
    par_data => model%get_par_real_ptr (i)
    call model%par(i)%init_unused (par_data, name)
    call var_list_append_real (model%var_list, &
        name, locked=.true., intrinsic=.true.)

```

```

    model%max_par_name_length = max (model%max_par_name_length, len (name))
end subroutine model_set_parameter_unused

```

Make a copy of a parameter. We assume that the `model_data_t` parameter arrays have already been copied, so names and values are available in the current model, and can be used as targets. The eval tree should not be copied, since it should refer to the new variable list. The safe solution is to make use of the above initializers, which also take care of the building a new variable list.

```

<Models: model: TBP>+≡
    procedure, private :: copy_parameter => model_copy_parameter

<Models: procedures>+≡
    subroutine model_copy_parameter (model, i, par)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(parameter_t), intent(in) :: par
        type(string_t) :: name
        real(default) :: value
        name = par%data%get_name ()
        select case (par%type)
        case (PAR_INDEPENDENT)
            if (associated (par%pn)) then
                call model%set_parameter_parse_node (i, name, par%pn, &
                    constant = .true.)
            else
                value = par%data%get_real ()
                call model%set_parameter_constant (i, name, value)
            end if
            if (allocated (par%block_index)) then
                model%par(i)%block_name = par%block_name
                model%par(i)%block_index = par%block_index
            end if
        case (PAR_DERIVED)
            call model%set_parameter_parse_node (i, name, par%pn, &
                constant = .false.)
        case (PAR_EXTERNAL)
            call model%set_parameter_external (i, name)
        case (PAR_UNUSED)
            call model%set_parameter_unused (i, name)
        end select
    end subroutine model_copy_parameter

```

Recalculate all derived parameters.

```

<Models: model: TBP>+≡
    procedure :: update_parameters => model_parameters_update

<Models: procedures>+≡
    subroutine model_parameters_update (model)
        class(model_t), intent(inout) :: model
        integer :: i
        real(default), dimension(:), allocatable :: par
        do i = 1, size (model%par)
            call model%par(i)%reset_derived ()
        end do
    end subroutine model_parameters_update

```

```

end do
if (associated (model%init_external_parameters)) then
  allocate (par (model%get_n_real ()))
  call model%real_parameters_to_c_array (par)
  call model%init_external_parameters (par)
  call model%real_parameters_from_c_array (par)
  if (model%get_name() == var_str ("SM_tt_threshold")) &
    call set_threshold_parameters ()
end if
contains
subroutine set_threshold_parameters ()
  real(default) :: mpole, wtop
  !!! !!! !!! Workaround for OS-X and BSD which do not load
  !!! !!! !!! the global values created previously. Therefore
  !!! !!! !!! a second initialization for the threshold model,
  !!! !!! !!! where M1S is required to compute the top mass.
  call init_parameters (mpole, wtop, &
    par(20), par(21), par(22), &
    par(19), par(39), par(4), par(1), &
    par(2), par(10), par(24), par(25), &
    par(23), par(26), par(27), par(29), &
    par(30), par(31), par(32), par(33), &
    par(36) > 0._default, par(28))
end subroutine set_threshold_parameters
end subroutine model_parameters_update

```

Initialize field data with PDG long name and PDG code.

```

<Models: model: TBP>+≡
  procedure, private :: init_field => model_init_field

<Models: procedures>+≡
  subroutine model_init_field (model, i, longname, pdg)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: longname
    integer, intent(in) :: pdg
    type(field_data_t), pointer :: field
    field => model%get_field_ptr_by_index (i)
    call field%init (longname, pdg)
  end subroutine model_init_field

```

Copy field data for index i from another particle which serves as a template.
The name should be the unique long name.

```

<Models: model: TBP>+≡
  procedure, private :: copy_field => model_copy_field

<Models: procedures>+≡
  subroutine model_copy_field (model, i, name_src)
    class(model_t), intent(inout), target :: model
    integer, intent(in) :: i
    type(string_t), intent(in) :: name_src
    type(field_data_t), pointer :: field_src, field
    field_src => model%get_field_ptr (name_src)
    field => model%get_field_ptr_by_index (i)

```

```

    call field%copy_from (field_src)
end subroutine model_copy_field

```

28.4.5 Model Access via Variables

Write the model variable list.

```

<Models: model: TBP>+≡
    procedure :: write_var_list => model_write_var_list

<Models: procedures>+≡
    subroutine model_write_var_list (model, unit, follow_link)
        class(model_t), intent(in) :: model
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: follow_link
        call var_list_write (model%var_list, unit, follow_link)
    end subroutine model_write_var_list

```

Link a variable list to the model variables.

```

<Models: model: TBP>+≡
    procedure :: link_var_list => model_link_var_list

<Models: procedures>+≡
    subroutine model_link_var_list (model, var_list)
        class(model_t), intent(inout) :: model
        type(var_list_t), intent(in), target :: var_list
        call model%var_list%link (var_list)
    end subroutine model_link_var_list

```

Check if the model contains a named variable.

```

<Models: model: TBP>+≡
    procedure :: var_exists => model_var_exists

<Models: procedures>+≡
    function model_var_exists (model, name) result (flag)
        class(model_t), intent(in) :: model
        type(string_t), intent(in) :: name
        logical :: flag
        flag = model%var_list%contains (name, follow_link=.false.)
    end function model_var_exists

```

Check if the model variable is a derived parameter, i.e., locked.

```

<Models: model: TBP>+≡
    procedure :: var_is_locked => model_var_is_locked

<Models: procedures>+≡
    function model_var_is_locked (model, name) result (flag)
        class(model_t), intent(in) :: model
        type(string_t), intent(in) :: name
        logical :: flag
        flag = model%var_list%is_locked (name, follow_link=.false.)
    end function model_var_is_locked

```


Set a model parameter via the named variable. We assume that the variable exists and is writable, i.e., non-locked. We update the model and variable list, so independent and derived parameters are always synchronized.

```

<Models: model: TBP>+≡
  procedure :: set_real => model_var_set_real

<Models: procedures>+≡
  subroutine model_var_set_real (model, name, rval, verbose, pacified)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in) :: name
    real(default), intent(in) :: rval
    logical, intent(in), optional :: verbose, pacified
    call model%var_list%set_real (name, rval, &
      is_known=.true., ignore=.false., &
      verbose=verbose, model_name=model%get_name (), pacified=pacified)
    call model%update_parameters ()
  end subroutine model_var_set_real

```

Retrieve a model parameter value.

```

<Models: model: TBP>+≡
  procedure :: get_rval => model_var_get_rval

<Models: procedures>+≡
  function model_var_get_rval (model, name) result (rval)
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: name
    real(default) :: rval
    rval = model%var_list%get_rval (name, follow_link=.false.)
  end function model_var_get_rval

```

[To be deleted] Return a pointer to the variable list.

```

<Models: model: TBP>+≡
  procedure :: get_var_list_ptr => model_get_var_list_ptr

<Models: procedures>+≡
  function model_get_var_list_ptr (model) result (var_list)
    type(var_list_t), pointer :: var_list
    class(model_t), intent(in), target :: model
    var_list => model%var_list
  end function model_get_var_list_ptr

```

28.4.6 UFO models

A single flag identifies a model as a UFO model. There is no other distinction, but the flag allows us to handle built-in and UFO models with the same name in parallel.

```

<Models: model: TBP>+≡
  procedure :: is_ufo_model => model_is_ufo_model

```

```

<Models: procedures>+≡
function model_is_ufo_model (model) result (flag)
  class(model_t), intent(in) :: model
  logical :: flag
  flag = model%ufo_model
end function model_is_ufo_model

```

Return the UFO path used for fetching the UFO source.

```

<Models: model: TBP>+≡
  procedure :: get_ufo_path => model_get_ufo_path

<Models: procedures>+≡
function model_get_ufo_path (model) result (path)
  class(model_t), intent(in) :: model
  type(string_t) :: path
  if (model%ufo_model) then
    path = model%ufo_path
  else
    path = ""
  end if
end function model_get_ufo_path

```

Call Omega and generate a model file from an UFO source file. We start with a file name; the model name is expected to be the base name, stripping extensions.

The path search either takes `ufo_path_requested`, or searches first in the working directory, then in a hard-coded UFO model directory.

```

<Models: procedures>+≡
subroutine model_generate_ufo (filename, os_data, ufo_path, &
  ufo_path_requested)
  type(string_t), intent(in) :: filename
  type(os_data_t), intent(in) :: os_data
  type(string_t), intent(out) :: ufo_path
  type(string_t), intent(in), optional :: ufo_path_requested
  type(string_t) :: model_name, omega_path, ufo_dir, ufo_init
  logical :: exist
  call get_model_name (filename, model_name)
  call msg_message ("Model: Generating model '" // char (model_name) &
    // "' from UFO sources")
  if (present (ufo_path_requested)) then
    call msg_message ("Model: Searching for UFO sources in '" &
      // char (ufo_path_requested) // "'")
    ufo_path = ufo_path_requested
    ufo_dir = ufo_path_requested // "/" // model_name
    ufo_init = ufo_dir // "/" // "__init__.py"
    inquire (file = char (ufo_init), exist = exist)
  else
    call msg_message ("Model: Searching for UFO sources in &
      &working directory")
    ufo_path = "."
    ufo_dir = ufo_path // "/" // model_name
    ufo_init = ufo_dir // "/" // "__init__.py"
    inquire (file = char (ufo_init), exist = exist)
    if (.not. exist) then

```

```

        ufo_path = char (os_data%whizard_modelpath_ufo)
        ufo_dir = ufo_path // "/" // model_name
        ufo_init = ufo_dir // "/" // "__init__.py"
        call msg_message ("Model: Searching for UFO sources in '" &
            // char (os_data%whizard_modelpath_ufo) // "'")
        inquire (file = char (ufo_init), exist = exist)
    end if
end if
if (exist) then
    call msg_message ("Model: Found UFO sources for model '" &
        // char (model_name) // "'")
else
    call msg_fatal ("Model: UFO sources for model '" &
        // char (model_name) // "' not found")
end if
omega_path = os_data%whizard_omega_binpath // "/omega_UFO.opt"
call os_system_call (omega_path &
    // " -model:UFO_dir " // ufo_dir &
    // " -model:exec" &
    // " -model:write_WHIZARD" &
    // " > " // filename)
inquire (file = char (filename), exist = exist)
if (exist) then
    call msg_message ("Model: Model file '" // char (filename) //&
        "' generated")
else
    call msg_fatal ("Model: Model file '" // char (filename) &
        // "' could not be generated")
end if
contains
subroutine get_model_name (filename, model_name)
    type(string_t), intent(in) :: filename
    type(string_t), intent(out) :: model_name
    type(string_t) :: string
    string = filename
    call split (string, model_name, ".")
end subroutine get_model_name
end subroutine model_generate_ufo

```

28.4.7 Scheme handling

A model can specify a set of allowed schemes that steer the setup of model variables. The model file can contain scheme-specific declarations that are selected by a `select scheme` clause. Scheme support is optional.

If enabled, the model object contains a list of allowed schemes, and the model reader takes the active scheme as an argument. After the model has been read, the scheme is fixed and can no longer be modified.

The model supports schemes if the scheme array is allocated.

(Models: model: TBP)+≡

```
procedure :: has_schemes => model_has_schemes
```

(Models: procedures)+≡

```

function model_has_schemes (model) result (flag)
  logical :: flag
  class(model_t), intent(in) :: model
  flag = allocated (model%schemes)
end function model_has_schemes

```

Enable schemes: fix the list of allowed schemes.

```

<Models: model: TBP>+≡
  procedure :: enable_schemes => model_enable_schemes

<Models: procedures>+≡
  subroutine model_enable_schemes (model, scheme)
    class(model_t), intent(inout) :: model
    type(string_t), dimension(:), intent(in) :: scheme
    allocate (model%schemes (size (scheme)), source = scheme)
  end subroutine model_enable_schemes

```

Find the scheme. Check if the scheme is allowed. The numeric index of the selected scheme is stored in the `model_data_t` base object.

If no argument is given, select the first scheme. The numeric scheme ID will then be 1, while a model without schemes retains 0.

```

<Models: model: TBP>+≡
  procedure :: set_scheme => model_set_scheme

<Models: procedures>+≡
  subroutine model_set_scheme (model, scheme)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in), optional :: scheme
    logical :: ok
    integer :: i
    if (model%has_schemes ()) then
      if (present (scheme)) then
        ok = .false.
        CHECK_SCHEME: do i = 1, size (model%schemes)
          if (scheme == model%schemes(i)) then
            allocate (model%selected_scheme, source = scheme)
            call model%set_scheme_num (i)
            ok = .true.
            exit CHECK_SCHEME
          end if
        end do CHECK_SCHEME
      if (.not. ok) then
        call msg_fatal &
          ("Model '" // char (model%get_name ()) &
           // "': scheme '" // char (scheme) // "' not supported")
      end if
    else
      allocate (model%selected_scheme, source = model%schemes(1))
      call model%set_scheme_num (1)
    end if
  else
    if (present (scheme)) then
      call msg_error &
        ("Model '" // char (model%get_name ()) &

```

```

// '' does not support schemes")
    end if
  end if
end subroutine model_set_scheme

```

Get the scheme. Note that the base `model_data_t` provides a `get_scheme_num` getter function.

```

<Models: model: TBP>+≡
  procedure :: get_scheme => model_get_scheme

<Models: procedures>+≡
  function model_get_scheme (model) result (scheme)
    class(model_t), intent(in) :: model
    type(string_t) :: scheme
    if (allocated (model%selected_scheme)) then
      scheme = model%selected_scheme
    else
      scheme = ""
    end if
  end function model_get_scheme

```

Check if a model has been set up with a specific name and (if applicable) scheme. This helps in determining whether we need a new model object.

A UFO model is considered to be distinct from a non-UFO model. We assume that if `ufo` is asked for, there is no scheme argument. Furthermore, if there is an `ufo_path` requested, it must coincide with the `ufo_path` of the model. If not, the model `ufo_path` is not checked.

```

<Models: model: TBP>+≡
  procedure :: matches => model_matches

<Models: procedures>+≡
  function model_matches (model, name, scheme, ufo, ufo_path) result (flag)
    logical :: flag
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: scheme
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path
    logical :: ufo_model
    ufo_model = .false.; if (present (ufo)) ufo_model = ufo
    if (name /= model%get_name ()) then
      flag = .false.
    else if (ufo_model .neqv. model%is_ufo_model ()) then
      flag = .false.
    else if (ufo_model) then
      if (present (ufo_path)) then
        flag = model%get_ufo_path () == ufo_path
      else
        flag = .true.
      end if
    else if (model%has_schemes ()) then
      if (present (scheme)) then
        flag = model%get_scheme () == scheme
      end if
    end if
  end function model_matches

```

```

        else
            flag = model%get_scheme_num () == 1
        end if
    else if (present (scheme)) then
        flag = .false.
    else
        flag = .true.
    end if
end function model_matches

```

28.4.8 SLHA-type interface

Abusing the original strict SUSY Les Houches Accord (SLHA), we support reading parameter data from some custom SLHA-type input file. To this end, the `model` object stores a list of model-specific block names together with information how to find a parameter in the model record, given a block name and index vector.

Check if the model supports custom SLHA block info. This is the case if `n_slha_block` is nonzero, i.e., after SLHA block names have been parsed and registered.

```

<Models: model: TBP>+≡
    procedure :: supports_custom_slha => model_supports_custom_slha

<Models: procedures>+≡
    function model_supports_custom_slha (model) result (flag)
        class(model_t), intent(in) :: model
        logical :: flag

        flag = model%n_slha_block > 0

    end function model_supports_custom_slha

```

Return the block names for all SLHA block references.

```

<Models: model: TBP>+≡
    procedure :: get_custom_slha_blocks => model_get_custom_slha_blocks

<Models: procedures>+≡
    subroutine model_get_custom_slha_blocks (model, block_name)
        class(model_t), intent(in) :: model
        type(string_t), dimension(:), allocatable :: block_name

        integer :: i

        allocate (block_name (model%n_slha_block))
        do i = 1, size (block_name)
            block_name(i) = model%slha_block(i)%name
        end do

    end subroutine model_get_custom_slha_blocks

```

This routine registers a SLHA block reference. We have the index of a (new) parameter entry and a parse node from the model file which specifies a block name and an index array.

(Models: procedures)+≡

```

subroutine model_record_slha_block_entry (model, i_par, node)
  class(model_t), intent(inout) :: model
  integer, intent(in) :: i_par
  type(parse_node_t), intent(in), target :: node

  type(parse_node_t), pointer :: node_block_name, node_index
  type(string_t) :: block_name
  integer :: n_index, i, i_block
  integer, dimension(:), allocatable :: block_index

  node_block_name => node%get_sub_ptr (2)
  select case (char (node_block_name%get_rule_key ()))
  case ("block_name")
    block_name = node_block_name%get_string ()
  case ("QNUMBERS")
    block_name = "QNUMBERS"
  case default
    block_name = node_block_name%get_string ()
  end select
  n_index = node%get_n_sub () - 2
  allocate (block_index (n_index))
  node_index => node_block_name%get_next_ptr ()
  do i = 1, n_index
    block_index(i) = node_index%get_integer ()
    node_index => node_index%get_next_ptr ()
  end do
  i_block = 0
  FIND_BLOCK: do i = 1, model%n_slha_block
    if (model%slha_block(i)%name == block_name) then
      i_block = i
      exit FIND_BLOCK
    end if
  end do FIND_BLOCK
  if (i_block == 0) then
    call model_add_slha_block (model, block_name)
    i_block = model%n_slha_block
  end if
  associate (b => model%slha_block(i_block))
    call add_slha_block_entry (b, block_index, i_par)
  end associate
  model%par(i_par)%block_name = block_name
  model%par(i_par)%block_index = block_index
end subroutine model_record_slha_block_entry

```

Add a new entry to the SLHA block register, increasing the array size if necessary

(Models: procedures)+≡

```

subroutine model_add_slha_block (model, block_name)
  class(model_t), intent(inout) :: model

```

```

type(string_t), intent(in) :: block_name

if (.not. allocated (model%slha_block)) allocate (model%slha_block (1))
if (model%n_slha_block == size (model%slha_block)) call grow
model%n_slha_block = model%n_slha_block + 1
associate (b => model%slha_block(model%n_slha_block))
    b%name = block_name
    allocate (b%entry (1))
end associate

contains

subroutine grow
    type(slha_block_t), dimension(:), allocatable :: b_tmp
    call move_alloc (model%slha_block, b_tmp)
    allocate (model%slha_block (2 * size (b_tmp)))
    model%slha_block(:size (b_tmp)) = b_tmp(:)
end subroutine grow

end subroutine model_add_slha_block

```

Add a new entry to a block-register record. The entry establishes a pointer-target relation between an index array within the SLHA block and a parameter-data record. We increase the entry array as needed.

(Models: procedures)+≡

```

subroutine add_slha_block_entry (b, block_index, i_par)
    type(slha_block_t), intent(inout) :: b
    integer, dimension(:), intent(in) :: block_index
    integer, intent(in) :: i_par

    if (b%n_entry == size (b%entry)) call grow
    b%n_entry = b%n_entry + 1
    associate (entry => b%entry(b%n_entry))
        entry%block_index = block_index
        entry%i_par = i_par
    end associate

contains

subroutine grow
    type(slha_entry_t), dimension(:), allocatable :: entry_tmp
    call move_alloc (b%entry, entry_tmp)
    allocate (b%entry (2 * size (entry_tmp)))
    b%entry(:size (entry_tmp)) = entry_tmp(:)
end subroutine grow

end subroutine add_slha_block_entry

```

The lookup routine returns a pointer to the appropriate `par_data` record, if `block_name` and `block_index` are valid. The latter point to the `slha_block_t` register within the `model_t` object, if it is allocated.

This should only be needed during I/O (i.e., while reading the SLHA file), so a simple linear search for each parameter should not be a performance problem.


```

<Models: model: TBP>+≡
  procedure :: slha_lookup => model_slha_lookup

<Models: procedures>+≡
  subroutine model_slha_lookup (model, block_name, block_index, par_data)
    class(model_t), intent(in) :: model
    type(string_t), intent(in) :: block_name
    integer, dimension(:), intent(in) :: block_index
    class(modelpar_data_t), pointer, intent(out) :: par_data

    integer :: i, j

    par_data => null ()
    if (allocated (model%slha_block)) then
      do i = 1, model%n_slha_block
        associate (block => model%slha_block(i))
          if (block%name == block_name) then
            do j = 1, block%n_entry
              associate (entry => block%entry(j))
                if (size (entry%block_index) == size (block_index)) then
                  if (all (entry%block_index == block_index)) then
                    par_data => model%par(entry%i_par)%data
                    return
                  end if
                end if
              end if
            end associate
          end do
        end if
      end associate
    end do
  end if

end subroutine model_slha_lookup

```

Modify the value of a parameter, identified by block name and index array.

```

<Models: model: TBP>+≡
  procedure :: slha_set_par => model_slha_set_par

<Models: procedures>+≡
  subroutine model_slha_set_par (model, block_name, block_index, value)
    class(model_t), intent(inout) :: model
    type(string_t), intent(in) :: block_name
    integer, dimension(:), intent(in) :: block_index
    real(default), intent(in) :: value

    class(modelpar_data_t), pointer :: par_data

    call model%slha_lookup (block_name, block_index, par_data)
    if (associated (par_data)) then
      par_data = value
    end if

  end subroutine model_slha_set_par

```

28.4.9 Reading models from file

This procedure defines the model-file syntax for the parser, returning an internal file (ifile).

Note that arithmetic operators are defined as keywords in the expression syntax, so we exclude them here.

(Models: procedures)+≡

```
subroutine define_model_file_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "SEQ model_def = model_name_def " // &
    "scheme_header parameters external_pars particles vertices")
  call ifile_append (ifile, "SEQ model_name_def = model model_name")
  call ifile_append (ifile, "KEY model")
  call ifile_append (ifile, "QUO model_name = '...'"")
  call ifile_append (ifile, "SEQ scheme_header = scheme_decl?")
  call ifile_append (ifile, "SEQ scheme_decl = schemes '=' scheme_list")
  call ifile_append (ifile, "KEY schemes")
  call ifile_append (ifile, "LIS scheme_list = scheme_name+")
  call ifile_append (ifile, "QUO scheme_name = '...'"")
  call ifile_append (ifile, "SEQ parameters = generic_par_def*")
  call ifile_append (ifile, "ALT generic_par_def = &
    &parameter_def | derived_def | unused_def | scheme_block")
  call ifile_append (ifile, "SEQ parameter_def = parameter par_name " // &
    "'=' any_real_value slha_annotation?")
  call ifile_append (ifile, "ALT any_real_value = " &
    // "neg_real_value | pos_real_value | real_value")
  call ifile_append (ifile, "SEQ neg_real_value = '-' real_value")
  call ifile_append (ifile, "SEQ pos_real_value = '+' real_value")
  call ifile_append (ifile, "KEY parameter")
  call ifile_append (ifile, "IDE par_name")
  ! call ifile_append (ifile, "KEY '='")          !!! Key already exists
  call ifile_append (ifile, "SEQ slha_annotation = " // &
    "slha_entry slha_block_name slha_entry_index*")
  call ifile_append (ifile, "KEY slha_entry")
  call ifile_append (ifile, "IDE slha_block_name")
  call ifile_append (ifile, "INT slha_entry_index")
  call ifile_append (ifile, "SEQ derived_def = derived par_name " // &
    "'=' expr")
  call ifile_append (ifile, "KEY derived")
  call ifile_append (ifile, "SEQ unused_def = unused par_name")
  call ifile_append (ifile, "KEY unused")
  call ifile_append (ifile, "SEQ external_pars = external_def*")
  call ifile_append (ifile, "SEQ external_def = external par_name")
  call ifile_append (ifile, "KEY external")
  call ifile_append (ifile, "SEQ scheme_block = &
    &scheme_block_beg scheme_block_body scheme_block_end")
  call ifile_append (ifile, "SEQ scheme_block_beg = select scheme")
  call ifile_append (ifile, "SEQ scheme_block_body = scheme_block_case*")
  call ifile_append (ifile, "SEQ scheme_block_case = &
    &scheme scheme_id parameters")
  call ifile_append (ifile, "ALT scheme_id = scheme_list | other")
  call ifile_append (ifile, "SEQ scheme_block_end = end select")
  call ifile_append (ifile, "KEY select")
  call ifile_append (ifile, "KEY scheme")
end subroutine
```

```

call ifile_append (ifile, "KEY other")
call ifile_append (ifile, "KEY end")
call ifile_append (ifile, "SEQ particles = particle_def*")
call ifile_append (ifile, "SEQ particle_def = particle name_def " // &
    "prt_pdg prt_details")
call ifile_append (ifile, "KEY particle")
call ifile_append (ifile, "SEQ prt_pdg = signed_int")
call ifile_append (ifile, "ALT prt_details = prt_src | prt_properties")
call ifile_append (ifile, "SEQ prt_src = like name_def prt_properties")
call ifile_append (ifile, "KEY like")
call ifile_append (ifile, "SEQ prt_properties = prt_property*")
call ifile_append (ifile, "ALT prt_property = " // &
    "parton | invisible | gauge | left | right | " // &
    "prt_name | prt_anti | prt_tex_name | prt_tex_anti | " // &
    "prt_spin | prt_isospin | prt_charge | " // &
    "prt_color | prt_mass | prt_width")
call ifile_append (ifile, "KEY parton")
call ifile_append (ifile, "KEY invisible")
call ifile_append (ifile, "KEY gauge")
call ifile_append (ifile, "KEY left")
call ifile_append (ifile, "KEY right")
call ifile_append (ifile, "SEQ prt_name = name name_def+")
call ifile_append (ifile, "SEQ prt_anti = anti name_def+")
call ifile_append (ifile, "SEQ prt_tex_name = tex_name name_def")
call ifile_append (ifile, "SEQ prt_tex_anti = tex_anti name_def")
call ifile_append (ifile, "KEY name")
call ifile_append (ifile, "KEY anti")
call ifile_append (ifile, "KEY tex_name")
call ifile_append (ifile, "KEY tex_anti")
call ifile_append (ifile, "ALT name_def = name_string | name_id")
call ifile_append (ifile, "QUO name_string = '...'"")
call ifile_append (ifile, "IDE name_id")
call ifile_append (ifile, "SEQ prt_spin = spin frac")
call ifile_append (ifile, "KEY spin")
call ifile_append (ifile, "SEQ prt_isospin = isospin frac")
call ifile_append (ifile, "KEY isospin")
call ifile_append (ifile, "SEQ prt_charge = charge frac")
call ifile_append (ifile, "KEY charge")
call ifile_append (ifile, "SEQ prt_color = color integer_literal")
call ifile_append (ifile, "KEY color")
call ifile_append (ifile, "SEQ prt_mass = mass par_name")
call ifile_append (ifile, "KEY mass")
call ifile_append (ifile, "SEQ prt_width = width par_name")
call ifile_append (ifile, "KEY width")
call ifile_append (ifile, "SEQ vertices = vertex_def*")
call ifile_append (ifile, "SEQ vertex_def = vertex name_def+")
call ifile_append (ifile, "KEY vertex")
call define_expr_syntax (ifile, particles=.false., analysis=.false.)
end subroutine define_model_file_syntax

```

The model-file syntax and lexer are fixed, therefore stored as module variables:

```

(Models: variables)≡
    type(syntax_t), target, save :: syntax_model_file

```

```

<Models: public>+≡
    public :: syntax_model_file_init

<Models: procedures>+≡
    subroutine syntax_model_file_init ()
        type(ifile_t) :: ifile
        call define_model_file_syntax (ifile)
        call syntax_init (syntax_model_file, ifile)
        call ifile_final (ifile)
    end subroutine syntax_model_file_init

<Models: procedures>+≡
    subroutine lexer_init_model_file (lexer)
        type(lexer_t), intent(out) :: lexer
        call lexer_init (lexer, &
            comment_chars = "#!", &
            quote_chars = '"{', &
            quote_match = '"}', &
            single_chars = ":(, ", &
            special_class = [ "+-*/^", "<>= " ], &
            keyword_list = syntax_get_keyword_list_ptr (syntax_model_file))
    end subroutine lexer_init_model_file

<Models: public>+≡
    public :: syntax_model_file_final

<Models: procedures>+≡
    subroutine syntax_model_file_final ()
        call syntax_final (syntax_model_file)
    end subroutine syntax_model_file_final

<Models: public>+≡
    public :: syntax_model_file_write

<Models: procedures>+≡
    subroutine syntax_model_file_write (unit)
        integer, intent(in), optional :: unit
        call syntax_write (syntax_model_file, unit)
    end subroutine syntax_model_file_write

```

Read a model from file. Handle all syntax and respect the provided scheme.

The `ufo` flag just says that the model object should be tagged as being derived from an UFO model. The UFO model path may be requested by the caller. If not, we use a standard path search for UFO models. There is no difference in the contents of the file or the generated model object.

```

<Models: model: TBP>+≡
    procedure :: read => model_read

<Models: procedures>+≡
    subroutine model_read (model, filename, os_data, exist, &
        scheme, ufo, ufo_path_requested, rebuild_md1)
        class(model_t), intent(out), target :: model
        type(string_t), intent(in) :: filename
        type(os_data_t), intent(in) :: os_data

```

```

logical, intent(out), optional :: exist
type(string_t), intent(in), optional :: scheme
logical, intent(in), optional :: ufo
type(string_t), intent(in), optional :: ufo_path_requested
logical, intent(in), optional :: rebuild_mdl
type(string_t) :: file
type(stream_t), target :: stream
type(lexer_t) :: lexer
integer :: unit
character(32) :: model_md5sum
type(parse_node_t), pointer :: nd_model_def, nd_model_name_def
type(parse_node_t), pointer :: nd_schemes, nd_scheme_decl
type(parse_node_t), pointer :: nd_parameters
type(parse_node_t), pointer :: nd_external_pars
type(parse_node_t), pointer :: nd_particles, nd_vertices
type(string_t) :: model_name, lib_name
integer :: n_parblock, n_par, i_par, n_ext, n_prt, n_vtx
type(parse_node_t), pointer :: nd_par_def
type(parse_node_t), pointer :: nd_ext_def
type(parse_node_t), pointer :: nd_prt
type(parse_node_t), pointer :: nd_vtx
logical :: ufo_model, model_exist, rebuild
ufo_model = .false.; if (present (ufo)) ufo_model = ufo
rebuild = .true.; if (present (rebuild_mdl)) rebuild = rebuild_mdl
file = filename
inquire (file=char(file), exist=model_exist)
if ((.not. model_exist) .and. (.not. os_data%use_testfiles)) then
    file = os_data%whizard_modelpath_local // "/" // filename
    inquire (file = char (file), exist = model_exist)
end if
if (.not. model_exist) then
    file = os_data%whizard_modelpath // "/" // filename
    inquire (file = char (file), exist = model_exist)
end if
if (ufo_model .and. rebuild) then
    file = filename
    call model_generate_ufo (filename, os_data, model%ufo_path, &
        ufo_path_requested=ufo_path_requested)
    inquire (file = char (file), exist = model_exist)
end if
if (.not. model_exist) then
    call msg_fatal ("Model file '" // char (filename) // "' not found")
    if (present (exist)) exist = .false.
    return
end if
if (present (exist)) exist = .true.

if (logging) call msg_message ("Reading model file '" // char (file) // "'")

unit = free_unit ()
open (file=char(file), unit=unit, action="read", status="old")
model_md5sum = md5sum (unit)
close (unit)

```

```

call lexer_init_model_file (lexer)
call stream_init (stream, char (file))
call lexer_assign_stream (lexer, stream)
call parse_tree_init (model%parse_tree, syntax_model_file, lexer)
call stream_final (stream)
call lexer_final (lexer)

nd_model_def => model%parse_tree%get_root_ptr ()
nd_model_name_def => parse_node_get_sub_ptr (nd_model_def)
model_name = parse_node_get_string &
    (parse_node_get_sub_ptr (nd_model_name_def, 2))
nd_schemes => nd_model_name_def%get_next_ptr ()

call find_block &
    ("scheme_header", nd_schemes, nd_scheme_decl, nd_next=nd_parameters)
call find_block &
    ("parameters", nd_parameters, nd_par_def, n_parblock, nd_external_pars)
call find_block &
    ("external_pars", nd_external_pars, nd_ext_def, n_ext, nd_particles)
call find_block &
    ("particles", nd_particles, nd_prt, n_prt, nd_vertices)
call find_block &
    ("vertices", nd_vertices, nd_vtx, n_vtx)

if (associated (nd_external_pars)) then
    lib_name = "external." // model_name
else
    lib_name = ""
end if

if (associated (nd_scheme_decl)) then
    call handle_schemes (nd_scheme_decl, scheme)
end if

n_par = 0
call count_parameters (nd_par_def, n_parblock, n_par)

call model%init &
    (model_name, lib_name, os_data, n_par + n_ext, n_prt, n_vtx, ufo)
model%md5sum = model_md5sum

if (associated (nd_par_def)) then
    i_par = 0
    call handle_parameters (nd_par_def, n_parblock, i_par)
end if
if (associated (nd_ext_def)) then
    call handle_external (nd_ext_def, n_par, n_ext)
end if
call model%update_parameters ()
if (associated (nd_prt)) then
    call handle_fields (nd_prt, n_prt)
end if
if (associated (nd_vtx)) then
    call handle_vertices (nd_vtx, n_vtx)

```

```

end if

call model%freeze_vertices ()
call model%append_field_vars ()

contains

subroutine find_block (key, nd, nd_item, n_item, nd_next)
  character(*), intent(in) :: key
  type(parse_node_t), pointer, intent(inout) :: nd
  type(parse_node_t), pointer, intent(out) :: nd_item
  integer, intent(out), optional :: n_item
  type(parse_node_t), pointer, intent(out), optional :: nd_next
  if (associated (nd)) then
    if (nd%get_rule_key () == key) then
      nd_item => nd%get_sub_ptr ()
      if (present (n_item)) n_item = nd%get_n_sub ()
      if (present (nd_next)) nd_next => nd%get_next_ptr ()
    else
      nd_item => null ()
      if (present (n_item)) n_item = 0
      if (present (nd_next)) nd_next => nd
      nd => null ()
    end if
  else
    nd_item => null ()
    if (present (n_item)) n_item = 0
    if (present (nd_next)) nd_next => null ()
  end if
end subroutine find_block

subroutine handle_schemes (nd_scheme_decl, scheme)
  type(parse_node_t), pointer, intent(in) :: nd_scheme_decl
  type(string_t), intent(in), optional :: scheme
  type(parse_node_t), pointer :: nd_list, nd_entry
  type(string_t), dimension(:), allocatable :: schemes
  integer :: i, n_schemes
  nd_list => nd_scheme_decl%get_sub_ptr (3)
  nd_entry => nd_list%get_sub_ptr ()
  n_schemes = nd_list%get_n_sub ()
  allocate (schemes (n_schemes))
  do i = 1, n_schemes
    schemes(i) = nd_entry%get_string ()
    nd_entry => nd_entry%get_next_ptr ()
  end do
  if (present (scheme)) then
    do i = 1, n_schemes
      if (schemes(i) == scheme) goto 10 ! block exit
    end do
    call msg_fatal ("Scheme '" // char (scheme) &
      // "' is not supported by model '" // char (model_name) // "'")
  end if
10 continue
call model%enable_schemes (schemes)

```

```

        call model%set_scheme (scheme)
end subroutine handle_schemes

subroutine select_scheme (nd_scheme_block, n_parblock_sub, nd_par_def)
    type(parse_node_t), pointer, intent(in) :: nd_scheme_block
    integer, intent(out) :: n_parblock_sub
    type(parse_node_t), pointer, intent(out) :: nd_par_def
    type(parse_node_t), pointer :: nd_scheme_body
    type(parse_node_t), pointer :: nd_scheme_case, nd_scheme_id, nd_scheme
    type(string_t) :: scheme
    integer :: n_cases, i
    scheme = model%get_scheme ()
    nd_scheme_body => nd_scheme_block%get_sub_ptr (2)
    nd_parameters => null ()
    select case (char (nd_scheme_body%get_rule_key ()))
    case ("scheme_block_body")
        n_cases = nd_scheme_body%get_n_sub ()
        FIND_SCHEME: do i = 1, n_cases
            nd_scheme_case => nd_scheme_body%get_sub_ptr (i)
            nd_scheme_id => nd_scheme_case%get_sub_ptr (2)
            select case (char (nd_scheme_id%get_rule_key ()))
            case ("scheme_list")
                nd_scheme => nd_scheme_id%get_sub_ptr ()
                do while (associated (nd_scheme))
                    if (scheme == nd_scheme%get_string ()) then
                        nd_parameters => nd_scheme_id%get_next_ptr ()
                        exit FIND_SCHEME
                    end if
                    nd_scheme => nd_scheme%get_next_ptr ()
                end do
            case ("other")
                nd_parameters => nd_scheme_id%get_next_ptr ()
                exit FIND_SCHEME
            case default
                print *, "'", char (nd_scheme_id%get_rule_key ()), "'"
                call msg_bug ("Model read: impossible scheme rule")
            end select
        end do FIND_SCHEME
    end select
    if (associated (nd_parameters)) then
        select case (char (nd_parameters%get_rule_key ()))
        case ("parameters")
            n_parblock_sub = nd_parameters%get_n_sub ()
            if (n_parblock_sub > 0) then
                nd_par_def => nd_parameters%get_sub_ptr ()
            else
                nd_par_def => null ()
            end if
        case default
            n_parblock_sub = 0
            nd_par_def => null ()
        end select
    else
        n_parblock_sub = 0
    end if
end subroutine

```



```

        nd_par_def => null ()
    end if
end subroutine select_scheme

recursive subroutine count_parameters (nd_par_def_in, n_parblock, n_par)
    type(parse_node_t), pointer, intent(in) :: nd_par_def_in
    integer, intent(in) :: n_parblock
    integer, intent(inout) :: n_par
    type(parse_node_t), pointer :: nd_par_def, nd_par_key
    type(parse_node_t), pointer :: nd_par_def_sub
    integer :: n_parblock_sub
    integer :: i
    nd_par_def => nd_par_def_in
    do i = 1, n_parblock
        nd_par_key => nd_par_def%get_sub_ptr ()
        select case (char (nd_par_key%get_rule_key ()))
            case ("parameter", "derived", "unused")
                n_par = n_par + 1
            case ("scheme_block_beg")
                call select_scheme (nd_par_def, n_parblock_sub, nd_par_def_sub)
                if (n_parblock_sub > 0) then
                    call count_parameters (nd_par_def_sub, n_parblock_sub, n_par)
                end if
            case default
                print *, "'", char (nd_par_key%get_rule_key ()), "'"
                call msg_bug ("Model read: impossible parameter rule")
            end select
        nd_par_def => parse_node_get_next_ptr (nd_par_def)
    end do
end subroutine count_parameters

recursive subroutine handle_parameters (nd_par_def_in, n_parblock, i_par)
    type(parse_node_t), pointer, intent(in) :: nd_par_def_in
    integer, intent(in) :: n_parblock
    integer, intent(inout) :: i_par
    type(parse_node_t), pointer :: nd_par_def, nd_par_key
    type(parse_node_t), pointer :: nd_par_def_sub
    integer :: n_parblock_sub
    integer :: i
    nd_par_def => nd_par_def_in
    do i = 1, n_parblock
        nd_par_key => nd_par_def%get_sub_ptr ()
        select case (char (nd_par_key%get_rule_key ()))
            case ("parameter")
                i_par = i_par + 1
                call model%read_parameter (i_par, nd_par_def)
            case ("derived")
                i_par = i_par + 1
                call model%read_derived (i_par, nd_par_def)
            case ("unused")
                i_par = i_par + 1
                call model%read_unused (i_par, nd_par_def)
            case ("scheme_block_beg")
                call select_scheme (nd_par_def, n_parblock_sub, nd_par_def_sub)
        end select
    end do
end subroutine handle_parameters

```

```

        if (n_parblock_sub > 0) then
            call handle_parameters (nd_par_def_sub, n_parblock_sub, i_par)
        end if
    end select
    nd_par_def => parse_node_get_next_ptr (nd_par_def)
end do
end subroutine handle_parameters

subroutine handle_external (nd_ext_def, n_par, n_ext)
    type(parse_node_t), pointer, intent(inout) :: nd_ext_def
    integer, intent(in) :: n_par, n_ext
    integer :: i
    do i = n_par + 1, n_par + n_ext
        call model%read_external (i, nd_ext_def)
        nd_ext_def => parse_node_get_next_ptr (nd_ext_def)
    end do
!   real(c_default_float), dimension(:), allocatable :: par
!   if (associated (model%init_external_parameters)) then
!       allocate (par (model%get_n_real ()))
!       call model%real_parameters_to_c_array (par)
!       call model%init_external_parameters (par)
!       call model%real_parameters_from_c_array (par)
!   end if
end subroutine handle_external

subroutine handle_fields (nd_prt, n_prt)
    type(parse_node_t), pointer, intent(inout) :: nd_prt
    integer, intent(in) :: n_prt
    integer :: i
    do i = 1, n_prt
        call model%read_field (i, nd_prt)
        nd_prt => parse_node_get_next_ptr (nd_prt)
    end do
end subroutine handle_fields

subroutine handle_vertices (nd_vtx, n_vtx)
    type(parse_node_t), pointer, intent(inout) :: nd_vtx
    integer, intent(in) :: n_vtx
    integer :: i
    do i = 1, n_vtx
        call model%read_vertex (i, nd_vtx)
        nd_vtx => parse_node_get_next_ptr (nd_vtx)
    end do
end subroutine handle_vertices

end subroutine model_read

```

Parameters are real values (literal) with an optional unit.

<Models: model: TBP>+≡

```
    procedure, private :: read_parameter => model_read_parameter
```

<Models: procedures>+≡

```
    subroutine model_read_parameter (model, i, node)
        class(model_t), intent(inout), target :: model

```

```

integer, intent(in) :: i
type(parse_node_t), intent(in), target :: node
type(parse_node_t), pointer :: node_name, node_val, node_slha_entry
type(string_t) :: name
node_name => parse_node_get_sub_ptr (node, 2)
name = parse_node_get_string (node_name)
node_val => parse_node_get_next_ptr (node_name, 2)
call model%set_parameter_parse_node (i, name, node_val, constant=.true.)
node_slha_entry => parse_node_get_next_ptr (node_val)
if (associated (node_slha_entry)) then
    call model_record_slha_block_entry (model, i, node_slha_entry)
end if
end subroutine model_read_parameter

```

Derived parameters have any numeric expression as their definition. Don't evaluate the expression, yet.

```

<Models: model: TBP>+≡
    procedure, private :: read_derived => model_read_derived

<Models: procedures>+≡
    subroutine model_read_derived (model, i, node)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(parse_node_t), intent(in), target :: node
        type(string_t) :: name
        type(parse_node_t), pointer :: pn_expr
        name = parse_node_get_string (parse_node_get_sub_ptr (node, 2))
        pn_expr => parse_node_get_sub_ptr (node, 4)
        call model%set_parameter_parse_node (i, name, pn_expr, constant=.false.)
    end subroutine model_read_derived

```

External parameters have no definition; they are handled by an external library.

```

<Models: model: TBP>+≡
    procedure, private :: read_external => model_read_external

<Models: procedures>+≡
    subroutine model_read_external (model, i, node)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i
        type(parse_node_t), intent(in), target :: node
        type(string_t) :: name
        name = parse_node_get_string (parse_node_get_sub_ptr (node, 2))
        call model%set_parameter_external (i, name)
    end subroutine model_read_external

```

Ditto for unused parameters, they are there just for reserving the name.

```

<Models: model: TBP>+≡
    procedure, private :: read_unused => model_read_unused

<Models: procedures>+≡
    subroutine model_read_unused (model, i, node)
        class(model_t), intent(inout), target :: model
        integer, intent(in) :: i

```

```

type(parse_node_t), intent(in), target :: node
type(string_t) :: name
name = parse_node_get_string (parse_node_get_sub_ptr (node, 2))
call model%set_parameter_unused (i, name)
end subroutine model_read_unused

```

<Models: model: TBP>+≡

```

procedure, private :: read_field => model_read_field

```

<Models: procedures>+≡

```

subroutine model_read_field (model, i, node)
class(model_t), intent(inout), target :: model
integer, intent(in) :: i
type(parse_node_t), intent(in) :: node
type(parse_node_t), pointer :: nd_src, nd_props, nd_prop
type(string_t) :: longname
integer :: pdg
type(string_t) :: name_src
type(string_t), dimension(:), allocatable :: name
type(field_data_t), pointer :: field, field_src
longname = parse_node_get_string (parse_node_get_sub_ptr (node, 2))
pdg = read_frac (parse_node_get_sub_ptr (node, 3))
field => model%get_field_ptr_by_index (i)
call field%init (longname, pdg)
nd_src => parse_node_get_sub_ptr (node, 4)
if (associated (nd_src)) then
  if (parse_node_get_rule_key (nd_src) == "prt_src") then
    name_src = parse_node_get_string (parse_node_get_sub_ptr (nd_src, 2))
    field_src => model%get_field_ptr (name_src, check=.true.)
    call field%copy_from (field_src)
    nd_props => parse_node_get_sub_ptr (nd_src, 3)
  else
    nd_props => nd_src
  end if
nd_prop => parse_node_get_sub_ptr (nd_props)
do while (associated (nd_prop))
  select case (char (parse_node_get_rule_key (nd_prop)))
  case ("invisible")
    call field%set (is_visible=.false.)
  case ("parton")
    call field%set (is_parton=.true.)
  case ("gauge")
    call field%set (is_gauge=.true.)
  case ("left")
    call field%set (is_left_handed=.true.)
  case ("right")
    call field%set (is_right_handed=.true.)
  case ("prt_name")
    call read_names (nd_prop, name)
    call field%set (name=name)
  case ("prt_anti")
    call read_names (nd_prop, name)
    call field%set (anti=name)
  case ("prt_tex_name")

```

```

        call field%set ( &
            tex_name = parse_node_get_string &
            (parse_node_get_sub_ptr (nd_prop, 2)))
    case ("prt_tex_anti")
        call field%set ( &
            tex_anti = parse_node_get_string &
            (parse_node_get_sub_ptr (nd_prop, 2)))
    case ("prt_spin")
        call field%set ( &
            spin_type = read_frac &
            (parse_node_get_sub_ptr (nd_prop, 2), 2))
    case ("prt_isospin")
        call field%set ( &
            isospin_type = read_frac &
            (parse_node_get_sub_ptr (nd_prop, 2), 2))
    case ("prt_charge")
        call field%set ( &
            charge_type = read_frac &
            (parse_node_get_sub_ptr (nd_prop, 2), 3))
    case ("prt_color")
        call field%set ( &
            color_type = parse_node_get_integer &
            (parse_node_get_sub_ptr (nd_prop, 2)))
    case ("prt_mass")
        call field%set ( &
            mass_data = model%get_par_data_ptr &
            (parse_node_get_string &
            (parse_node_get_sub_ptr (nd_prop, 2))))
    case ("prt_width")
        call field%set ( &
            width_data = model%get_par_data_ptr &
            (parse_node_get_string &
            (parse_node_get_sub_ptr (nd_prop, 2))))
    case default
        call msg_bug (" Unknown particle property '" &
            // char (parse_node_get_rule_key (nd_prop)) // "'")
    end select
    if (allocated (name)) deallocate (name)
    nd_prop => parse_node_get_next_ptr (nd_prop)
end do
end if
call field%freeze ()
end subroutine model_read_field

```

<Models: model: TBP>+≡

```

    procedure, private :: read_vertex => model_read_vertex

```

<Models: procedures>+≡

```

    subroutine model_read_vertex (model, i, node)
        class(model_t), intent(inout) :: model
        integer, intent(in) :: i
        type(parse_node_t), intent(in) :: node
        type(string_t), dimension(:), allocatable :: name
        call read_names (node, name)
    end subroutine

```

```

        call model%set_vertex (i, name)
    end subroutine model_read_vertex

```

(Models: procedures)+≡

```

subroutine read_names (node, name)
    type(parse_node_t), intent(in) :: node
    type(string_t), dimension(:), allocatable, intent(inout) :: name
    type(parse_node_t), pointer :: nd_name
    integer :: n_names, i
    n_names = parse_node_get_n_sub (node) - 1
    allocate (name (n_names))
    nd_name => parse_node_get_sub_ptr (node, 2)
    do i = 1, n_names
        name(i) = parse_node_get_string (nd_name)
        nd_name => parse_node_get_next_ptr (nd_name)
    end do
end subroutine read_names

```

There is an optional argument for the base.

(Models: procedures)+≡

```

function read_frac (nd_frac, base) result (qn_type)
    integer :: qn_type
    type(parse_node_t), intent(in) :: nd_frac
    integer, intent(in), optional :: base
    type(parse_node_t), pointer :: nd_num, nd_den
    integer :: num, den
    nd_num => parse_node_get_sub_ptr (nd_frac)
    nd_den => parse_node_get_next_ptr (nd_num)
    select case (char (parse_node_get_rule_key (nd_num)))
    case ("integer_literal")
        num = parse_node_get_integer (nd_num)
    case ("neg_int")
        num = - parse_node_get_integer (parse_node_get_sub_ptr (nd_num, 2))
    case ("pos_int")
        num = parse_node_get_integer (parse_node_get_sub_ptr (nd_num, 2))
    case default
        call parse_tree_bug (nd_num, "int|neg_int|pos_int")
    end select
    if (associated (nd_den)) then
        den = parse_node_get_integer (parse_node_get_sub_ptr (nd_den, 2))
    else
        den = 1
    end if
    if (present (base)) then
        if (den == 1) then
            qn_type = sign (1 + abs (num) * base, num)
        else if (den == base) then
            qn_type = sign (abs (num) + 1, num)
        else
            call parse_node_write_rec (nd_frac)
            call msg_fatal (" Fractional quantum number: wrong denominator")
        end if
    else

```

```

        if (den == 1) then
            qn_type = num
        else
            call parse_node_write_rec (nd_frac)
            call msg_fatal (" Wrong type: no fraction expected")
        end if
    end if
end if
end function read_frac

```

Append field (PDG-array) variables to the variable list, based on the field content.

(Models: model: TBP)+≡

```

    procedure, private :: append_field_vars => model_append_field_vars

```

(Models: procedures)+≡

```

subroutine model_append_field_vars (model)
    class(model_t), intent(inout) :: model
    type(pdg_array_t) :: aval
    type(field_data_t), dimension(:), pointer :: field_array
    type(field_data_t), pointer :: field
    type(string_t) :: name
    type(string_t), dimension(:), allocatable :: name_array
    integer, dimension(:), allocatable :: pdg
    logical, dimension(:), allocatable :: mask
    integer :: i, j
    field_array => model%get_field_array_ptr ()
    aval = UNDEFINED
    call var_list_append_pdg_array &
        (model%var_list, var_str ("particle"), &
            aval, locked = .true., intrinsic=.true.)
    do i = 1, size (field_array)
        aval = field_array(i)%get_pdg ()
        name = field_array(i)%get_longname ()
        call var_list_append_pdg_array &
            (model%var_list, name, aval, locked=.true., intrinsic=.true.)
        call field_array(i)%get_name_array (.false., name_array)
        do j = 1, size (name_array)
            call var_list_append_pdg_array &
                (model%var_list, name_array(j), &
                    aval, locked=.true., intrinsic=.true.)
        end do
        model%max_field_name_length = &
            max (model%max_field_name_length, len (name_array(1)))
        aval = - field_array(i)%get_pdg ()
        call field_array(i)%get_name_array (.true., name_array)
        do j = 1, size (name_array)
            call var_list_append_pdg_array &
                (model%var_list, name_array(j), &
                    aval, locked=.true., intrinsic=.true.)
        end do
    end do
    if (size (name_array) > 0) then
        model%max_field_name_length = &
            max (model%max_field_name_length, len (name_array(1)))
    end if
end if

```

```

end do
call model%get_all_pdg (pdg)
allocate (mask (size (pdg)))
do i = 1, size (pdg)
    field => model%get_field_ptr (pdg(i))
    mask(i) = field%get_charge_type () /= 1
end do
aval = pack (pdg, mask)
call var_list_append_pdg_array &
    (model%var_list, var_str ("charged"), &
    aval, locked = .true., intrinsic=.true.)
do i = 1, size (pdg)
    field => model%get_field_ptr (pdg(i))
    mask(i) = field%get_charge_type () == 1
end do
aval = pack (pdg, mask)
call var_list_append_pdg_array &
    (model%var_list, var_str ("neutral"), &
    aval, locked = .true., intrinsic=.true.)
do i = 1, size (pdg)
    field => model%get_field_ptr (pdg(i))
    mask(i) = field%get_color_type () /= 1
end do
aval = pack (pdg, mask)
call var_list_append_pdg_array &
    (model%var_list, var_str ("colored"), &
    aval, locked = .true., intrinsic=.true.)
end subroutine model_append_field_vars

```

28.4.10 Test models

(Models: public)+≡

```
public :: create_test_model
```

(Models: procedures)+≡

```

subroutine create_test_model (model_name, test_model)
    type(string_t), intent(in) :: model_name
    type(model_t), intent(out), pointer :: test_model
    type(os_data_t) :: os_data
    type(model_list_t):: model_list
    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
        (model_name, model_name // var_str (".mdl"), os_data, test_model)
end subroutine create_test_model

```

28.4.11 Model list

List of currently active models

(Models: types)+≡

```
type, extends (model_t) :: model_entry_t
```



```

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

    <Models: public>+≡
        public :: model_list_t
    <Models: types>+≡
        type :: model_list_t
            type(model_entry_t), pointer :: first => null ()
            type(model_entry_t), pointer :: last => null ()
            type(model_list_t), pointer :: context => null ()
        contains
            <Models: model list: TBP>
        end type model_list_t

```

Write an account of the model list. We write linked lists first, starting from the global context.

```

    <Models: model list: TBP>≡
        procedure :: write => model_list_write

    <Models: procedures>+≡
        recursive subroutine model_list_write (object, unit, verbose, follow_link)
            class(model_list_t), intent(in) :: object
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: verbose
            logical, intent(in), optional :: follow_link
            type(model_entry_t), pointer :: current
            logical :: rec
            integer :: u
            u = given_output_unit (unit); if (u < 0) return
            rec = .true.; if (present (follow_link)) rec = follow_link
            if (rec .and. associated (object%context)) then
                call object%context%write (unit, verbose, follow_link)
            end if
            current => object%first
            if (associated (current)) then
                do while (associated (current))
                    call current%write (unit, verbose)
                    current => current%next
                    if (associated (current)) write (u, *)
                end do
            end if
        end subroutine model_list_write

```

Link this list to another one.

```

    <Models: model list: TBP>+≡
        procedure :: link => model_list_link

    <Models: procedures>+≡
        subroutine model_list_link (model_list, context)
            class(model_list_t), intent(inout) :: model_list
            type(model_list_t), intent(in), target :: context
            model_list%context => context
        end subroutine model_list_link

```

(Private, used below:) Append an existing model, for which we have allocated a pointer entry, to the model list. The original pointer becomes disassociated, and the model should now be considered as part of the list. We assume that this model is not yet part of the list.

If we provide a `model` argument, this returns a pointer to the new entry.

```

<Models: model list: TBP>+≡
  procedure, private :: import => model_list_import

<Models: procedures>+≡
  subroutine model_list_import (model_list, current, model)
    class(model_list_t), intent(inout) :: model_list
    type(model_entry_t), pointer, intent(inout) :: current
    type(model_t), optional, pointer, intent(out) :: model
    if (associated (current)) then
      if (associated (model_list%first)) then
        model_list%last%next => current
      else
        model_list%first => current
      end if
      model_list%last => current
      if (present (model)) model => current%model_t
      current => null ()
    end if
  end subroutine model_list_import

```

Currently test only:

Add a new model with given `name` to the list, if it does not yet exist. If successful, return a pointer to the new model.

```

<Models: model list: TBP>+≡
  procedure :: add => model_list_add

<Models: procedures>+≡
  subroutine model_list_add (model_list, &
    name, os_data, n_par, n_prt, n_vtx, model)
    class(model_list_t), intent(inout) :: model_list
    type(string_t), intent(in) :: name
    type(os_data_t), intent(in) :: os_data
    integer, intent(in) :: n_par, n_prt, n_vtx
    type(model_t), pointer :: model
    type(model_entry_t), pointer :: current
    if (model_list%model_exists (name, follow_link=.false.)) then
      model => null ()
    else
      allocate (current)
      call current%init (name, var_str (""), os_data, &
        n_par, n_prt, n_vtx)
      call model_list%import (current, model)
    end if
  end subroutine model_list_add

```

Read a new model from file and add to the list, if it does not yet exist. Finalize the model by allocating the vertex table. Return a pointer to the new model. If unsuccessful, return the original pointer.

The model is always inserted in the last link of a chain of model lists. This way, we avoid loading models twice from different contexts. When a model is modified, we should first allocate a local copy.

```

<Models: model list: TBP>+≡
  procedure :: read_model => model_list_read_model

<Models: procedures>+≡
  subroutine model_list_read_model &
    (model_list, name, filename, os_data, model, &
     scheme, ufo, ufo_path, rebuild_mdl)
    class(model_list_t), intent(inout), target :: model_list
    type(string_t), intent(in) :: name, filename
    type(os_data_t), intent(in) :: os_data
    type(model_t), pointer, intent(inout) :: model
    type(string_t), intent(in), optional :: scheme
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path
    logical, intent(in), optional :: rebuild_mdl
    class(model_list_t), pointer :: global_model_list
    type(model_entry_t), pointer :: current
    logical :: exist
    if (.not. model_list%model_exists (name, &
     scheme, ufo, ufo_path, follow_link=.true.)) then
      allocate (current)
      call current%read (filename, os_data, exist, &
       scheme=scheme, ufo=ufo, ufo_path_requested=ufo_path, &
       rebuild_mdl=rebuild_mdl)
      if (.not. exist) return
      if (current%get_name () /= name) then
        call msg_fatal ("Model file '" // char (filename) // &
         "' contains model '" // char (current%get_name ()) // &
         "' instead of '" // char (name) // "'")
        call current%final (); deallocate (current)
        return
      end if
      global_model_list => model_list
      do while (associated (global_model_list%context))
        global_model_list => global_model_list%context
      end do
      call global_model_list%import (current, model)
    else
      model => model_list%get_model_ptr (name, scheme, ufo, ufo_path)
    end if
  end subroutine model_list_read_model

```

Append a copy of an existing model to a model list. Optionally, return pointer to the new entry.

```

<Models: model list: TBP>+≡
  procedure :: append_copy => model_list_append_copy

<Models: procedures>+≡
  subroutine model_list_append_copy (model_list, orig, model)
    class(model_list_t), intent(inout) :: model_list
    type(model_t), intent(in), target :: orig

```

```

    type(model_t), intent(out), pointer, optional :: model
    type(model_entry_t), pointer :: copy
    allocate (copy)
    call copy%init_instance (orig)
    call model_list%import (copy, model)
end subroutine model_list_append_copy

```

Check if a model exists by examining the list. Check recursively unless told otherwise.

```

<Models: model list: TBP>+≡
    procedure :: model_exists => model_list_model_exists

<Models: procedures>+≡
    recursive function model_list_model_exists &
        (model_list, name, scheme, ufo, ufo_path, follow_link) result (exists)
    class(model_list_t), intent(in) :: model_list
    logical :: exists
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: scheme
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path
    logical, intent(in), optional :: follow_link
    type(model_entry_t), pointer :: current
    logical :: rec
    rec = .true.; if (present (follow_link)) rec = follow_link
    current => model_list%first
    do while (associated (current))
        if (current%matches (name, scheme, ufo, ufo_path)) then
            exists = .true.
            return
        end if
        current => current%next
    end do
    if (rec .and. associated (model_list%context)) then
        exists = model_list%context%model_exists (name, &
            scheme, ufo, ufo_path, follow_link)
    else
        exists = .false.
    end if
end function model_list_model_exists

```

Return a pointer to a named model. Search recursively unless told otherwise.

```

<Models: model list: TBP>+≡
    procedure :: get_model_ptr => model_list_get_model_ptr

<Models: procedures>+≡
    recursive function model_list_get_model_ptr &
        (model_list, name, scheme, ufo, ufo_path, follow_link) result (model)
    class(model_list_t), intent(in) :: model_list
    type(model_t), pointer :: model
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: scheme
    logical, intent(in), optional :: ufo
    type(string_t), intent(in), optional :: ufo_path

```

```

logical, intent(in), optional :: follow_link
type(model_entry_t), pointer :: current
logical :: rec
rec = .true.; if (present (follow_link)) rec = follow_link
current => model_list%first
do while (associated (current))
    if (current%matches (name, scheme, ufo, ufo_path)) then
        model => current%model_t
        return
    end if
    current => current%next
end do
if (rec .and. associated (model_list%context)) then
    model => model_list%context%get_model_ptr (name, &
        scheme, ufo, ufo_path, follow_link)
else
    model => null ()
end if
end function model_list_get_model_ptr

```

Delete the list of models. No recursion.

```

<Models: model list: TBP>+≡
    procedure :: final => model_list_final

<Models: procedures>+≡
    subroutine model_list_final (model_list)
        class(model_list_t), intent(inout) :: model_list
        type(model_entry_t), pointer :: current
        model_list%last => null ()
        do while (associated (model_list%first))
            current => model_list%first
            model_list%first => model_list%first%next
            call current%final ()
            deallocate (current)
        end do
    end subroutine model_list_final

```

28.4.12 Model instances

A model instance is a copy of a model object. The parameters are true copies. The particle data and the variable list pointers should point to the copy, so modifying the parameters has only a local effect. Hence, we build them up explicitly. The vertex array is also rebuilt, it contains particle pointers. Finally, the vertex hash table can be copied directly since it contains no pointers.

The **multiplicity** entry depends on the association of the **mass_data** entry and therefore has to be set at the end.

The instance must carry the **target** attribute.

Parameters: the **copy_parameter** method essentially copies the parameter decorations (parse node, expression etc.). The current parameter values are part of the **model_data_t** base type and are copied afterwards via its **copy_from** method.

Note: the parameter set is initialized for real parameters only.

In order for the local model to be able to use the correct UFO model setup, UFO model information has to be transferred.

```

<Models: model: TBP>+≡
  procedure :: init_instance => model_copy

<Models: procedures>+≡
  subroutine model_copy (model, orig)
    class(model_t), intent(out), target :: model
    type(model_t), intent(in) :: orig
    integer :: n_par, n_prt, n_vtx
    integer :: i
    n_par = orig%get_n_real ()
    n_prt = orig%get_n_field ()
    n_vtx = orig%get_n_vtx ()
    call model%basic_init (orig%get_name (), n_par, n_prt, n_vtx)
    if (allocated (orig%schemes)) then
      model%schemes = orig%schemes
      if (allocated (orig%selected_scheme)) then
        model%selected_scheme = orig%selected_scheme
        call model%set_scheme_num (orig%get_scheme_num ())
      end if
    end if
    if (allocated (orig%slha_block)) then
      model%slha_block = orig%slha_block
    end if
    model%md5sum = orig%md5sum
    model%ufo_model = orig%ufo_model
    model%ufo_path = orig%ufo_path
    if (allocated (orig%par)) then
      do i = 1, n_par
        call model%copy_parameter (i, orig%par(i))
      end do
    end if
    model%init_external_parameters => orig%init_external_parameters
    call model%model_data_t%copy_from (orig)
    model%max_par_name_length = orig%max_par_name_length
    call model%append_field_vars ()
  end subroutine model_copy

```

28.4.13 Unit tests

Test module, followed by the corresponding implementation module.

```

<models_ut.f90>≡
  <File header>

  module models_ut
    use unit_tests
    use models_util

    <Standard module head>

```

```

    <Models: public test>

contains

    <Models: test driver>

    end module models_ut
<models_uti.f90>≡
    <File header>

    module models_uti

    <Use kinds>
    <Use strings>
        use file_utils, only: delete_file
        use physics_defs, only: SCALAR, SPINOR
        use os_interface
        use model_data
        use variables

        use models

    <Standard module head>

    <Models: test declarations>

contains

    <Models: tests>

    end module models_uti
API: driver for the unit tests below.
<Models: public test>≡
    public :: models_test
<Models: test driver>≡
    subroutine models_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Models: execute tests>
    end subroutine models_test

```

Construct a Model

Here, we construct a toy model explicitly without referring to a file.

```

<Models: execute tests>≡
    call test (models_1, "models_1", &
        "construct model", &
        u, results)
<Models: test declarations>≡
    public :: models_1

```

```

<Models: tests>≡
subroutine models_1 (u)
  integer, intent(in) :: u
  type(os_data_t) :: os_data
  type(model_list_t) :: model_list
  type(model_t), pointer :: model
  type(string_t) :: model_name
  type(string_t) :: x_longname
  type(string_t), dimension(2) :: parname
  type(string_t), dimension(2) :: x_name
  type(string_t), dimension(1) :: x_anti
  type(string_t) :: x_tex_name, x_tex_anti
  type(string_t) :: y_longname
  type(string_t), dimension(2) :: y_name
  type(string_t) :: y_tex_name
  type(field_data_t), pointer :: field

  write (u, "(A)")  "* Test output: models_1"
  write (u, "(A)")  "* Purpose: create a model"
  write (u, *)

  model_name = "Test model"
  call model_list%add (model_name, os_data, 2, 2, 3, model)
  parname(1) = "mx"
  parname(2) = "coup"
  call model%set_parameter_constant (1, parname(1), 10._default)
  call model%set_parameter_constant (2, parname(2), 1.3_default)
  x_longname = "X_LEPTON"
  x_name(1) = "X"
  x_name(2) = "x"
  x_anti(1) = "Xbar"
  x_tex_name = "X^+"
  x_tex_anti = "X^-"
  field => model%get_field_ptr_by_index (1)
  call field%init (x_longname, 99)
  call field%set ( &
    .true., .false., .false., .false., .false., &
    name=x_name, anti=x_anti, tex_name=x_tex_name, tex_anti=x_tex_anti, &
    spin_type=SPINOR, isospin_type=-3, charge_type=2, &
    mass_data=model%get_par_data_ptr (parname(1)))
  y_longname = "Y_COLORON"
  y_name(1) = "Y"
  y_name(2) = "yc"
  y_tex_name = "Y^0"
  field => model%get_field_ptr_by_index (2)
  call field%init (y_longname, 97)
  call field%set ( &
    .false., .false., .true., .false., .false., &
    name=y_name, tex_name=y_tex_name, &
    spin_type=SCALAR, isospin_type=2, charge_type=1, color_type=8)
  call model%set_vertex (1, [99, 99, 99])
  call model%set_vertex (2, [99, 99, 99, 99])
  call model%set_vertex (3, [99, 97, 99])
  call model_list%write (u)

```



```

call model_list%final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_1"

end subroutine models_1

```

Read a Model

Read a predefined model from file.

```

<Models: execute tests>+≡
call test (models_2, "models_2", &
    "read model", &
    u, results)

<Models: test declarations>+≡
public :: models_2

<Models: tests>+≡
subroutine models_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(var_list_t), pointer :: var_list
    type(model_t), pointer :: model

    write (u, "(A)")  "* Test output: models_2"
    write (u, "(A)")  "* Purpose: read a model from file"
    write (u, *)

    call syntax_model_file_init ()
    call os_data%init ()

    call model_list%read_model (var_str ("Test"), var_str ("Test.mdl"), &
        os_data, model)
    call model_list%write (u)

    write (u, *)
    write (u, "(A)")  "* Variable list"
    write (u, *)

    var_list => model%get_var_list_ptr ()
    call var_list%write (u)

    write (u, *)
    write (u, "(A)")  "* Cleanup"

    call model_list%final ()
    call syntax_model_file_final ()

    write (u, *)
    write (u, "(A)")  "* Test output end: models_2"

```

```
end subroutine models_2
```

Model Instance

Read a predefined model from file and create an instance.

```

<Models: execute tests>+≡
  call test (models_3, "models_3", &
    "model instance", &
    u, results)

<Models: test declarations>+≡
  public :: models_3

<Models: tests>+≡
  subroutine models_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(var_list_t), pointer :: var_list
    type(model_t), pointer :: instance

    write (u, "(A)")  "* Test output: models_3"
    write (u, "(A)")  "* Purpose: create a model instance"
    write (u, *)

    call syntax_model_file_init ()
    call os_data%init ()

    call model_list%read_model (var_str ("Test"), var_str ("Test.mdl"), &
      os_data, model)
    allocate (instance)
    call instance%init_instance (model)

    call model%write (u)

    write (u, *)
    write (u, "(A)")  "* Variable list"
    write (u, *)

    var_list => instance%get_var_list_ptr ()
    call var_list%write (u)

    write (u, *)
    write (u, "(A)")  "* Cleanup"

    call instance%final ()
    deallocate (instance)

    call model_list%final ()
    call syntax_model_file_final ()

    write (u, *)
    write (u, "(A)")  "* Test output end: models_3"

```

```
end subroutine models_3
```

Unstable and Polarized Particles

Read a predefined model from file and define decays and polarization.

```

<Models: execute tests>+≡
  call test (models_4, "models_4", &
    "handle decays and polarization", &
    u, results)

<Models: test declarations>+≡
  public :: models_4

<Models: tests>+≡
  subroutine models_4 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model, model_instance
    character(32) :: md5sum

    write (u, "(A)")  "* Test output: models_4"
    write (u, "(A)")  "* Purpose: set and unset decays and polarization"
    write (u, *)

    call syntax_model_file_init ()
    call os_data%init ()

    write (u, "(A)")  "* Read model from file"

    call model_list%read_model (var_str ("Test"), var_str ("Test.mdl"), &
      os_data, model)

    md5sum = model%get_parameters_md5sum ()
    write (u, *)
    write (u, "(1x,3A)")  "MD5 sum (parameters) = '", md5sum, "'"

    write (u, *)
    write (u, "(A)")  "* Set particle decays and polarization"
    write (u, *)

    call model%set_unstable (25, [var_str ("dec1"), var_str ("dec2")])
    call model%set_polarized (6)
    call model%set_unstable (-6, [var_str ("fdec")])

    call model%write (u)

    md5sum = model%get_parameters_md5sum ()
    write (u, *)
    write (u, "(1x,3A)")  "MD5 sum (parameters) = '", md5sum, "'"

    write (u, *)
    write (u, "(A)")  "* Create a model instance"

```

```

allocate (model_instance)
call model_instance%init_instance (model)

write (u, *)
write (u, "(A)")  "* Revert particle decays and polarization"
write (u, *)

call model%set_stable (25)
call model%set_unpolarized (6)
call model%set_stable (-6)

call model%write (u)

md5sum = model%get_parameters_md5sum ()
write (u, *)
write (u, "(1x,3A)")  "MD5 sum (parameters) = '", md5sum, "'"

write (u, *)
write (u, "(A)")  "* Show the model instance"
write (u, *)

call model_instance%write (u)

md5sum = model_instance%get_parameters_md5sum ()
write (u, *)
write (u, "(1x,3A)")  "MD5 sum (parameters) = '", md5sum, "'"

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_instance%final ()
deallocate (model_instance)
call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_4"

end subroutine models_4

```

Model Variables

Read a predefined model from file and modify some parameters.

Note that the MD5 sum is not modified by this.

```

<Models: execute tests>+≡
  call test (models_5, "models_5", &
    "handle parameters", &
    u, results)

<Models: test declarations>+≡
  public :: models_5

```

```

<Models: tests>+≡
subroutine models_5 (u)
  integer, intent(in) :: u
  type(os_data_t) :: os_data
  type(model_list_t) :: model_list
  type(model_t), pointer :: model, model_instance
  character(32) :: md5sum

  write (u, "(A)")  "* Test output: models_5"
  write (u, "(A)")  "* Purpose: access and modify model variables"
  write (u, *)

  call syntax_model_file_init ()
  call os_data%init ()

  write (u, "(A)")  "* Read model from file"

  call model_list%read_model (var_str ("Test"), var_str ("Test.mdl"), &
    os_data, model)

  write (u, *)

  call model%write (u, &
    show_md5sum = .true., &
    show_variables = .true., &
    show_parameters = .true., &
    show_particles = .false., &
    show_vertices = .false.)

  write (u, *)
  write (u, "(A)")  "* Check parameter status"
  write (u, *)

  write (u, "(1x,A,L1)") "xy exists = ", model%var_exists (var_str ("xx"))
  write (u, "(1x,A,L1)") "ff exists = ", model%var_exists (var_str ("ff"))
  write (u, "(1x,A,L1)") "mf exists = ", model%var_exists (var_str ("mf"))
  write (u, "(1x,A,L1)") "ff locked = ", model%var_is_locked (var_str ("ff"))
  write (u, "(1x,A,L1)") "mf locked = ", model%var_is_locked (var_str ("mf"))

  write (u, *)
  write (u, "(1x,A,F6.2)") "ff = ", model%get_rval (var_str ("ff"))
  write (u, "(1x,A,F6.2)") "mf = ", model%get_rval (var_str ("mf"))

  write (u, *)
  write (u, "(A)")  "* Modify parameter"
  write (u, *)

  call model%set_real (var_str ("ff"), 1._default)

  call model%write (u, &
    show_md5sum = .true., &
    show_variables = .true., &
    show_parameters = .true., &
    show_particles = .false., &

```

```

        show_vertices = .false.)

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_5"

end subroutine models_5

```

Read model with disordered parameters

Read a model from file where the ordering of independent and derived parameters is non-canonical.

```

<Models: execute tests>+≡
    call test (models_6, "models_6", &
        "read model parameters", &
        u, results)

<Models: test declarations>+≡
    public :: models_6

<Models: tests>+≡
    subroutine models_6 (u)
        integer, intent(in) :: u
        integer :: um
        character(80) :: buffer
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(var_list_t), pointer :: var_list
        type(model_t), pointer :: model

        write (u, "(A)")  "* Test output: models_6"
        write (u, "(A)")  "* Purpose: read a model from file &
            &with non-canonical parameter ordering"
        write (u, *)

        open (newunit=um, file="Test6.mdl", status="replace", action="readwrite")
        write (um, "(A)")  'model "Test6"'
        write (um, "(A)")  ' parameter a = 1.0000000000000E+00'
        write (um, "(A)")  ' derived b = 2 * a'
        write (um, "(A)")  ' parameter c = 3.0000000000000E+00'
        write (um, "(A)")  ' unused d'

        rewind (um)
        do
            read (um, "(A)", end=1) buffer
            write (u, "(A)") trim (buffer)
        end do
1    continue

```

```

close (um)

call syntax_model_file_init ()
call os_data%init ()

call model_list%read_model (var_str ("Test6"), var_str ("Test6.mdl"), &
    os_data, model)

write (u, *)
write (u, "(A)")  "* Variable list"
write (u, *)

var_list => model%get_var_list_ptr ()
call var_list%write (u)

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_6"

end subroutine models_6

```

Read model with schemes

Read a model from file which supports scheme selection in the parameter list.

```

<Models: execute tests>+≡
    call test (models_7, "models_7", &
        "handle schemes", &
        u, results)

<Models: test declarations>+≡
    public :: models_7

<Models: tests>+≡
    subroutine models_7 (u)
        integer, intent(in) :: u
        integer :: um
        character(80) :: buffer
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(var_list_t), pointer :: var_list
        type(model_t), pointer :: model

        write (u, "(A)")  "* Test output: models_7"
        write (u, "(A)")  "* Purpose: read a model from file &
            &with scheme selection"
        write (u, *)

        open (newunit=um, file="Test7.mdl", status="replace", action="readwrite")
        write (um, "(A)")  'model "Test7"'

```

```

write (um, "(A)" ) ' schemes = "foo", "bar", "gee"'
write (um, "(A)" ) ''
write (um, "(A)" ) ' select scheme'
write (um, "(A)" ) ' scheme "foo"'
write (um, "(A)" ) ' parameter a = 1'
write (um, "(A)" ) ' derived b = 2 * a'
write (um, "(A)" ) ' scheme other'
write (um, "(A)" ) ' parameter b = 4'
write (um, "(A)" ) ' derived a = b / 2'
write (um, "(A)" ) ' end select'
write (um, "(A)" ) ''
write (um, "(A)" ) ' parameter c = 3'
write (um, "(A)" ) ''
write (um, "(A)" ) ' select scheme'
write (um, "(A)" ) ' scheme "foo", "gee"'
write (um, "(A)" ) ' derived d = b + c'
write (um, "(A)" ) ' scheme other'
write (um, "(A)" ) ' unused d'
write (um, "(A)" ) ' end select'

rewind (um)
do
  read (um, "(A)", end=1) buffer
  write (u, "(A)" ) trim (buffer)
end do
1 continue
close (um)

call syntax_model_file_init ()
call os_data%init ()

write (u, *)
write (u, "(A)" ) "* Model output, default scheme (= foo)"
write (u, *)

call model_list%read_model (var_str ("Test7"), var_str ("Test7.mdl"), &
  os_data, model)
call model%write (u, show_md5sum=.false.)
call show_var_list ()
call show_par_array ()

call model_list%final ()

write (u, *)
write (u, "(A)" ) "* Model output, scheme foo"
write (u, *)

call model_list%read_model (var_str ("Test7"), var_str ("Test7.mdl"), &
  os_data, model, scheme = var_str ("foo"))
call model%write (u, show_md5sum=.false.)
call show_var_list ()
call show_par_array ()

call model_list%final ()

```



```

write (u, *)
write (u, "(A)")  "* Model output, scheme bar"
write (u, *)

call model_list%read_model (var_str ("Test7"), var_str ("Test7.mdl"), &
    os_data, model, scheme = var_str ("bar"))
call model%write (u, show_md5sum=.false.)
call show_var_list ()
call show_par_array ()

call model_list%final ()

write (u, *)
write (u, "(A)")  "* Model output, scheme gee"
write (u, *)

call model_list%read_model (var_str ("Test7"), var_str ("Test7.mdl"), &
    os_data, model, scheme = var_str ("gee"))
call model%write (u, show_md5sum=.false.)
call show_var_list ()
call show_par_array ()

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_7"

contains

subroutine show_var_list ()
    write (u, *)
    write (u, "(A)")  "* Variable list"
    write (u, *)
    var_list => model%get_var_list_ptr ()
    call var_list%write (u)
end subroutine show_var_list

subroutine show_par_array ()
    real(default), dimension(:), allocatable :: par
    integer :: n
    write (u, *)
    write (u, "(A)")  "* Parameter array"
    write (u, *)
    n = model%get_n_real ()
    allocate (par (n))
    call model%real_parameters_to_array (par)
    write (u, 1) par
1   format (1X,F6.3)
end subroutine show_par_array

```

```
end subroutine models_7
```

Read and handle UFO model

Read a model from file which is considered as an UFO model. In fact, it is a mock model file which just follows our naming convention for UFO models. Compare this to an equivalent non-UFO model.

```

<Models: execute tests>+≡
    call test (models_8, "models_8", &
               "handle UFO-derived models", &
               u, results)

<Models: test declarations>+≡
    public :: models_8

<Models: tests>+≡
    subroutine models_8 (u)
        integer, intent(in) :: u
        integer :: um
        character(80) :: buffer
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(string_t) :: model_name
        type(model_t), pointer :: model

        write (u, "(A)")  "* Test output: models_8"
        write (u, "(A)")  "* Purpose: distinguish models marked as UFO-derived"
        write (u, *)

        call os_data%init ()

        call show_model_list_status ()
        model_name = "models_8_M"

        write (u, *)
        write (u, "(A)")  "* Write WHIZARD model"
        write (u, *)

        open (newunit=um, file=char (model_name // ".mdl"), &
              status="replace", action="readwrite")
        write (um, "(A)")  'model "models_8_M"'
        write (um, "(A)")  ' parameter a = 1'

        rewind (um)
        do
            read (um, "(A)", end=1) buffer
            write (u, "(A)") trim (buffer)
        end do
1    continue
        close (um)

        write (u, *)

```

```

write (u, "(A)")  "* Write UFO model"
write (u, *)

open (newunit=um, file=char (model_name // ".ufo.mdl"), &
      status="replace", action="readwrite")
write (um, "(A)")  'model "models_8_M"'
write (um, "(A)")  '  parameter a = 2'

rewind (um)
do
  read (um, "(A)", end=2)  buffer
  write (u, "(A)")  trim (buffer)
end do
2 continue
close (um)

call syntax_model_file_init ()
call os_data%init ()

write (u, *)
write (u, "(A)")  "* Read WHIZARD model"
write (u, *)

call model_list%read_model (model_name, model_name // ".mdl", &
  os_data, model)
call model%write (u, show_md5sum=.false.)

call show_model_list_status ()

write (u, *)
write (u, "(A)")  "* Read UFO model"
write (u, *)

call model_list%read_model (model_name, model_name // ".ufo.mdl", &
  os_data, model, ufo=.true., rebuild_mdl = .false.)
call model%write (u, show_md5sum=.false.)

call show_model_list_status ()

write (u, *)
write (u, "(A)")  "* Reload WHIZARD model"
write (u, *)

call model_list%read_model (model_name, model_name // ".mdl", &
  os_data, model)
call model%write (u, show_md5sum=.false.)

call show_model_list_status ()

write (u, *)
write (u, "(A)")  "* Reload UFO model"
write (u, *)

call model_list%read_model (model_name, model_name // ".ufo.mdl", &

```

```

        os_data, model, ufo=.true., rebuild_mdl = .false.)
call model%write (u, show_md5sum=.false.)

call show_model_list_status ()

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_8"

contains

subroutine show_model_list_status ()
    write (u, "(A)")  "* Model list status"
    write (u, *)
    write (u, "(A,1x,L1)")  "WHIZARD model exists =", &
        model_list%model_exists (model_name)
    write (u, "(A,1x,L1)")  "UFO model exists =", &
        model_list%model_exists (model_name, ufo=.true.)
end subroutine show_model_list_status

end subroutine models_8

```

Generate UFO model file

Generate the necessary .ufo.mdl file from source, calling OMega, and load the model.

Note: There must not be another unit test which works with the same UFO model. The model file is deleted explicitly at the end of this test.

```

<Models: execute tests>+≡
    call test (models_9, "models_9", &
        "generate UFO-derived model file", &
        u, results)

<Models: test declarations>+≡
    public :: models_9

<Models: tests>+≡
    subroutine models_9 (u)
        integer, intent(in) :: u
        integer :: um
        character(80) :: buffer
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(string_t) :: model_name, model_file_name
        type(model_t), pointer :: model

        write (u, "(A)")  "* Test output: models_9"
        write (u, "(A)")  "* Purpose: enable the UFO Standard Model (test version)"
    end subroutine models_9

```

```

write (u, *)

call os_data%init ()
call syntax_model_file_init ()

os_data%whizard_modelpath_ufo = "../models/UFO"

model_name = "SM"
model_file_name = model_name // ".models_9" // ".ufo.mdl"

write (u, "(A)")  "* Generate and read UFO model"
write (u, *)

call delete_file (char (model_file_name))

call model_list%read_model (model_name, model_file_name, os_data, model, ufo=.true.)
call model%write (u, show_md5sum=.false.)

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_9"

end subroutine models_9

```

Read model with schemes

Read a model from file which contains `slha_entry` qualifiers for parameters.

```

<Models: execute tests>+≡
  call test (models_10, "models_10", &
    "handle slha_entry option", &
    u, results)

<Models: test declarations>+≡
  public :: models_10

<Models: tests>+≡
  subroutine models_10 (u)
    integer, intent(in) :: u
    integer :: um
    character(80) :: buffer
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(var_list_t), pointer :: var_list
    type(model_t), pointer :: model
    type(string_t), dimension(:), allocatable :: slha_block_name
    integer :: i

    write (u, "(A)")  "* Test output: models_10"
    write (u, "(A)")  "*   Purpose: read a model from file &

```

```

        &with slha_entry options"
write (u, *)

open (newunit=um, file="Test10.mdl", status="replace", action="readwrite")
write (um, "(A)") 'model "Test10"'
write (um, "(A)") ' parameter a = 1    slha_entry F00 1'
write (um, "(A)") ' parameter b = 4    slha_entry BAR 2 1'

rewind (um)
do
    read (um, "(A)", end=1) buffer
    write (u, "(A)") trim (buffer)
end do
1 continue
close (um)

call syntax_model_file_init ()
call os_data%init ()

write (u, *)
write (u, "(A)")  "* Model output, default scheme (= foo)"
write (u, *)

call model_list%read_model (var_str ("Test10"), var_str ("Test10.mdl"), &
    os_data, model)
call model%write (u, show_md5sum=.false.)

write (u, *)
write (u, "(A)")  "* Check that model contains slha_entry options"
write (u, *)

write (u, "(A,1x,L1)") &
    "supports_custom_slha =", model%supports_custom_slha ()

write (u, *)
write (u, "(A)")  "custom_slha_blocks ="
call model%get_custom_slha_blocks (slha_block_name)
do i = 1, size (slha_block_name)
    write (u, "(1x,A)", advance="no") char (slha_block_name(i))
end do
write (u, *)

write (u, *)
write (u, "(A)")  "* Parameter lookup"
write (u, *)

call show_slha ("F00", [1])
call show_slha ("F00", [2])
call show_slha ("BAR", [2, 1])
call show_slha ("GEE", [3])

write (u, *)
write (u, "(A)")  "* Modify parameter via SLHA block interface"
write (u, *)

```

```

call model%slha_set_par (var_str ("F00"), [1], 7._default)
call show_slha ("F00", [1])

write (u, *)
write (u, "(A)")  "* Show var list with modified parameter"
write (u, *)

call show_var_list ()

write (u, *)
write (u, "(A)")  "* Cleanup"

call model_list%final ()
call syntax_model_file_final ()

write (u, *)
write (u, "(A)")  "* Test output end: models_10"

contains

subroutine show_slha (block_name, block_index)
  character(*), intent(in) :: block_name
  integer, dimension(:), intent(in) :: block_index
  class(modelpar_data_t), pointer :: par_data
  write (u, "(A,*(1x,I0))", advance="no") block_name, block_index
  write (u, "(' => ')", advance="no")
  call model%slha_lookup (var_str (block_name), block_index, par_data)
  if (associated (par_data)) then
    call par_data%write (u)
    write (u, *)
  else
    write (u, "(' - ')")
  end if
end subroutine show_slha

subroutine show_var_list ()
  var_list => model%get_var_list_ptr ()
  call var_list%write (u)
end subroutine show_var_list

end subroutine models_10

```

28.5 The SUSY Les Houches Accord

The SUSY Les Houches Accord defines a standard interfaces for storing the physics data of SUSY models. Here, we provide the means for reading, storing, and writing such data.

```
(slha_interface.f90)≡  
  <File header>  
  
  module slha_interface  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use constants  
    use string_utils, only: upper_case  
    use system_defs, only: VERSION_STRING  
    use system_defs, only: EOF  
    use diagnostics  
    use os_interface  
    use ifiles  
    use lexers  
    use syntax_rules  
    use parser  
    use variables  
    use models  
  
    <Standard module head>  
  
    <SLHA: public>  
  
    <SLHA: parameters>  
  
    <SLHA: variables>  
  
    save  
  
    contains  
  
    <SLHA: procedures>  
  
    <SLHA: tests>  
  
  end module slha_interface
```

28.5.1 Preprocessor

SLHA is a mixed-format standard. It should be read in assuming free format (but line-oriented), but it has some fixed-format elements.

To overcome this difficulty, we implement a preprocessing step which transforms the SLHA into a format that can be swallowed by our generic free-format lexer and parser. Each line with a blank first character is assumed to be a data line. We prepend a 'DATA' keyword to these lines. Furthermore, to enforce line-orientation, each line is appended a '\$' key which is recognized by the

parser. To do this properly, we first remove trailing comments, and skip lines consisting only of comments.

The preprocessor reads from a stream and puts out an `ifile`. Blocks that are not recognized are skipped. For some blocks, data items are quoted, so they can be read as strings if necessary.

A name clash occurs if the block name is identical to a keyword. This can happen for custom SLHA models and files. In that case, we prepend an underscore, which will be silently suppressed where needed.

$\langle SLHA: parameters \rangle \equiv$

```
integer, parameter :: MODE_SKIP = 0, MODE_DATA = 1, MODE_INFO = 2
```

$\langle SLHA: procedures \rangle \equiv$

```
subroutine slha_preprocess (stream, custom_block_name, ifile)
  type(stream_t), intent(inout), target :: stream
  type(string_t), dimension(:), intent(in) :: custom_block_name
  type(ifile_t), intent(out) :: ifile
  type(string_t) :: buffer, line, item
  integer :: iostat
  integer :: mode
  mode = MODE
  SCAN_FILE: do
    call stream_get_record (stream, buffer, iostat)
    select case (iostat)
    case (0)
      call split (buffer, line, "#")
      if (len_trim (line) == 0) cycle SCAN_FILE
      select case (char (extract (line, 1, 1)))
      case ("B", "b")
        call check_block_handling (line, custom_block_name, mode)
        call ifile_append (ifile, line // "$")
      case ("D", "d")
        mode = MODE_DATA
        call ifile_append (ifile, line // "$")
      case (" " )
        select case (mode)
        case (MODE_DATA)
          call ifile_append (ifile, "DATA" // line // "$")
        case (MODE_INFO)
          line = adjustl (line)
          call split (line, item, " ")
          call ifile_append (ifile, "INFO" // " " // item // " " &
            // ' ' // trim (adjustl (line)) // ' ' $)
          end select
        case default
          call msg_message (char (line))
          call msg_fatal ("SLHA: Incomprehensible line")
        end select
      case (EOF)
        exit SCAN_FILE
      case default
        call msg_fatal ("SLHA: I/O error occurred while reading SLHA input")
        end select
    end do SCAN_FILE
```

```
end subroutine slha_preprocess
```

Return the mode that we should treat this block with. We add the `custom_block_name` array to the set of supported blocks, which otherwise includes only hard-coded block names. Those custom blocks are data blocks.

Unknown blocks will be skipped altogether. The standard does not specify their internal format at all, so we must not parse their content.

If the name of a (custom) block clashes with a keyword of the SLHA syntax, we append an underscore to the block name, modifying the current line string. This should be silently suppressed when actually parsing block names.

(*SLHA: procedures*) +=

```
subroutine check_block_handling (line, custom_block_name, mode)
  type(string_t), intent(inout) :: line
  type(string_t), dimension(:), intent(in) :: custom_block_name
  integer, intent(out) :: mode
  type(string_t) :: buffer, key, block_name
  integer :: i
  buffer = trim (line)
  call split (buffer, key, " ")
  buffer = adjustl (buffer)
  call split (buffer, block_name, " ")
  buffer = adjustl (buffer)
  block_name = trim (adjustl (upper_case (block_name)))
  select case (char (block_name))
    case ("MODESEL", "MINPAR", "SMINPUTS")
      mode = MODE_DATA
    case ("MASS")
      mode = MODE_DATA
    case ("NMIX", "UMIX", "VMIX", "STOPMIX", "SBOTMIX", "STAUMIX")
      mode = MODE_DATA
    case ("NMHMIX", "NMAMIX", "NMNMIX", "NMSSMRUN")
      mode = MODE_DATA
    case ("ALPHA", "HMIX")
      mode = MODE_DATA
    case ("AU", "AD", "AE")
      mode = MODE_DATA
    case ("SPINFO", "DCINFO")
      mode = MODE_INFO
    case default
      mode = MODE_SKIP
      CHECK_CUSTOM_NAMES: do i = 1, size (custom_block_name)
        if (block_name == custom_block_name(i)) then
          mode = MODE_DATA
          call mangle_keywords (block_name)
          line = key // " " // block_name // " " // trim (buffer)
          exit CHECK_CUSTOM_NAMES
        end if
      end do CHECK_CUSTOM_NAMES
    end select
end subroutine check_block_handling
```

Append an underscore to specific block names:

```

<SLHA: procedures>+=
  subroutine mangle_keywords (name)
    type(string_t), intent(inout) :: name
    select case (char (name))
      case ("BLOCK", "DATA", "INFO", "DECAY")
        name = name // "_"
    end select
  end subroutine mangle_keywords

```

Remove the underscore again:

```

<SLHA: procedures>+=
  subroutine demangle_keywords (name)
    type(string_t), intent(inout) :: name
    select case (char (name))
      case ("BLOCK_", "DATA_", "INFO_", "DECAY_")
        name = extract (name, 1, len(name)-1)
    end select
  end subroutine demangle_keywords

```

28.5.2 Lexer and syntax

```

<SLHA: variables>=
  type(syntax_t), target :: syntax_slha

```

```

<SLHA: public>=
  public :: syntax_slha_init

```

```

<SLHA: procedures>+=
  subroutine syntax_slha_init ()
    type(ifile_t) :: ifile
    call define_slha_syntax (ifile)
    call syntax_init (syntax_slha, ifile)
    call ifile_final (ifile)
  end subroutine syntax_slha_init

```

```

<SLHA: public>+=
  public :: syntax_slha_final

```

```

<SLHA: procedures>+=
  subroutine syntax_slha_final ()
    call syntax_final (syntax_slha)
  end subroutine syntax_slha_final

```

```

<SLHA: public>+=
  public :: syntax_slha_write

```

```

<SLHA: procedures>+=
  subroutine syntax_slha_write (unit)
    integer, intent(in), optional :: unit
    call syntax_write (syntax_slha, unit)
  end subroutine syntax_slha_write

```

```

<SLHA: procedures> +=
subroutine define_slha_syntax (ifile)
  type(ifile_t), intent(inout) :: ifile
  call ifile_append (ifile, "SEQ slha = chunk*")
  call ifile_append (ifile, "ALT chunk = block_def | decay_def")
  call ifile_append (ifile, "SEQ block_def = " &
    // "BLOCK blockgen '$' block_line*")
  call ifile_append (ifile, "ALT blockgen = block_spec | q_spec")
  call ifile_append (ifile, "KEY BLOCK")
  call ifile_append (ifile, "SEQ q_spec = QNUMBERS pdg_code")
  call ifile_append (ifile, "KEY QNUMBERS")
  call ifile_append (ifile, "SEQ block_spec = block_name qvalue?")
  call ifile_append (ifile, "IDE block_name")
  call ifile_append (ifile, "SEQ qvalue = qname '=' real")
  call ifile_append (ifile, "IDE qname")
  call ifile_append (ifile, "KEY '='")
  call ifile_append (ifile, "REA real")
  call ifile_append (ifile, "KEY '$'")
  call ifile_append (ifile, "ALT block_line = block_data | block_info")
  call ifile_append (ifile, "SEQ block_data = DATA data_line '$'")
  call ifile_append (ifile, "KEY DATA")
  call ifile_append (ifile, "SEQ data_line = data_item+")
  call ifile_append (ifile, "ALT data_item = signed_number | number")
  call ifile_append (ifile, "SEQ signed_number = sign number")
  call ifile_append (ifile, "ALT sign = '+' | '-'")
  call ifile_append (ifile, "ALT number = integer | real")
  call ifile_append (ifile, "INT integer")
  call ifile_append (ifile, "KEY '-'")
  call ifile_append (ifile, "KEY '+'")
  call ifile_append (ifile, "SEQ block_info = INFO info_line '$'")
  call ifile_append (ifile, "KEY INFO")
  call ifile_append (ifile, "SEQ info_line = integer string_literal")
  call ifile_append (ifile, "QUO string_literal = '... '")
  call ifile_append (ifile, "SEQ decay_def = " &
    // "DECAY decay_spec '$' decay_data*")
  call ifile_append (ifile, "KEY DECAY")
  call ifile_append (ifile, "SEQ decay_spec = pdg_code data_item")
  call ifile_append (ifile, "ALT pdg_code = signed_integer | integer")
  call ifile_append (ifile, "SEQ signed_integer = sign integer")
  call ifile_append (ifile, "SEQ decay_data = DATA decay_line '$'")
  call ifile_append (ifile, "SEQ decay_line = data_item integer pdg_code+")
end subroutine define_slha_syntax

```

The SLHA specification allows for string data items in certain places. Currently, we do not interpret them, but the strings, which are not quoted, must be parsed somehow. The hack for this problem is to allow essentially all characters as special characters, so the string can be read before it is discarded.

```

<SLHA: public> +=
public :: lexer_init_slha

<SLHA: procedures> +=
subroutine lexer_init_slha (lexer)
  type(lexer_t), intent(out) :: lexer
  call lexer_init (lexer, &

```

```

        comment_chars = "#", &
        quote_chars = "'", &
        quote_match = "'", &
        single_chars = "+-=$", &
        special_class = [ " " ], &
        keyword_list = syntax_get_keyword_list_ptr (syntax_slha), &
        upper_case_keywords = .true.) ! $
end subroutine lexer_init_slha

```

28.5.3 Interpreter

Find blocks

From the parse tree, find the node that represents a particular block. If `required` is true, issue an error if not found. Since `block_name` is always invoked with capital letters, we have to capitalize `pn.block_name`.

```

<SLHA: procedures>+=
function slha_get_block_ptr &
    (parse_tree, block_name, required) result (pn_block)
    type(parse_node_t), pointer :: pn_block
    type(parse_tree_t), intent(in) :: parse_tree
    type(string_t), intent(in) :: block_name
    type(string_t) :: block_def
    logical, intent(in) :: required
    type(parse_node_t), pointer :: pn_root, pn_block_spec, pn_block_name
    pn_root => parse_tree%get_root_ptr ()
    pn_block => parse_node_get_sub_ptr (pn_root)
    do while (associated (pn_block))
        select case (char (parse_node_get_rule_key (pn_block)))
            case ("block_def")
                pn_block_spec => parse_node_get_sub_ptr (pn_block, 2)
                pn_block_name => parse_node_get_sub_ptr (pn_block_spec)
                select case (char (pn_block_name%get_rule_key ()))
                    case ("block_name")
                        block_def = trim (adjustl (upper_case &
                            (pn_block_name%get_string ())))
                    case ("QNUMBERS")
                        block_def = "QNUMBERS"
                    end select
                if (block_def == block_name) then
                    return
                end if
            end select
            pn_block => parse_node_get_next_ptr (pn_block)
        end do
    if (required) then
        call msg_fatal ("SLHA: block '" // char (block_name) // "' not found")
    end if
end function slha_get_block_ptr

```

Scan the file for the first/next DECAY block.

```

<SLHA: procedures>+=

```

```

function slha_get_first_decay_ptr (parse_tree) result (pn_decay)
  type(parse_node_t), pointer :: pn_decay
  type(parse_tree_t), intent(in) :: parse_tree
  type(parse_node_t), pointer :: pn_root
  pn_root => parse_tree%get_root_ptr ()
  pn_decay => parse_node_get_sub_ptr (pn_root)
  do while (associated (pn_decay))
    select case (char (parse_node_get_rule_key (pn_decay)))
      case ("decay_def")
        return
    end select
    pn_decay => parse_node_get_next_ptr (pn_decay)
  end do
end function slha_get_first_decay_ptr

function slha_get_next_decay_ptr (pn_block) result (pn_decay)
  type(parse_node_t), pointer :: pn_decay
  type(parse_node_t), intent(in), target :: pn_block
  pn_decay => parse_node_get_next_ptr (pn_block)
  do while (associated (pn_decay))
    select case (char (parse_node_get_rule_key (pn_decay)))
      case ("decay_def")
        return
    end select
    pn_decay => parse_node_get_next_ptr (pn_decay)
  end do
end function slha_get_next_decay_ptr

```

Extract and transfer data from blocks

Given the parse node of a block, find the parse node of a particular switch or data line. Return this node and the node of the data item following the integer code.

(*SLHA: procedures*) +=

```

subroutine slha_find_index_ptr (pn_block, pn_data, pn_item, code)
  type(parse_node_t), intent(in), target :: pn_block
  type(parse_node_t), intent(out), pointer :: pn_data
  type(parse_node_t), intent(out), pointer :: pn_item
  integer, intent(in) :: code
  pn_data => parse_node_get_sub_ptr (pn_block, 4)
  call slha_next_index_ptr (pn_data, pn_item, code)
end subroutine slha_find_index_ptr

subroutine slha_find_index_pair_ptr (pn_block, pn_data, pn_item, code1, code2)
  type(parse_node_t), intent(in), target :: pn_block
  type(parse_node_t), intent(out), pointer :: pn_data
  type(parse_node_t), intent(out), pointer :: pn_item
  integer, intent(in) :: code1, code2
  pn_data => parse_node_get_sub_ptr (pn_block, 4)
  call slha_next_index_pair_ptr (pn_data, pn_item, code1, code2)
end subroutine slha_find_index_pair_ptr

```

Starting from the pointer to a data line, find a data line with the given integer code.

(SLHA: procedures)+≡

```

subroutine slha_next_index_ptr (pn_data, pn_item, code)
  type(parse_node_t), intent(inout), pointer :: pn_data
  integer, intent(in) :: code
  type(parse_node_t), intent(out), pointer :: pn_item
  type(parse_node_t), pointer :: pn_line, pn_code
  do while (associated (pn_data))
    pn_line => parse_node_get_sub_ptr (pn_data, 2)
    pn_code => parse_node_get_sub_ptr (pn_line)
    select case (char (parse_node_get_rule_key (pn_code)))
    case ("integer")
      if (parse_node_get_integer (pn_code) == code) then
        pn_item => parse_node_get_next_ptr (pn_code)
        return
      end if
    end select
    pn_data => parse_node_get_next_ptr (pn_data)
  end do
  pn_item => null ()
end subroutine slha_next_index_ptr

```

Starting from the pointer to a data line, find a data line with the given integer code pair.

(SLHA: procedures)+≡

```

subroutine slha_next_index_pair_ptr (pn_data, pn_item, code1, code2)
  type(parse_node_t), intent(inout), pointer :: pn_data
  integer, intent(in) :: code1, code2
  type(parse_node_t), intent(out), pointer :: pn_item
  type(parse_node_t), pointer :: pn_line, pn_code1, pn_code2
  do while (associated (pn_data))
    pn_line => parse_node_get_sub_ptr (pn_data, 2)
    pn_code1 => parse_node_get_sub_ptr (pn_line)
    select case (char (parse_node_get_rule_key (pn_code1)))
    case ("integer")
      if (parse_node_get_integer (pn_code1) == code1) then
        pn_code2 => parse_node_get_next_ptr (pn_code1)
        if (associated (pn_code2)) then
          select case (char (parse_node_get_rule_key (pn_code2)))
          case ("integer")
            if (parse_node_get_integer (pn_code2) == code2) then
              pn_item => parse_node_get_next_ptr (pn_code2)
              return
            end if
          end select
        end if
      end if
    end select
    pn_data => parse_node_get_next_ptr (pn_data)
  end do
  pn_item => null ()
end subroutine slha_next_index_pair_ptr

```

Handle info data

Return all strings with index *i*. The result is an allocated string array. Since we do not know the number of matching entries in advance, we build an intermediate list which is transferred to the final array and deleted before exiting.

(SLHA: procedures)+≡

```
subroutine retrieve_strings_in_block (pn_block, code, str_array)
  type(parse_node_t), intent(in), target :: pn_block
  integer, intent(in) :: code
  type(string_t), dimension(:), allocatable, intent(out) :: str_array
  type(parse_node_t), pointer :: pn_data, pn_item
  type :: str_entry_t
    type(string_t) :: str
    type(str_entry_t), pointer :: next => null ()
  end type str_entry_t
  type(str_entry_t), pointer :: first => null ()
  type(str_entry_t), pointer :: current => null ()
  integer :: n
  n = 0
  call slha_find_index_ptr (pn_block, pn_data, pn_item, code)
  if (associated (pn_item)) then
    n = n + 1
    allocate (first)
    first%str = parse_node_get_string (pn_item)
    current => first
    do while (associated (pn_data))
      pn_data => parse_node_get_next_ptr (pn_data)
      call slha_next_index_ptr (pn_data, pn_item, code)
      if (associated (pn_item)) then
        n = n + 1
        allocate (current%next)
        current => current%next
        current%str = parse_node_get_string (pn_item)
      end if
    end do
    allocate (str_array (n))
    n = 0
    do while (associated (first))
      n = n + 1
      current => first
      str_array(n) = current%str
      first => first%next
      deallocate (current)
    end do
  else
    allocate (str_array (0))
  end if
end subroutine retrieve_strings_in_block
```


Transfer data from SLHA to variables

Extract real parameter with index *i*. If it does not exist, retrieve it from the variable list, using the given name.

(SLHA: procedures)+≡

```
function get_parameter_in_block (pn_block, code, name, var_list) result (var)
  real(default) :: var
  type(parse_node_t), intent(in), target :: pn_block
  integer, intent(in) :: code
  type(string_t), intent(in) :: name
  type(var_list_t), intent(in), target :: var_list
  type(parse_node_t), pointer :: pn_data, pn_item
  call slha_find_index_ptr (pn_block, pn_data, pn_item, code)
  if (associated (pn_item)) then
    var = get_real_parameter (pn_item)
  else
    var = var_list%get_rval (name)
  end if
end function get_parameter_in_block
```

Extract a real data item with index *i*. If it does exist, set it in the variable list, using the given name. If the variable is not present in the variable list, ignore it.

(SLHA: procedures)+≡

```
subroutine set_data_item (pn_block, code, name, var_list)
  type(parse_node_t), intent(in), target :: pn_block
  integer, intent(in) :: code
  type(string_t), intent(in) :: name
  type(var_list_t), intent(inout), target :: var_list
  type(parse_node_t), pointer :: pn_data, pn_item
  call slha_find_index_ptr (pn_block, pn_data, pn_item, code)
  if (associated (pn_item)) then
    call var_list%set_real (name, get_real_parameter (pn_item), &
      is_known=.true., ignore=.true.)
  end if
end subroutine set_data_item
```

Extract a real matrix element with index *i,j*. If it does exists, set it in the variable list, using the given name. If the variable is not present in the variable list, ignore it.

(SLHA: procedures)+≡

```
subroutine set_matrix_element (pn_block, code1, code2, name, var_list)
  type(parse_node_t), intent(in), target :: pn_block
  integer, intent(in) :: code1, code2
  type(string_t), intent(in) :: name
  type(var_list_t), intent(inout), target :: var_list
  type(parse_node_t), pointer :: pn_data, pn_item
  call slha_find_index_pair_ptr (pn_block, pn_data, pn_item, code1, code2)
  if (associated (pn_item)) then
    call var_list%set_real (name, get_real_parameter (pn_item), &
      is_known=.true., ignore=.true.)
  end if
end subroutine set_matrix_element
```

Transfer data from variables to SLHA

Get a real/integer parameter with index *i* from the variable list and write it to the current output file. In the integer case, we account for the fact that the variable is type real. If it does not exist, do nothing.

(SLHA: procedures)+≡

```
subroutine write_integer_data_item (u, code, name, var_list, comment)
  integer, intent(in) :: u
  integer, intent(in) :: code
  type(string_t), intent(in) :: name
  type(var_list_t), intent(in) :: var_list
  character(*), intent(in) :: comment
  integer :: item
  if (var_list%contains (name)) then
    item = nint (var_list%get_rval (name))
    call write_integer_parameter (u, code, item, comment)
  end if
end subroutine write_integer_data_item

subroutine write_real_data_item (u, code, name, var_list, comment)
  integer, intent(in) :: u
  integer, intent(in) :: code
  type(string_t), intent(in) :: name
  type(var_list_t), intent(in) :: var_list
  character(*), intent(in) :: comment
  real(default) :: item
  if (var_list%contains (name)) then
    item = var_list%get_rval (name)
    call write_real_parameter (u, code, item, comment)
  end if
end subroutine write_real_data_item
```

Get a real data item with two integer indices from the variable list and write it to the current output file. If it does not exist, do nothing.

(SLHA: procedures)+≡

```
subroutine write_matrix_element (u, code1, code2, name, var_list, comment)
  integer, intent(in) :: u
  integer, intent(in) :: code1, code2
  type(string_t), intent(in) :: name
  type(var_list_t), intent(in) :: var_list
  character(*), intent(in) :: comment
  real(default) :: item
  if (var_list%contains (name)) then
    item = var_list%get_rval (name)
    call write_real_matrix_element (u, code1, code2, item, comment)
  end if
end subroutine write_matrix_element
```

28.5.4 Auxiliary function

Write a block header.

```
(SLHA: procedures)+≡  
  subroutine write_block_header (u, name, comment)  
    integer, intent(in) :: u  
    character(*), intent(in) :: name, comment  
    write (u, "(A,1x,A,3x,'#',1x,A)") "BLOCK", name, comment  
  end subroutine write_block_header
```

Extract a real parameter that may be defined real or integer, signed or unsigned.

```
(SLHA: procedures)+≡  
  function get_real_parameter (pn_item) result (var)  
    real(default) :: var  
    type(parse_node_t), intent(in), target :: pn_item  
    type(parse_node_t), pointer :: pn_sign, pn_var  
    integer :: sign  
    select case (char (parse_node_get_rule_key (pn_item)))  
    case ("signed_number")  
      pn_sign => parse_node_get_sub_ptr (pn_item)  
      pn_var => parse_node_get_next_ptr (pn_sign)  
      select case (char (parse_node_get_key (pn_sign)))  
      case ("+"); sign = +1  
      case ("-"); sign = -1  
      end select  
    case default  
      sign = +1  
      pn_var => pn_item  
    end select  
    select case (char (parse_node_get_rule_key (pn_var)))  
    case ("integer"); var = sign * parse_node_get_integer (pn_var)  
    case ("real"); var = sign * parse_node_get_real (pn_var)  
    end select  
  end function get_real_parameter
```

Auxiliary: Extract an integer parameter that may be defined signed or unsigned.
A real value is an error.

```
(SLHA: procedures)+≡  
  function get_integer_parameter (pn_item) result (var)  
    integer :: var  
    type(parse_node_t), intent(in), target :: pn_item  
    type(parse_node_t), pointer :: pn_sign, pn_var  
    integer :: sign  
    select case (char (parse_node_get_rule_key (pn_item)))  
    case ("signed_integer")  
      pn_sign => parse_node_get_sub_ptr (pn_item)  
      pn_var => parse_node_get_next_ptr (pn_sign)  
      select case (char (parse_node_get_key (pn_sign)))  
      case ("+"); sign = +1  
      case ("-"); sign = -1  
      end select  
    case ("integer")  
      sign = +1
```

```

        pn_var => pn_item
    case default
        call parse_node_write (pn_var)
        call msg_error ("SLHA: Integer parameter expected")
        var = 0
        return
    end select
    var = sign * parse_node_get_integer (pn_var)
end function get_integer_parameter

```

Write an integer parameter with a single index directly to file, using the required output format.

<SLHA: procedures>+≡

```

subroutine write_integer_parameter (u, code, item, comment)
    integer, intent(in) :: u
    integer, intent(in) :: code
    integer, intent(in) :: item
    character(*), intent(in) :: comment
1   format (1x, I9, 3x, 3x, I9, 4x, 3x, '#', 1x, A)
    write (u, 1) code, item, comment
end subroutine write_integer_parameter

```

Write a real parameter with two indices directly to file, using the required output format.

<SLHA: procedures>+≡

```

subroutine write_real_parameter (u, code, item, comment)
    integer, intent(in) :: u
    integer, intent(in) :: code
    real(default), intent(in) :: item
    character(*), intent(in) :: comment
1   format (1x, I9, 3x, 1P, E16.8, 0P, 3x, '#', 1x, A)
    write (u, 1) code, item, comment
end subroutine write_real_parameter

```

Write a real parameter with a single index directly to file, using the required output format.

<SLHA: procedures>+≡

```

subroutine write_real_matrix_element (u, code1, code2, item, comment)
    integer, intent(in) :: u
    integer, intent(in) :: code1, code2
    real(default), intent(in) :: item
    character(*), intent(in) :: comment
1   format (1x, I2, 1x, I2, 3x, 1P, E16.8, 0P, 3x, '#', 1x, A)
    write (u, 1) code1, code2, item, comment
end subroutine write_real_matrix_element

```

The concrete SLHA interpreter

SLHA codes for particular physics models

<SLHA: parameters>+≡

```
integer, parameter :: MDL_MSSM = 0
integer, parameter :: MDL_NMSSM = 1
```

Take the parse tree and extract relevant data. Select the correct model and store all data that is present in the appropriate variable list. Finally, update the variable record.

We assume that if the model contains custom SLHA block names, we just have to scan those to get complete information. Block names could coincide with the SLHA standard block names, but we do not have to assume this. This will be the situation for an UFO-generated file. In particular, an UFO file should contain all expressions necessary for computing dependent parameters, so we can forget about the strict SLHA standard and its hard-coded conventions.

If there are no custom SLHA block names, we should assume that the model is a standard SUSY model, and the parameters and hard-coded blocks can be read as specified by the original SLHA standard. There are hard-coded block names and parameter calculations.

Public for use in unit test.

<SLHA: public>+≡

```
public :: slha_interpret_parse_tree
```

<SLHA: procedures>+≡

```
subroutine slha_interpret_parse_tree &
  (parse_tree, model, input, spectrum, decays)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model
  logical, intent(in) :: input, spectrum, decays
  logical :: errors
  integer :: mssm_type
  if (model%supports_custom_slha ()) then
    call slha_handle_custom_file (parse_tree, model)
  else
    call slha_handle_MODSEL (parse_tree, model, mssm_type)
    if (input) then
      call slha_handle_SMINPUTS (parse_tree, model)
      call slha_handle_MINPAR (parse_tree, model, mssm_type)
    end if
    if (spectrum) then
      call slha_handle_info_block (parse_tree, "SPINFO", errors)
      if (errors) return
      call slha_handle_MASS (parse_tree, model)
      call slha_handle_matrix_block (parse_tree, "NMIX", "mn_", 4, 4, model)
      call slha_handle_matrix_block (parse_tree, "NMNMIX", "mixn_", 5, 5, model)
      call slha_handle_matrix_block (parse_tree, "UMIX", "mu_", 2, 2, model)
      call slha_handle_matrix_block (parse_tree, "VMIX", "mv_", 2, 2, model)
      call slha_handle_matrix_block (parse_tree, "STOPMIX", "mt_", 2, 2, model)
      call slha_handle_matrix_block (parse_tree, "SBOTMIX", "mb_", 2, 2, model)
      call slha_handle_matrix_block (parse_tree, "STAUMIX", "ml_", 2, 2, model)
      call slha_handle_matrix_block (parse_tree, "NMHMIX", "mixh0_", 3, 3, model)
      call slha_handle_matrix_block (parse_tree, "NMAMIX", "mixa0_", 2, 3, model)
      call slha_handle_ALPHA (parse_tree, model)
      call slha_handle_HMIX (parse_tree, model)
      call slha_handle_NMSSMRUN (parse_tree, model)
      call slha_handle_matrix_block (parse_tree, "AU", "Au_", 3, 3, model)
      call slha_handle_matrix_block (parse_tree, "AD", "Ad_", 3, 3, model)
```

```

        call slha_handle_matrix_block (parse_tree, "AE", "Ae_", 3, 3, model)
    end if
end if
if (decays) then
    call slha_handle_info_block (parse_tree, "DCINFO", errors)
    if (errors) return
    call slha_handle_decays (parse_tree, model)
end if
end subroutine slha_interpret_parse_tree

```

Info blocks

Handle the informational blocks SPINFO and DCINFO. The first two items are program name and version. Items with index 3 are warnings. Items with index 4 are errors. We reproduce these as WHIZARD warnings and errors.

(SLHA: procedures)+≡

```

subroutine slha_handle_info_block (parse_tree, block_name, errors)
    type(parse_tree_t), intent(in) :: parse_tree
    character(*), intent(in) :: block_name
    logical, intent(out) :: errors
    type(parse_node_t), pointer :: pn_block
    type(string_t), dimension(:), allocatable :: msg
    integer :: i
    pn_block => slha_get_block_ptr &
        (parse_tree, var_str (block_name), required=.true.)
    if (.not. associated (pn_block)) then
        call msg_error ("SLHA: Missing info block '" &
            // trim (block_name) // "'; ignored.")
        errors = .true.
        return
    end if
    select case (block_name)
    case ("SPINFO")
        call msg_message ("SLHA: SUSY spectrum program info:")
    case ("DCINFO")
        call msg_message ("SLHA: SUSY decay program info:")
    end select
    call retrieve_strings_in_block (pn_block, 1, msg)
    do i = 1, size (msg)
        call msg_message ("SLHA: " // char (msg(i)))
    end do
    call retrieve_strings_in_block (pn_block, 2, msg)
    do i = 1, size (msg)
        call msg_message ("SLHA: " // char (msg(i)))
    end do
    call retrieve_strings_in_block (pn_block, 3, msg)
    do i = 1, size (msg)
        call msg_warning ("SLHA: " // char (msg(i)))
    end do
    call retrieve_strings_in_block (pn_block, 4, msg)
    do i = 1, size (msg)
        call msg_error ("SLHA: " // char (msg(i)))
    end do
end subroutine

```

```

end do
errors = size (msg) > 0
end subroutine slha_handle_info_block

```

MODSEL

Handle the overall model definition. Only certain models are recognized. The soft-breaking model templates that determine the set of input parameters.

This block used to be required, but for generic UFO model support we should allow for its absence. In that case, `mssm_type` will be set to a negative value. If the block is present, the model must be one of the following, or parsing ends with an error.

(SLHA: parameters)+≡

```

integer, parameter :: MSSM_GENERIC = 0
integer, parameter :: MSSM_SUGRA = 1
integer, parameter :: MSSM_GMSB = 2
integer, parameter :: MSSM_AMSB = 3

```

(SLHA: procedures)+≡

```

subroutine slha_handle_MODSEL (parse_tree, model, mssm_type)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(in), target :: model
  integer, intent(out) :: mssm_type
  type(parse_node_t), pointer :: pn_block, pn_data, pn_item
  type(string_t) :: model_name
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("MODSEL"), required=.false.)
  if (.not. associated (pn_block)) then
    mssm_type = -1
    return
  end if
  call slha_find_index_ptr (pn_block, pn_data, pn_item, 1)
  if (associated (pn_item)) then
    mssm_type = get_integer_parameter (pn_item)
  else
    mssm_type = MSSM_GENERIC
  end if
  call slha_find_index_ptr (pn_block, pn_data, pn_item, 3)
  if (associated (pn_item)) then
    select case (parse_node_get_integer (pn_item))
    case (MDL_MSSM); model_name = "MSSM"
    case (MDL_NMSSM); model_name = "NMSSM"
    case default
      call msg_fatal ("SLHA: unknown model code in MODSEL")
      return
    end select
  else
    model_name = "MSSM"
  end if
  call slha_find_index_ptr (pn_block, pn_data, pn_item, 4)
  if (associated (pn_item)) then
    call msg_fatal (" R-parity violation is currently not supported by WHIZARD.")
  end if
end subroutine

```

```

end if
call slha_find_index_ptr (pn_block, pn_data, pn_item, 5)
if (associated (pn_item)) then
    call msg_fatal (" CP violation is currently not supported by WHIZARD.")
end if
select case (char (model_name))
case ("MSSM")
    select case (char (model%get_name ()))
    case ("MSSM", "MSSM_CKM", "MSSM_Grav", "MSSM_Hgg")
        model_name = model%get_name ()
    case default
        call msg_fatal ("Selected model '" &
            // char (model%get_name ()) // "' does not match model '" &
            // char (model_name) // "' in SLHA input file.")
        return
    end select
case ("NMSSM")
    select case (char (model%get_name ()))
    case ("NMSSM", "NMSSM_CKM", "NMSSM_Hgg")
        model_name = model%get_name ()
    case default
        call msg_fatal ("Selected model '" &
            // char (model%get_name ()) // "' does not match model '" &
            // char (model_name) // "' in SLHA input file.")
        return
    end select
case default
    call msg_bug ("SLHA model name '" &
        // char (model_name) // "' not recognized.")
    return
end select
call msg_message ("SLHA: Initializing model '" // char (model_name) // "'")
end subroutine slha_handle_MODSEL

```

Write a MODSEL block, based on the contents of the current model.

(SLHA: procedures)+≡

```

subroutine slha_write_MODSEL (u, model, mssm_type)
    integer, intent(in) :: u
    type(model_t), intent(in), target :: model
    integer, intent(out) :: mssm_type
    type(var_list_t), pointer :: var_list
    integer :: model_id
    type(string_t) :: mtype_string
    var_list => model%get_var_list_ptr ()
    if (var_list%contains (var_str ("mtype"))) then
        mssm_type = nint (var_list%get_rval (var_str ("mtype")))
    else
        call msg_error ("SLHA: parameter 'mtype' (SUSY breaking scheme) " &
            // "is unknown in current model, no SLHA output possible")
        mssm_type = -1
        return
    end if
    call write_block_header (u, "MODSEL", "SUSY model selection")

```



```

select case (mssm_type)
case (0); mtype_string = "Generic MSSM"
case (1); mtype_string = "SUGRA"
case (2); mtype_string = "GMSB"
case (3); mtype_string = "AMSB"
case default
    mtype_string = "unknown"
end select
call write_integer_parameter (u, 1, mssm_type, &
    "SUSY-breaking scheme: " // char (mtype_string))
select case (char (model%get_name ()))
case ("MSSM"); model_id = MDL_MSSM
case ("NMSSM"); model_id = MDL_NMSSM
case default
    model_id = 0
end select
call write_integer_parameter (u, 3, model_id, &
    "SUSY model type: " // char (model%get_name ()))
end subroutine slha_write_MODSEL

```

SMINPUTS

Read SM parameters and update the variable list accordingly. If a parameter is not defined in the block, we use the previous value from the model variable list. For the basic parameters we have to do a small recalculation, since SLHA uses the G_F - α - m_Z scheme, while WHIZARD derives them from G_F , m_W , and m_Z .

(*SLHA: procedures*)+≡

```

subroutine slha_handle_SMINPUTS (parse_tree, model)
type(parse_tree_t), intent(in) :: parse_tree
type(model_t), intent(inout), target :: model
type(parse_node_t), pointer :: pn_block
real(default) :: alpha_em_i, GF, alphas, mZ
real(default) :: ee, vv, cw_sw, cw2, mW
real(default) :: mb, mtop, mtau
type(var_list_t), pointer :: var_list
var_list => model%get_var_list_ptr ()
pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("SMINPUTS"), required=.true.)
if (.not. (associated (pn_block))) return
alpha_em_i = &
    get_parameter_in_block (pn_block, 1, var_str ("alpha_em_i"), var_list)
GF = get_parameter_in_block (pn_block, 2, var_str ("GF"), var_list)
alphas = &
    get_parameter_in_block (pn_block, 3, var_str ("alphas"), var_list)
mZ = get_parameter_in_block (pn_block, 4, var_str ("mZ"), var_list)
mb = get_parameter_in_block (pn_block, 5, var_str ("mb"), var_list)
mtop = get_parameter_in_block (pn_block, 6, var_str ("mtop"), var_list)
mtau = get_parameter_in_block (pn_block, 7, var_str ("mtau"), var_list)
ee = sqrt (4 * pi / alpha_em_i)
vv = 1 / sqrt (sqrt (2._default) * GF)
cw_sw = ee * vv / (2 * mZ)
if (2*cw_sw <= 1) then

```

```

      cw2 = (1 + sqrt (1 - 4 * cw_sw**2)) / 2
      mW = mZ * sqrt (cw2)
      call var_list%set_real (var_str ("GF"), GF, .true.)
      call var_list%set_real (var_str ("mZ"), mZ, .true.)
      call var_list%set_real (var_str ("mW"), mW, .true.)
      call var_list%set_real (var_str ("mtau"), mtau, .true.)
      call var_list%set_real (var_str ("mb"), mb, .true.)
      call var_list%set_real (var_str ("mtop"), mtop, .true.)
      call var_list%set_real (var_str ("alphas"), alphas, .true.)
    else
      call msg_fatal ("SLHA: Unphysical SM parameter values")
      return
    end if
  end subroutine slha_handle_SMINPUTS

```

Write a SMINPUTS block.

```

<SLHA: procedures>+≡
subroutine slha_write_SMINPUTS (u, model)
  integer, intent(in) :: u
  type(model_t), intent(in), target :: model
  type(var_list_t), pointer :: var_list
  var_list => model%get_var_list_ptr ()
  call write_block_header (u, "SMINPUTS", "SM input parameters")
  call write_real_data_item (u, 1, var_str ("alpha_em_i"), var_list, &
    "Inverse electromagnetic coupling alpha (Z pole)")
  call write_real_data_item (u, 2, var_str ("GF"), var_list, &
    "Fermi constant")
  call write_real_data_item (u, 3, var_str ("alphas"), var_list, &
    "Strong coupling alpha_s (Z pole)")
  call write_real_data_item (u, 4, var_str ("mZ"), var_list, &
    "Z mass")
  call write_real_data_item (u, 5, var_str ("mb"), var_list, &
    "b running mass (at mb)")
  call write_real_data_item (u, 6, var_str ("mtop"), var_list, &
    "top mass")
  call write_real_data_item (u, 7, var_str ("mtau"), var_list, &
    "tau mass")
end subroutine slha_write_SMINPUTS

```

MINPAR

The block of SUSY input parameters. They are accessible to WHIZARD, but they only get used when an external spectrum generator is invoked. The precise set of parameters depends on the type of SUSY breaking, which by itself is one of the parameters.

```

<SLHA: procedures>+≡
subroutine slha_handle_MINPAR (parse_tree, model, mssm_type)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model
  integer, intent(in) :: mssm_type
  type(var_list_t), pointer :: var_list
  type(parse_node_t), pointer :: pn_block

```

```

var_list => model%get_var_list_ptr ()
call var_list%set_real &
    (var_str ("mtype"), real(mssm_type, default), is_known=.true.)
pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("MINPAR"), required=.true.)
select case (mssm_type)
case (MSSM_SUGRA)
    call set_data_item (pn_block, 1, var_str ("m_zero"), var_list)
    call set_data_item (pn_block, 2, var_str ("m_half"), var_list)
    call set_data_item (pn_block, 3, var_str ("tanb"), var_list)
    call set_data_item (pn_block, 4, var_str ("sgn_mu"), var_list)
    call set_data_item (pn_block, 5, var_str ("A0"), var_list)
case (MSSM_GMSB)
    call set_data_item (pn_block, 1, var_str ("Lambda"), var_list)
    call set_data_item (pn_block, 2, var_str ("M_mes"), var_list)
    call set_data_item (pn_block, 3, var_str ("tanb"), var_list)
    call set_data_item (pn_block, 4, var_str ("sgn_mu"), var_list)
    call set_data_item (pn_block, 5, var_str ("N_5"), var_list)
    call set_data_item (pn_block, 6, var_str ("c_grav"), var_list)
case (MSSM_AMSB)
    call set_data_item (pn_block, 1, var_str ("m_zero"), var_list)
    call set_data_item (pn_block, 2, var_str ("m_grav"), var_list)
    call set_data_item (pn_block, 3, var_str ("tanb"), var_list)
    call set_data_item (pn_block, 4, var_str ("sgn_mu"), var_list)
case default
    call set_data_item (pn_block, 3, var_str ("tanb"), var_list)
end select
end subroutine slha_handle_MINPAR

```

Write a MINPAR block as appropriate for the current model type.

(SLHA: procedures)+≡

```

subroutine slha_write_MINPAR (u, model, mssm_type)
    integer, intent(in) :: u
    type(model_t), intent(in), target :: model
    integer, intent(in) :: mssm_type
    type(var_list_t), pointer :: var_list
    var_list => model%get_var_list_ptr ()
    call write_block_header (u, "MINPAR", "Basic SUSY input parameters")
    select case (mssm_type)
    case (MSSM_SUGRA)
        call write_real_data_item (u, 1, var_str ("m_zero"), var_list, &
            "Common scalar mass")
        call write_real_data_item (u, 2, var_str ("m_half"), var_list, &
            "Common gaugino mass")
        call write_real_data_item (u, 3, var_str ("tanb"), var_list, &
            "tan(beta)")
        call write_integer_data_item (u, 4, &
            var_str ("sgn_mu"), var_list, &
            "Sign of mu")
        call write_real_data_item (u, 5, var_str ("A0"), var_list, &
            "Common trilinear coupling")
    case (MSSM_GMSB)
        call write_real_data_item (u, 1, var_str ("Lambda"), var_list, &
            "Soft-breaking scale")
    end select
end subroutine slha_write_MINPAR

```

```

    call write_real_data_item (u, 2, var_str ("M_mes"), var_list, &
        "Messenger scale")
    call write_real_data_item (u, 3, var_str ("tanb"), var_list, &
        "tan(beta)")
    call write_integer_data_item (u, 4, &
        var_str ("sgn_mu"), var_list, &
        "Sign of mu")
    call write_integer_data_item (u, 5, var_str ("N_5"), var_list, &
        "Messenger index")
    call write_real_data_item (u, 6, var_str ("c_grav"), var_list, &
        "Gravitino mass factor")
case (MSSM_AMSB)
    call write_real_data_item (u, 1, var_str ("m_zero"), var_list, &
        "Common scalar mass")
    call write_real_data_item (u, 2, var_str ("m_grav"), var_list, &
        "Gravitino mass")
    call write_real_data_item (u, 3, var_str ("tanb"), var_list, &
        "tan(beta)")
    call write_integer_data_item (u, 4, &
        var_str ("sgn_mu"), var_list, &
        "Sign of mu")
case default
    call write_real_data_item (u, 3, var_str ("tanb"), var_list, &
        "tan(beta)")
end select
end subroutine slha_write_MINPAR

```

Mass spectrum

Set masses. Since the particles are identified by PDG code, read the line and try to set the appropriate particle mass in the current model. At the end, update parameters, just in case the W or Z mass was included.

(*SLHA: procedures*)+≡

```

subroutine slha_handle_MASS (parse_tree, model)
    type(parse_tree_t), intent(in) :: parse_tree
    type(model_t), intent(inout), target :: model
    type(parse_node_t), pointer :: pn_block, pn_data, pn_line, pn_code
    type(parse_node_t), pointer :: pn_mass
    integer :: pdg
    real(default) :: mass
    pn_block => slha_get_block_ptr &
        (parse_tree, var_str ("MASS"), required=.true.)
    if (.not. (associated (pn_block))) return
    pn_data => parse_node_get_sub_ptr (pn_block, 4)
    do while (associated (pn_data))
        pn_line => parse_node_get_sub_ptr (pn_data, 2)
        pn_code => parse_node_get_sub_ptr (pn_line)
        if (associated (pn_code)) then
            pdg = get_integer_parameter (pn_code)
            pn_mass => parse_node_get_next_ptr (pn_code)
            if (associated (pn_mass)) then
                mass = get_real_parameter (pn_mass)
            end if
        end if
        pn_data => parse_node_get_next_ptr (pn_data)
    end do
end subroutine slha_handle_MASS

```

```

        call model%set_field_mass (pdg, mass)
    else
        call msg_error ("SLHA: Block MASS: Missing mass value")
    end if
else
    call msg_error ("SLHA: Block MASS: Missing PDG code")
end if
pn_data => parse_node_get_next_ptr (pn_data)
end do
end subroutine slha_handle_MASS

```

Widths

Set widths. For each DECAY block, extract the header, read the PDG code and width, and try to set the appropriate particle width in the current model.

(SLHA: procedures) +=

```

subroutine slha_handle_decays (parse_tree, model)
    type(parse_tree_t), intent(in) :: parse_tree
    type(model_t), intent(inout), target :: model
    type(parse_node_t), pointer :: pn_decay, pn_decay_spec, pn_code, pn_width
    integer :: pdg
    real(default) :: width
    pn_decay => slha_get_first_decay_ptr (parse_tree)
    do while (associated (pn_decay))
        pn_decay_spec => parse_node_get_sub_ptr (pn_decay, 2)
        pn_code => parse_node_get_sub_ptr (pn_decay_spec)
        pdg = get_integer_parameter (pn_code)
        pn_width => parse_node_get_next_ptr (pn_code)
        width = get_real_parameter (pn_width)
        call model%set_field_width (pdg, width)
        pn_decay => slha_get_next_decay_ptr (pn_decay)
    end do
end subroutine slha_handle_decays

```

Mixing matrices

Read mixing matrices. We can treat all matrices by a single procedure if we just know the block name, variable prefix, and matrix dimension. The matrix dimension must be less than 10. For the pseudoscalar Higgses in NMSSM-type models we need off-diagonal matrices, so we generalize the definition.

(SLHA: procedures) +=

```

subroutine slha_handle_matrix_block &
    (parse_tree, block_name, var_prefix, dim1, dim2, model)
    type(parse_tree_t), intent(in) :: parse_tree
    character(*), intent(in) :: block_name, var_prefix
    integer, intent(in) :: dim1, dim2
    type(model_t), intent(inout), target :: model
    type(parse_node_t), pointer :: pn_block
    type(var_list_t), pointer :: var_list
    integer :: i, j
    character(len=len(var_prefix)+2) :: var_name

```

```

var_list => model%get_var_list_ptr ()
pn_block => slha_get_block_ptr &
    (parse_tree, var_str (block_name), required=.false.)
if (.not. (associated (pn_block))) return
do i = 1, dim1
    do j = 1, dim2
        write (var_name, "(A,I1,I1)") var_prefix, i, j
        call set_matrix_element (pn_block, i, j, var_str (var_name), var_list)
    end do
end do
end subroutine slha_handle_matrix_block

```

Higgs data

Read the block ALPHA which holds just the Higgs mixing angle.

```

<SLHA: procedures>+=
subroutine slha_handle_ALPHA (parse_tree, model)
    type(parse_tree_t), intent(in) :: parse_tree
    type(model_t), intent(inout), target :: model
    type(parse_node_t), pointer :: pn_block, pn_line, pn_data, pn_item
    type(var_list_t), pointer :: var_list
    real(default) :: al_h
    var_list => model%get_var_list_ptr ()
    pn_block => slha_get_block_ptr &
        (parse_tree, var_str ("ALPHA"), required=.false.)
    if (.not. (associated (pn_block))) return
    pn_data => parse_node_get_sub_ptr (pn_block, 4)
    pn_line => parse_node_get_sub_ptr (pn_data, 2)
    pn_item => parse_node_get_sub_ptr (pn_line)
    if (associated (pn_item)) then
        al_h = get_real_parameter (pn_item)
        call var_list%set_real (var_str ("al_h"), al_h, &
            is_known=.true., ignore=.true.)
    end if
end subroutine slha_handle_ALPHA

```

Read the block HMX for the Higgs mixing parameters

```

<SLHA: procedures>+=
subroutine slha_handle_HMX (parse_tree, model)
    type(parse_tree_t), intent(in) :: parse_tree
    type(model_t), intent(inout), target :: model
    type(parse_node_t), pointer :: pn_block
    type(var_list_t), pointer :: var_list
    var_list => model%get_var_list_ptr ()
    pn_block => slha_get_block_ptr &
        (parse_tree, var_str ("HMX"), required=.false.)
    if (.not. (associated (pn_block))) return
    call set_data_item (pn_block, 1, var_str ("mu_h"), var_list)
    call set_data_item (pn_block, 2, var_str ("tanb_h"), var_list)
end subroutine slha_handle_HMX

```

Read the block NMSSMRUN for the specific NMSSM parameters

```

<SLHA: procedures>+=
subroutine slha_handle_NMSSMRUN (parse_tree, model)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model
  type(parse_node_t), pointer :: pn_block
  type(var_list_t), pointer :: var_list
  var_list => model%get_var_list_ptr ()
  pn_block => slha_get_block_ptr &
    (parse_tree, var_str ("NMSSMRUN"), required=.false.)
  if (.not. (associated (pn_block))) return
  call set_data_item (pn_block, 1, var_str ("ls"), var_list)
  call set_data_item (pn_block, 2, var_str ("ks"), var_list)
  call set_data_item (pn_block, 3, var_str ("a_ls"), var_list)
  call set_data_item (pn_block, 4, var_str ("a_ks"), var_list)
  call set_data_item (pn_block, 5, var_str ("nmu"), var_list)
end subroutine slha_handle_NMSSMRUN

```

28.5.5 Parsing custom SLHA files

With the introduction of UFO models, we support custom files in generic SLHA format that reset model parameters. In contrast to strict SLHA files, the order and naming of blocks is arbitrary.

We scan the complete file (i.e., preprocessed parse tree), parsing all blocks that contain data lines. For each data line, we identify index array and associated value. Then we set the model parameter that is associated with that block name and index array, if it exists.

```

<SLHA: procedures>+=
subroutine slha_handle_custom_file (parse_tree, model)
  type(parse_tree_t), intent(in) :: parse_tree
  type(model_t), intent(inout), target :: model

  type(parse_node_t), pointer :: pn_root, pn_block
  type(parse_node_t), pointer :: pn_block_spec, pn_block_name
  type(parse_node_t), pointer :: pn_data, pn_line, pn_code, pn_item
  type(string_t) :: block_name
  integer, dimension(:), allocatable :: block_index
  integer :: n_index, i
  real(default) :: value

  pn_root => parse_tree%get_root_ptr ()
  pn_block => pn_root%get_sub_ptr ()
  HANDLE_BLOCKS: do while (associated (pn_block))
    select case (char (pn_block%get_rule_key ()))
      case ("block_def")
        call slha_handle_custom_block (pn_block, model)
    end select
    pn_block => pn_block%get_next_ptr ()
  end do HANDLE_BLOCKS

end subroutine slha_handle_custom_file

```

```

<SLHA: procedures> +=
subroutine slha_handle_custom_block (pn_block, model)
  type(parse_node_t), intent(in), target :: pn_block
  type(model_t), intent(inout), target :: model

  type(parse_node_t), pointer :: pn_block_spec, pn_block_name
  type(parse_node_t), pointer :: pn_data, pn_line, pn_code, pn_item
  type(string_t) :: block_name
  integer, dimension(:), allocatable :: block_index
  integer :: n_index, i
  real(default) :: value

  pn_block_spec => parse_node_get_sub_ptr (pn_block, 2)
  pn_block_name => parse_node_get_sub_ptr (pn_block_spec)
  select case (char (parse_node_get_rule_key (pn_block_name)))
  case ("block_name")
    block_name = trim (adjustl (upper_case (pn_block_name%get_string ())))
  case ("QNUMBERS")
    block_name = "QNUMBERS"
  end select
  call demangle_keywords (block_name)
  pn_data => pn_block%get_sub_ptr (4)
  HANDLE_LINES: do while (associated (pn_data))
    select case (char (pn_data%get_rule_key ()))
    case ("block_data")
      pn_line => pn_data%get_sub_ptr (2)
      n_index = pn_line%get_n_sub () - 1
      allocate (block_index (n_index))
      pn_code => pn_line%get_sub_ptr ()
      READ_LINE: do i = 1, n_index
        select case (char (pn_code%get_rule_key ()))
        case ("integer"); block_index(i) = pn_code%get_integer ()
        case default
          pn_code => null ()
          exit READ_LINE
        end select
        pn_code => pn_code%get_next_ptr ()
      end do READ_LINE
      if (associated (pn_code)) then
        value = get_real_parameter (pn_code)
        call model%slha_set_par (block_name, block_index, value)
      end if
      deallocate (block_index)
    end select
    pn_data => pn_data%get_next_ptr ()
  end do HANDLE_LINES

end subroutine slha_handle_custom_block

```

28.5.6 Parser

Read a SLHA file from stream, including preprocessing, and make up a parse tree.

<SLHA: procedures>+≡

```

subroutine slha_parse_stream (stream, custom_block_name, parse_tree)
  type(stream_t), intent(inout), target :: stream
  type(string_t), dimension(:), intent(in) :: custom_block_name
  type(parse_tree_t), intent(out) :: parse_tree
  type(ifile_t) :: ifile
  type(lexer_t) :: lexer
  type(stream_t), target :: stream_tmp
  call slha_preprocess (stream, custom_block_name, ifile)
  call stream_init (stream_tmp, ifile)
  call lexer_init_slha (lexer)
  call lexer_assign_stream (lexer, stream_tmp)
  call parse_tree_init (parse_tree, syntax_slha, lexer)
  call lexer_final (lexer)
  call stream_final (stream_tmp)
  call ifile_final (ifile)
end subroutine slha_parse_stream

```

Read a SLHA file chosen by name. Check first the current directory, then the directory where SUSY input files should be located.

The `default_mode` applies to unknown blocks in the SLHA file: this is either `MODE_SKIP` or `MODE_DATA`, corresponding to genuine SUSY and custom file content, respectively.

<SLHA: public>+≡

```

public :: slha_parse_file

```

<SLHA: procedures>+≡

```

subroutine slha_parse_file (file, custom_block_name, os_data, parse_tree)
  type(string_t), intent(in) :: file
  type(string_t), dimension(:), intent(in) :: custom_block_name
  type(os_data_t), intent(in) :: os_data
  type(parse_tree_t), intent(out) :: parse_tree
  logical :: exist
  type(string_t) :: filename
  type(stream_t), target :: stream
  call msg_message ("Reading SLHA input file '" // char (file) // "'")
  filename = file
  inquire (file=char(filename), exist=exist)
  if (.not. exist) then
    filename = os_data%whizard_susypath // "/" // file
    inquire (file=char(filename), exist=exist)
    if (.not. exist) then
      call msg_fatal ("SLHA input file '" // char (file) // "' not found")
      return
    end if
  end if
  call stream_init (stream, char (filename))
  call slha_parse_stream (stream, custom_block_name, parse_tree)
  call stream_final (stream)
end subroutine slha_parse_file

```

28.5.7 API

Read the SLHA file, parse it, and interpret the parse tree. The model parameters retrieved from the file will be inserted into the appropriate model, which is loaded and modified in the background. The pointer to this model is returned as the last argument.

```

<SLHA: public>+≡
    public :: slha_read_file

<SLHA: procedures>+≡
    subroutine slha_read_file &
        (file, os_data, model, input, spectrum, decays)
        type(string_t), intent(in) :: file
        type(os_data_t), intent(in) :: os_data
        type(model_t), intent(inout), target :: model
        logical, intent(in) :: input, spectrum, decays
        type(string_t), dimension(:), allocatable :: custom_block_name
        type(parse_tree_t) :: parse_tree
        call model%get_custom_slha_blocks (custom_block_name)
        call slha_parse_file (file, custom_block_name, os_data, parse_tree)
        if (associated (parse_tree%get_root_ptr ())) then
            call slha_interpret_parse_tree &
                (parse_tree, model, input, spectrum, decays)
            call parse_tree_final (parse_tree)
            call model%update_parameters ()
        end if
    end subroutine slha_read_file

```

Write the SLHA contents, as far as possible, to external file.

```

<SLHA: public>+≡
    public :: slha_write_file

<SLHA: procedures>+≡
    subroutine slha_write_file (file, model, input, spectrum, decays)
        type(string_t), intent(in) :: file
        type(model_t), target, intent(in) :: model
        logical, intent(in) :: input, spectrum, decays
        integer :: mssm_type
        integer :: u
        u = free_unit ()
        call msg_message ("Writing SLHA output file '" // char (file) // "'")
        open (unit=u, file=char(file), action="write", status="replace")
        write (u, "(A)")  "# SUSY Les Houches Accord"
        write (u, "(A)")  "# Output generated by " // trim (VERSION_STRING)
        call slha_write_MODSEL (u, model, mssm_type)
        if (input) then
            call slha_write_SMINPUTS (u, model)
            call slha_write_MINPAR (u, model, mssm_type)
        end if
        if (spectrum) then
            call msg_bug ("SLHA: spectrum output not supported yet")
        end if
        if (decays) then
            call msg_bug ("SLHA: decays output not supported yet")
        end if
    end subroutine slha_write_file

```

```

        end if
        close (u)
    end subroutine slha_write_file

```

28.5.8 Dispatch

```

<SLHA: public>+≡
    public :: dispatch_slha

<SLHA: procedures>+≡
    subroutine dispatch_slha (var_list, input, spectrum, decays)
        type(var_list_t), intent(inout), target :: var_list
        logical, intent(out) :: input, spectrum, decays
        input = var_list%get_lval (var_str ("?slha_read_input"))
        spectrum = var_list%get_lval (var_str ("?slha_read_spectrum"))
        decays = var_list%get_lval (var_str ("?slha_read_decays"))
    end subroutine dispatch_slha

```

28.5.9 Unit tests

Test module, followed by the corresponding implementation module.

```

<slha_interface_ut.f90>≡
    <File header>

    module slha_interface_ut
        use unit_tests
        use slha_interface_uti

    <Standard module head>

    <SLHA: public test>

    contains

    <SLHA: test driver>

    end module slha_interface_ut

<slha_interface_uti.f90>≡
    <File header>

    module slha_interface_uti

    <Use strings>
        use io_units
        use os_interface
        use parser
        use model_data
        use variables
        use models

        use slha_interface

```

<Standard module head>

<SLHA: test declarations>

contains

<SLHA: tests>

end module slha_interface_util

API: driver for the unit tests below.

<SLHA: public test>≡

public :: slha_test

<SLHA: test driver>≡

subroutine slha_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<SLHA: execute tests>

end subroutine slha_test

Checking the basics of the SLHA interface.

<SLHA: execute tests>≡

call test (slha_1, "slha_1", &
"check SLHA interface", &
u, results)

<SLHA: test declarations>≡

public :: slha_1

<SLHA: tests>≡

subroutine slha_1 (u)

integer, intent(in) :: u

type(os_data_t), pointer :: os_data => null ()

type(parse_tree_t), pointer :: parse_tree => null ()

integer :: u_file, iostat

character(80) :: buffer

character(*), parameter :: file_slha = "slha_test.dat"

type(model_list_t) :: model_list

type(model_t), pointer :: model => null ()

type(string_t), dimension(0) :: empty_string_array

write (u, "(A)") "* Test output: SLHA Interface"

write (u, "(A)") "* Purpose: test SLHA file reading and writing"

write (u, "(A)")

write (u, "(A)") "* Initializing"

write (u, "(A)")

allocate (os_data)

allocate (parse_tree)

call os_data%init ()

call syntax_model_file_init ()

call model_list%read_model &

(var_str("MSSM"), var_str("MSSM.mdl"), os_data, model)

```

call syntax_slha_init ()

write (u, "(A)")  "* Reading SLHA file sps1ap_decays.slha"
write (u, "(A)")

call slha_parse_file (var_str ("sps1ap_decays.slha"), &
    empty_string_array, os_data, parse_tree)

write (u, "(A)")  "* Writing the parse tree:"
write (u, "(A)")

call parse_tree_write (parse_tree, u)

write (u, "(A)")  "* Interpreting the parse tree"
write (u, "(A)")

call slha_interpret_parse_tree (parse_tree, model, &
    input=.true., spectrum=.true., decays=.true.)
call parse_tree_final (parse_tree)

write (u, "(A)")  "* Writing out the list of variables (reals only):"
write (u, "(A)")

call var_list_write (model%get_var_list_ptr (), &
    only_type = V_REAL, unit = u)

write (u, "(A)")
write (u, "(A)")  "* Writing SLHA output to '" // file_slha // "'"
write (u, "(A)")

call slha_write_file (var_str (file_slha), model, input=.true., &
    spectrum=.false., decays=.false.)
u_file = free_unit ()
open (u_file, file = file_slha, action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat) buffer
    if (buffer(1:37) == "# Output generated by WHIZARD version") then
        buffer = "[...]"
    end if
    if (iostat /= 0) exit
    write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call parse_tree_final (parse_tree)
deallocate (parse_tree)
deallocate (os_data)

write (u, "(A)")  "* Test output end: slha_1"
write (u, "(A)")

```

```
end subroutine slha_1
```

SLHA interface

This rather trivial sets all input values for the SLHA interface to **false**.

```
<SLHA: execute tests>+≡
  call test (slha_2, "slha_2", &
    "SLHA interface", &
    u, results)

<SLHA: test declarations>+≡
  public :: slha_2

<SLHA: tests>+≡
  subroutine slha_2 (u)
    integer, intent(in) :: u
    type(var_list_t) :: var_list
    logical :: input, spectrum, decays

    write (u, "(A)")  "* Test output: slha_2"
    write (u, "(A)")  "* Purpose: SLHA interface settings"
    write (u, "(A)")

    write (u, "(A)")  "* Default settings"
    write (u, "(A)")

    call var_list%init_defaults (0)
    call dispatch_slha (var_list, &
      input = input, spectrum = spectrum, decays = decays)

    write (u, "(A,1x,L1)")  " slha_read_input      =", input
    write (u, "(A,1x,L1)")  " slha_read_spectrum    =", spectrum
    write (u, "(A,1x,L1)")  " slha_read_decays      =", decays

    call var_list%final ()
    call var_list%init_defaults (0)

    write (u, "(A)")
    write (u, "(A)")  "* Set all entries to [false]"
    write (u, "(A)")

    call var_list%set_log (var_str ("?slha_read_input"), &
      .false., is_known = .true.)
    call var_list%set_log (var_str ("?slha_read_spectrum"), &
      .false., is_known = .true.)
    call var_list%set_log (var_str ("?slha_read_decays"), &
      .false., is_known = .true.)

    call dispatch_slha (var_list, &
      input = input, spectrum = spectrum, decays = decays)

    write (u, "(A,1x,L1)")  " slha_read_input      =", input
    write (u, "(A,1x,L1)")  " slha_read_spectrum    =", spectrum
```

```
write (u, "(A,1x,L1)" " slha_read_decays    =", decays

call var_list%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: slha_2"

end subroutine slha_2
```

Chapter 29

Infrastructure for threshold processes

```
<interpolation.f90>≡  
  <File header>  
  
  module interpolation  
    use kinds  
    implicit none  
    save  
    private  
  
    public :: interpolate_linear, strictly_monotonous  
  
    interface interpolate_linear  
      module procedure interpolate_linear_1D_complex_array, &  
        interpolate_linear_1D_complex_scalar, &  
        interpolate_linear_1D_real_array, &  
        interpolate_linear_1D_real_scalar, &  
        interpolate_linear_2D_complex_array, &  
        interpolate_linear_2D_complex_scalar, &  
        interpolate_linear_2D_real_array, &  
        interpolate_linear_2D_real_scalar, &  
        interpolate_linear_3D_complex_array, &  
        interpolate_linear_3D_complex_scalar, &  
        interpolate_linear_3D_real_array, &  
        interpolate_linear_3D_real_scalar  
    end interface  
  
    interface strictly_monotonous  
      module procedure monotonous  
    end interface strictly_monotonous  
  
    interface find_nearest_left  
      !!! recursive bisection is slower  
      module procedure find_nearest_left_loop  
    end interface find_nearest_left
```

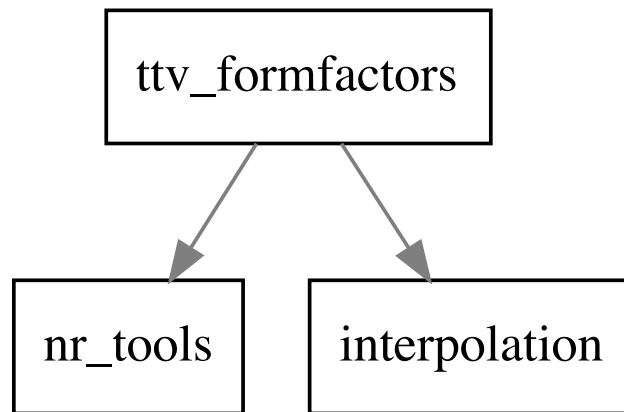



Figure 29.1: Module dependencies in `src/threshold`.

contains

```

pure subroutine interpolate_linear_1D_complex_scalar (xa, ya, x, y)
  real(default), dimension(:), intent(in) :: xa
  complex(default), dimension(:), intent(in) :: ya
  real(default), intent(in) :: x
  complex(default), intent(out) :: y
  integer :: ixl
  real(default) :: t
  y = 0.0_default
  !!! don't check this at runtime:
  ! if ( .not.monotonous(xa) ) return
  if ( out_of_range(xa, x) ) return
  ixl = 0
  call find_nearest_left (xa, x, ixl)
  t = ( x - xa(ixl) ) / ( xa(ixl+1) - xa(ixl) )
  y = (1.-t)*ya(ixl) + t*ya(ixl+1)
end subroutine interpolate_linear_1D_complex_scalar

pure subroutine interpolate_linear_2D_complex_scalar (x1a, x2a, ya, x1, x2, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  complex(default), dimension(:, :), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  complex(default), intent(out) :: y

```

```

integer :: ix1l, ix2l
real(default) :: t, u
y = 0.0_default
!!! don't check this at runtime:
! if ( (.not.monotonous(x1a)) .or. (.not.monotonous(x2a)) ) return
if ( out_of_range(x1a, x1) .or. out_of_range(x2a, x2) ) return
ix1l = 0
call find_nearest_left (x1a, x1, ix1l)
ix2l = 0
call find_nearest_left (x2a, x2, ix2l)
t = ( x1 - x1a(ix1l) ) / ( x1a(ix1l+1) - x1a(ix1l) )
u = ( x2 - x2a(ix2l) ) / ( x2a(ix2l+1) - x2a(ix2l) )
y = (1.-t)*(1.-u)*ya(ix1l ,ix2l ) &
+ t *(1.-u)*ya(ix1l+1,ix2l ) &
+ t * u *ya(ix1l+1,ix2l+1) &
+(1.-t)* u *ya(ix1l ,ix2l+1)
end subroutine interpolate_linear_2D_complex_scalar

pure subroutine interpolate_linear_3D_complex_scalar (x1a, x2a, x3a, ya, x1, x2, x3, y)
real(default), dimension(:), intent(in) :: x1a
real(default), dimension(:), intent(in) :: x2a
real(default), dimension(:), intent(in) :: x3a
complex(default), dimension(:,:), intent(in) :: ya
real(default), intent(in) :: x1
real(default), intent(in) :: x2
real(default), intent(in) :: x3
complex(default), intent(out) :: y
integer :: ix1l, ix2l, ix3l
real(default) :: t, u, v
y = 0.0_default
!!! don't check this at runtime:
! if ( (.not.monotonous(x1a)) .or. (.not.monotonous(x2a)) ) return
if ( out_of_range(x1a, x1) .or. out_of_range(x2a, x2) .or. out_of_range(x3a, x3) ) return
ix1l = 0
call find_nearest_left (x1a, x1, ix1l)
ix2l = 0
call find_nearest_left (x2a, x2, ix2l)
ix3l = 0
call find_nearest_left (x3a, x3, ix3l)
t = ( x1 - x1a(ix1l) ) / ( x1a(ix1l+1) - x1a(ix1l) )
u = ( x2 - x2a(ix2l) ) / ( x2a(ix2l+1) - x2a(ix2l) )
v = ( x3 - x3a(ix3l) ) / ( x3a(ix3l+1) - x3a(ix3l) )
y = (1.-t)*(1.-u)*(1.-v)*ya(ix1l ,ix2l ,ix3l ) &
+(1.-t)*(1.-u)* v *ya(ix1l ,ix2l ,ix3l+1) &
+(1.-t)* u *(1.-v)*ya(ix1l ,ix2l+1,ix3l ) &
+(1.-t)* u * v *ya(ix1l ,ix2l+1,ix3l+1) &
+ t *(1.-u)*(1.-v)*ya(ix1l+1,ix2l ,ix3l ) &
+ t *(1.-u)* v *ya(ix1l+1,ix2l ,ix3l+1) &
+ t * u *(1.-v)*ya(ix1l+1,ix2l+1,ix3l ) &
+ t * u * v *ya(ix1l+1,ix2l+1,ix3l+1)
end subroutine interpolate_linear_3D_complex_scalar

pure subroutine find_nearest_left_loop (xa, x, ixl)
real(default), dimension(:), intent(in) :: xa

```

```

real(default), intent(in) :: x
integer, intent(out) :: ixl
integer :: ixm, ixr
ixl = 1
ixr = size(xa)
do
  if ( ixr-ixl <= 1 ) return
  ixm = (ixr+ixl) / 2
  if ( x < xa(ixm) ) then
    ixr = ixm
  else
    ixl = ixm
  end if
end do
end subroutine find_nearest_left_loop

pure recursive subroutine find_nearest_left_rec (xa, x, ixl)
  real(default), dimension(:), intent(in) :: xa
  real(default), intent(in) :: x
  integer, intent(inout) :: ixl
  integer :: nx, bs
  real(default), dimension(:), allocatable :: xa_new
  nx = size(xa)
  bs = nx/2 + 1
  if ( nx < 3 ) then
    ixl = ixl + bs - 1
    return
  else
    if ( x < xa(bs) ) then
      allocate( xa_new(1:bs) )
      xa_new = xa(1:bs)
    else
      ixl = ixl + bs - 1
      allocate( xa_new(bs:nx) )
      xa_new = xa(bs:nx)
    end if
    call find_nearest_left_rec (xa_new, x, ixl)
    deallocate( xa_new )
  end if
end subroutine find_nearest_left_rec

pure function monotonous (xa) result (flag)
  real(default), dimension(:), intent(in) :: xa
  integer :: ix
  logical :: flag
  flag = .false.
  do ix = 1, size(xa)-1
    flag = ( xa(ix) < xa(ix+1) )
    if ( .not. flag ) return
  end do
end function monotonous

pure function out_of_range (xa, x) result (flag)
  real(default), dimension(:), intent(in) :: xa

```

```

    real(default), intent(in) :: x
    logical :: flag
    flag = ( x < xa(1) .or. x > xa(size(xa)) )
end function out_of_range

pure subroutine interpolate_linear_1D_complex_array (xa, ya, x, y)
    real(default), dimension(:), intent(in) :: xa
    complex(default), dimension(:,:), intent(in) :: ya
    real(default), intent(in) :: x
    complex(default), dimension(size(ya(1,:))), intent(out) :: y
    integer :: iy
    do iy=1, size(y)
        call interpolate_linear_1D_complex_scalar (xa, ya(:,iy), x, y(iy))
    end do
end subroutine interpolate_linear_1D_complex_array

pure subroutine interpolate_linear_1D_real_array (xa, ya, x, y)
    real(default), dimension(:), intent(in) :: xa
    real(default), dimension(:,:), intent(in) :: ya
    real(default), intent(in) :: x
    real(default), dimension(:), intent(out) :: y
    complex(default), dimension(size(ya(1,:))) :: y_c
    call interpolate_linear_1D_complex_array (xa, cmplx(ya,kind=default), x, y_c)
    y = real(y_c,kind=default)
end subroutine interpolate_linear_1D_real_array

pure subroutine interpolate_linear_1D_real_scalar (xa, ya, x, y)
    real(default), dimension(:), intent(in) :: xa
    real(default), dimension(:), intent(in) :: ya
    real(default), intent(in) :: x
    real(default), intent(out) :: y
    complex(default), dimension(size(ya)) :: ya_c
    complex(default) :: y_c
    ya_c = cmplx(ya,kind=default)
    call interpolate_linear_1D_complex_scalar (xa, ya_c, x, y_c)
    y = real(y_c,kind=default)
end subroutine interpolate_linear_1D_real_scalar

pure subroutine interpolate_linear_2D_complex_array (x1a, x2a, ya, x1, x2, y)
    real(default), dimension(:), intent(in) :: x1a
    real(default), dimension(:), intent(in) :: x2a
    complex(default), dimension(:,:,:), intent(in) :: ya
    real(default), intent(in) :: x1
    real(default), intent(in) :: x2
    complex(default), dimension(size(ya(1,1,:))), intent(out) :: y
    integer :: iy
    do iy=1, size(y)
        call interpolate_linear_2D_complex_scalar (x1a, x2a, ya(:, :, iy), x1, x2, y(iy))
    end do
end subroutine interpolate_linear_2D_complex_array

pure subroutine interpolate_linear_2D_real_array (x1a, x2a, ya, x1, x2, y)
    real(default), dimension(:), intent(in) :: x1a
    real(default), dimension(:), intent(in) :: x2a

```

```

real(default), dimension(:,:,:), intent(in) :: ya
real(default), intent(in) :: x1
real(default), intent(in) :: x2
real(default), dimension(:), intent(out) :: y
complex(default), dimension(size(ya(1,1,:))) :: y_c
call interpolate_linear_2D_complex_array (x1a, x2a, cmplx(ya,kind=default), x1, x2, y_c)
y = real(y_c,kind=default)
end subroutine interpolate_linear_2D_real_array

pure subroutine interpolate_linear_2D_real_scalar (x1a, x2a, ya, x1, x2, y)
real(default), dimension(:), intent(in) :: x1a
real(default), dimension(:), intent(in) :: x2a
real(default), dimension(:,:), intent(in) :: ya
real(default), intent(in) :: x1
real(default), intent(in) :: x2
real(default), intent(out) :: y
complex(default), dimension(size(ya(:,1)),size(ya(1,:))) :: ya_c
complex(default) :: y_c
ya_c = reshape (ya_c, shape(ya))
ya_c = cmplx(ya,kind=default)
call interpolate_linear_2D_complex_scalar (x1a, x2a, ya_c, x1, x2, y_c)
y = real(y_c,kind=default)
end subroutine interpolate_linear_2D_real_scalar

pure subroutine interpolate_linear_3D_complex_array (x1a, x2a, x3a, ya, x1, x2, x3, y)
real(default), dimension(:), intent(in) :: x1a
real(default), dimension(:), intent(in) :: x2a
real(default), dimension(:), intent(in) :: x3a
complex(default), dimension(:,:,:), intent(in) :: ya
real(default), intent(in) :: x1
real(default), intent(in) :: x2
real(default), intent(in) :: x3
complex(default), dimension(size(ya(1,1,1,:))), intent(out) :: y
integer :: iy
do iy=1, size(y)
    call interpolate_linear_3D_complex_scalar &
        (x1a, x2a, x3a, ya(:, :, :, iy), x1, x2, x3, y(iy))
end do
end subroutine interpolate_linear_3D_complex_array

pure subroutine interpolate_linear_3D_real_array (x1a, x2a, x3a, ya, x1, x2, x3, y)
real(default), dimension(:), intent(in) :: x1a
real(default), dimension(:), intent(in) :: x2a
real(default), dimension(:), intent(in) :: x3a
real(default), dimension(:,:,:), intent(in) :: ya
real(default), intent(in) :: x1
real(default), intent(in) :: x2
real(default), intent(in) :: x3
real(default), dimension(:), intent(out) :: y
complex(default), dimension(size(ya(1,1,1,:))) :: y_c
call interpolate_linear_3D_complex_array &
    (x1a, x2a, x3a, cmplx(ya,kind=default), x1, x2, x3, y_c)
y = real(y_c,kind=default)
end subroutine interpolate_linear_3D_real_array

```

```

pure subroutine interpolate_linear_3D_real_scalar (x1a, x2a, x3a, ya, x1, x2, x3, y)
  real(default), dimension(:), intent(in) :: x1a
  real(default), dimension(:), intent(in) :: x2a
  real(default), dimension(:), intent(in) :: x3a
  real(default), dimension(:,:,:), intent(in) :: ya
  real(default), intent(in) :: x1
  real(default), intent(in) :: x2
  real(default), intent(in) :: x3
  real(default), intent(out) :: y
  complex(default), dimension(size(ya(:,1,1)),size(ya(1,:,1)),size(ya(1,1,:))) :: ya_c
  complex(default) :: y_c
  ya_c = cmplx(ya,kind=default)
  call interpolate_linear_3D_complex_scalar (x1a, x2a, x3a, ya_c, x1, x2, x3, y_c)
  y = real(y_c,kind=default)
end subroutine interpolate_linear_3D_real_scalar
end module interpolation

(nr_tools.f90)≡
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
! WHIZARD Version Date

! routine hypgeo and other useful procedures from:
!
! Numerical Recipes in Fortran 77 and 90 (Second Edition)
!
! Book and code Copyright (c) 1986-2001,
! William H. Press, Saul A. Teukolsky,
! William T. Vetterling, Brian P. Flannery.
!
! Information at http://www.nr.com
!
!
!
! FB: -replaced tabs by 2 whitespaces
!      -reduced hardcoded default stepsize for subroutine 'odeint'
!      called by hypgeo, cf. line 4751
!      -added explicit interface for function 'qgaus' to main module 'nr'
!      -renamed function 'locate' to 'locatenr' to avoid segfault (???)
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

MODULE nrtype
  INTEGER, PARAMETER :: I4B = SELECTED_INT_KIND(9)
  INTEGER, PARAMETER :: I2B = SELECTED_INT_KIND(4)
  INTEGER, PARAMETER :: I1B = SELECTED_INT_KIND(2)
  INTEGER, PARAMETER :: SP = KIND(1.0)
  INTEGER, PARAMETER :: DP = KIND(1.0D0)
  INTEGER, PARAMETER :: SPC = KIND((1.0,1.0))
  INTEGER, PARAMETER :: DPC = KIND((1.0D0,1.0D0))
  INTEGER, PARAMETER :: LGT = KIND(.true.)
  REAL(SP), PARAMETER :: PI=3.141592653589793238462643383279502884197_sp
  REAL(SP), PARAMETER :: PI02=1.57079632679489661923132169163975144209858_sp

```

```

REAL(SP), PARAMETER :: TWOPI=6.283185307179586476925286766559005768394_sp
REAL(SP), PARAMETER :: SQRT2=1.41421356237309504880168872420969807856967_sp
REAL(SP), PARAMETER :: EULER=0.5772156649015328606065120900824024310422_sp
REAL(DP), PARAMETER :: PI_D=3.141592653589793238462643383279502884197_dp
REAL(DP), PARAMETER :: PI02_D=1.57079632679489661923132169163975144209858_dp
REAL(DP), PARAMETER :: TWOPI_D=6.283185307179586476925286766559005768394_dp
TYPE sprs2_sp
  INTEGER(I4B) :: n,len
  REAL(SP), DIMENSION(:), POINTER :: val
  INTEGER(I4B), DIMENSION(:), POINTER :: irow
  INTEGER(I4B), DIMENSION(:), POINTER :: jcol
END TYPE sprs2_sp
TYPE sprs2_dp
  INTEGER(I4B) :: n,len
  REAL(DP), DIMENSION(:), POINTER :: val
  INTEGER(I4B), DIMENSION(:), POINTER :: irow
  INTEGER(I4B), DIMENSION(:), POINTER :: jcol
END TYPE sprs2_dp
END MODULE nrtype

MODULE nrutil
  USE nrtype
  IMPLICIT NONE
  INTEGER(I4B), PARAMETER :: NPAR_ARTH=16,NPAR2_ARTH=8
  INTEGER(I4B), PARAMETER :: NPAR_GEOP=4,NPAR2_GEOP=2
  INTEGER(I4B), PARAMETER :: NPAR_CUMSUM=16
  INTEGER(I4B), PARAMETER :: NPAR_CUMPROD=8
  INTEGER(I4B), PARAMETER :: NPAR_POLY=8
  INTEGER(I4B), PARAMETER :: NPAR_POLYTERM=8
  INTERFACE array_copy
    MODULE PROCEDURE array_copy_r, array_copy_d, array_copy_i
  END INTERFACE
  INTERFACE swap
    MODULE PROCEDURE swap_i,swap_r,swap_rv,swap_c, &
      swap_cv,swap_cm,swap_z,swap_zv,swap_zm, &
      masked_swap_rs,masked_swap_rv,masked_swap_rm
  END INTERFACE
  INTERFACE reallocate
    MODULE PROCEDURE reallocate_rv,reallocate_rm,&
      reallocate_iv,reallocate_im,reallocate_hv
  END INTERFACE
  INTERFACE imaxloc
    MODULE PROCEDURE imaxloc_r,imaxloc_i
  END INTERFACE
  INTERFACE assert
    MODULE PROCEDURE assert1,assert2,assert3,assert4,assert_v
  END INTERFACE
  INTERFACE assert_eq
    MODULE PROCEDURE assert_eq2,assert_eq3,assert_eq4,assert_eqn
  END INTERFACE
  INTERFACE arth
    MODULE PROCEDURE arth_r, arth_d, arth_i
  END INTERFACE
  INTERFACE geop

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MODULE PROCEDURE geop_r, geop_d, geop_i, geop_c, geop_dv
END INTERFACE
INTERFACE cumsum
MODULE PROCEDURE cumsum_r, cumsum_i
END INTERFACE
INTERFACE poly
MODULE PROCEDURE poly_rr, poly_rrv, poly_dd, poly_ddv, &
poly_rc, poly_cc, poly_msk_rrv, poly_msk_ddv
END INTERFACE
INTERFACE poly_term
MODULE PROCEDURE poly_term_rr, poly_term_cc
END INTERFACE
INTERFACE outerprod
MODULE PROCEDURE outerprod_r, outerprod_d
END INTERFACE
INTERFACE outerdiff
MODULE PROCEDURE outerdiff_r, outerdiff_d, outerdiff_i
END INTERFACE
INTERFACE scatter_add
MODULE PROCEDURE scatter_add_r, scatter_add_d
END INTERFACE
INTERFACE scatter_max
MODULE PROCEDURE scatter_max_r, scatter_max_d
END INTERFACE
INTERFACE diagadd
MODULE PROCEDURE diagadd_rv, diagadd_r
END INTERFACE
INTERFACE diagmult
MODULE PROCEDURE diagmult_rv, diagmult_r
END INTERFACE
INTERFACE get_diag
MODULE PROCEDURE get_diag_rv, get_diag_dv
END INTERFACE
INTERFACE put_diag
MODULE PROCEDURE put_diag_rv, put_diag_r
END INTERFACE
CONTAINS
!BL
SUBROUTINE array_copy_r(src, dest, n_copied, n_not_copied)
REAL(SP), DIMENSION(:), INTENT(IN) :: src
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
n_copied=min(size(src), size(dest))
n_not_copied=size(src)-n_copied
dest(1:n_copied)=src(1:n_copied)
END SUBROUTINE array_copy_r
!BL
SUBROUTINE array_copy_d(src, dest, n_copied, n_not_copied)
REAL(DP), DIMENSION(:), INTENT(IN) :: src
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
n_copied=min(size(src), size(dest))
n_not_copied=size(src)-n_copied
dest(1:n_copied)=src(1:n_copied)

```



```

      END SUBROUTINE array_copy_d
!BL
      SUBROUTINE array_copy_i(src,dest,n_copied,n_not_copied)
      INTEGER(I4B), DIMENSION(:), INTENT(IN) :: src
      INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: dest
      INTEGER(I4B), INTENT(OUT) :: n_copied, n_not_copied
      n_copied=min(size(src),size(dest))
      n_not_copied=size(src)-n_copied
      dest(1:n_copied)=src(1:n_copied)
      END SUBROUTINE array_copy_i
!BL
!BL
      SUBROUTINE swap_i(a,b)
      INTEGER(I4B), INTENT(INOUT) :: a,b
      INTEGER(I4B) :: dum
      dum=a
      a=b
      b=dum
      END SUBROUTINE swap_i
!BL
      SUBROUTINE swap_r(a,b)
      REAL(SP), INTENT(INOUT) :: a,b
      REAL(SP) :: dum
      dum=a
      a=b
      b=dum
      END SUBROUTINE swap_r
!BL
      SUBROUTINE swap_rv(a,b)
      REAL(SP), DIMENSION(:), INTENT(INOUT) :: a,b
      REAL(SP), DIMENSION(SIZE(a)) :: dum
      dum=a
      a=b
      b=dum
      END SUBROUTINE swap_rv
!BL
      SUBROUTINE swap_c(a,b)
      COMPLEX(SPC), INTENT(INOUT) :: a,b
      COMPLEX(SPC) :: dum
      dum=a
      a=b
      b=dum
      END SUBROUTINE swap_c
!BL
      SUBROUTINE swap_cv(a,b)
      COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: a,b
      COMPLEX(SPC), DIMENSION(SIZE(a)) :: dum
      dum=a
      a=b
      b=dum
      END SUBROUTINE swap_cv
!BL
      SUBROUTINE swap_cm(a,b)
      COMPLEX(SPC), DIMENSION(:,,:), INTENT(INOUT) :: a,b

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        COMPLEX(SPC), DIMENSION(size(a,1),size(a,2)) :: dum
        dum=a
        a=b
        b=dum
    END SUBROUTINE swap_cm
!BL
    SUBROUTINE swap_z(a,b)
    COMPLEX(DPC), INTENT(INOUT) :: a,b
    COMPLEX(DPC) :: dum
    dum=a
    a=b
    b=dum
    END SUBROUTINE swap_z
!BL
    SUBROUTINE swap_zv(a,b)
    COMPLEX(DPC), DIMENSION(:), INTENT(INOUT) :: a,b
    COMPLEX(DPC), DIMENSION(SIZE(a)) :: dum
    dum=a
    a=b
    b=dum
    END SUBROUTINE swap_zv
!BL
    SUBROUTINE swap_zm(a,b)
    COMPLEX(DPC), DIMENSION(:,:), INTENT(INOUT) :: a,b
    COMPLEX(DPC), DIMENSION(size(a,1),size(a,2)) :: dum
    dum=a
    a=b
    b=dum
    END SUBROUTINE swap_zm
!BL
    SUBROUTINE masked_swap_rs(a,b,mask)
    REAL(SP), INTENT(INOUT) :: a,b
    LOGICAL(LGT), INTENT(IN) :: mask
    REAL(SP) :: swp
    if (mask) then
        swp=a
        a=b
        b=swp
    end if
    END SUBROUTINE masked_swap_rs
!BL
    SUBROUTINE masked_swap_rv(a,b,mask)
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: a,b
    LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
    REAL(SP), DIMENSION(size(a)) :: swp
    where (mask)
        swp=a
        a=b
        b=swp
    end where
    END SUBROUTINE masked_swap_rv
!BL
    SUBROUTINE masked_swap_rm(a,b,mask)
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a,b

```

```

LOGICAL(LGT), DIMENSION(:,:), INTENT(IN) :: mask
REAL(SP), DIMENSION(size(a,1),size(a,2)) :: swp
where (mask)
    swp=a
    a=b
    b=swp
end where
END SUBROUTINE masked_swap_rm
!BL
!BL
FUNCTION reallocate_rv(p,n)
REAL(SP), DIMENSION(:), POINTER :: p, reallocate_rv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_rv(n),stat=ierr)
if (ierr /= 0) call &
    nrerror('reallocate_rv: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p)
reallocate_rv(1:min(nold,n))=p(1:min(nold,n))
deallocate(p)
END FUNCTION reallocate_rv
!BL
FUNCTION reallocate_iv(p,n)
INTEGER(I4B), DIMENSION(:), POINTER :: p, reallocate_iv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_iv(n),stat=ierr)
if (ierr /= 0) call &
    nrerror('reallocate_iv: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p)
reallocate_iv(1:min(nold,n))=p(1:min(nold,n))
deallocate(p)
END FUNCTION reallocate_iv
!BL
FUNCTION reallocate_hv(p,n)
CHARACTER(1), DIMENSION(:), POINTER :: p, reallocate_hv
INTEGER(I4B), INTENT(IN) :: n
INTEGER(I4B) :: nold,ierr
allocate(reallocate_hv(n),stat=ierr)
if (ierr /= 0) call &
    nrerror('reallocate_hv: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p)
reallocate_hv(1:min(nold,n))=p(1:min(nold,n))
deallocate(p)
END FUNCTION reallocate_hv
!BL
FUNCTION reallocate_rm(p,n,m)
REAL(SP), DIMENSION(:,:), POINTER :: p, reallocate_rm
INTEGER(I4B), INTENT(IN) :: n,m
INTEGER(I4B) :: nold,mold,ierr
allocate(reallocate_rm(n,m),stat=ierr)

```

```

    if (ierr /= 0) call &
        nrerror('reallocate_rm: problem in attempt to allocate memory')
    if (.not. associated(p)) RETURN
    nold=size(p,1)
    mold=size(p,2)
    reallocate_rm(1:min(nold,n),1:min(mold,m))=&
        p(1:min(nold,n),1:min(mold,m))
    deallocate(p)
END FUNCTION reallocate_rm
!BL
FUNCTION reallocate_im(p,n,m)
INTEGER(I4B), DIMENSION(:,:), POINTER :: p, reallocate_im
INTEGER(I4B), INTENT(IN) :: n,m
INTEGER(I4B) :: nold,mold,ierr
allocate(reallocate_im(n,m),stat=ierr)
if (ierr /= 0) call &
    nrerror('reallocate_im: problem in attempt to allocate memory')
if (.not. associated(p)) RETURN
nold=size(p,1)
mold=size(p,2)
reallocate_im(1:min(nold,n),1:min(mold,m))=&
    p(1:min(nold,n),1:min(mold,m))
deallocate(p)
END FUNCTION reallocate_im
!BL
FUNCTION ifirstloc(mask)
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
INTEGER(I4B) :: ifirstloc
INTEGER(I4B), DIMENSION(1) :: loc
loc=maxloc(merge(1,0,mask))
ifirstloc=loc(1)
if (.not. mask(ifirstloc)) ifirstloc=size(mask)+1
END FUNCTION ifirstloc
!BL
FUNCTION imaxloc_r(arr)
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B) :: imaxloc_r
INTEGER(I4B), DIMENSION(1) :: imax
imax=maxloc(arr(:))
imaxloc_r=imax(1)
END FUNCTION imaxloc_r
!BL
FUNCTION imaxloc_i(iarr)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: iarr
INTEGER(I4B), DIMENSION(1) :: imax
INTEGER(I4B) :: imaxloc_i
imax=maxloc(iarr(:))
imaxloc_i=imax(1)
END FUNCTION imaxloc_i
!BL
FUNCTION iminloc(arr)
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B), DIMENSION(1) :: imin
INTEGER(I4B) :: iminloc

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```

imin=minloc(arr(:))
iminloc=imin(1)
END FUNCTION iminloc
!BL
SUBROUTINE assert1(n1,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1
if (.not. n1) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert1'
end if
END SUBROUTINE assert1
!BL
SUBROUTINE assert2(n1,n2,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2
if (.not. (n1 .and. n2)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert2'
end if
END SUBROUTINE assert2
!BL
SUBROUTINE assert3(n1,n2,n3,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2,n3
if (.not. (n1 .and. n2 .and. n3)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert3'
end if
END SUBROUTINE assert3
!BL
SUBROUTINE assert4(n1,n2,n3,n4,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, INTENT(IN) :: n1,n2,n3,n4
if (.not. (n1 .and. n2 .and. n3 .and. n4)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert4'
end if
END SUBROUTINE assert4
!BL
SUBROUTINE assert_v(n,string)
CHARACTER(LEN=*), INTENT(IN) :: string
LOGICAL, DIMENSION(:), INTENT(IN) :: n
if (.not. all(n)) then
    write (*,*) 'nrerror: an assertion failed with this tag:', &
        string
    STOP 'program terminated by assert_v'
end if
END SUBROUTINE assert_v
!BL

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```

FUNCTION assert_eq2(n1,n2,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2
INTEGER :: assert_eq2
if (n1 == n2) then
    assert_eq2=n1
else
    write (*,*) 'nrerror: an assert_eq failed with this tag:', &
        string
    STOP 'program terminated by assert_eq2'
end if
END FUNCTION assert_eq2
!BL
FUNCTION assert_eq3(n1,n2,n3,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2,n3
INTEGER :: assert_eq3
if (n1 == n2 .and. n2 == n3) then
    assert_eq3=n1
else
    write (*,*) 'nrerror: an assert_eq failed with this tag:', &
        string
    STOP 'program terminated by assert_eq3'
end if
END FUNCTION assert_eq3
!BL
FUNCTION assert_eq4(n1,n2,n3,n4,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, INTENT(IN) :: n1,n2,n3,n4
INTEGER :: assert_eq4
if (n1 == n2 .and. n2 == n3 .and. n3 == n4) then
    assert_eq4=n1
else
    write (*,*) 'nrerror: an assert_eq failed with this tag:', &
        string
    STOP 'program terminated by assert_eq4'
end if
END FUNCTION assert_eq4
!BL
FUNCTION assert_eqn(nn,string)
CHARACTER(LEN=*), INTENT(IN) :: string
INTEGER, DIMENSION(:), INTENT(IN) :: nn
INTEGER :: assert_eqn
if (all(nn(2:) == nn(1))) then
    assert_eqn=nn(1)
else
    write (*,*) 'nrerror: an assert_eq failed with this tag:', &
        string
    STOP 'program terminated by assert_eqn'
end if
END FUNCTION assert_eqn
!BL
SUBROUTINE nrerror(string)
CHARACTER(LEN=*), INTENT(IN) :: string

```

```

write (*,*) 'nrerror: ',string
STOP 'program terminated by nrerror'
END SUBROUTINE nrerror
!BL
FUNCTION arth_r(first,increment,n)
REAL(SP), INTENT(IN) :: first,increment
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(n) :: arth_r
INTEGER(I4B) :: k,k2
REAL(SP) :: temp
if (n > 0) arth_r(1)=first
if (n <= NPAR_ARTH) then
do k=2,n
arth_r(k)=arth_r(k-1)+increment
end do
else
do k=2,NPAR2_ARTH
arth_r(k)=arth_r(k-1)+increment
end do
temp=increment*NPAR2_ARTH
k=NPAR2_ARTH
do
if (k >= n) exit
k2=k+k
arth_r(k+1:min(k2,n))=temp+arth_r(1:min(k,n-k))
temp=temp+temp
k=k2
end do
end if
END FUNCTION arth_r
!BL
FUNCTION arth_d(first,increment,n)
REAL(DP), INTENT(IN) :: first,increment
INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(n) :: arth_d
INTEGER(I4B) :: k,k2
REAL(DP) :: temp
if (n > 0) arth_d(1)=first
if (n <= NPAR_ARTH) then
do k=2,n
arth_d(k)=arth_d(k-1)+increment
end do
else
do k=2,NPAR2_ARTH
arth_d(k)=arth_d(k-1)+increment
end do
temp=increment*NPAR2_ARTH
k=NPAR2_ARTH
do
if (k >= n) exit
k2=k+k
arth_d(k+1:min(k2,n))=temp+arth_d(1:min(k,n-k))
temp=temp+temp
k=k2
end do

```

```

        end do
    end if
END FUNCTION arth_d
!BL
FUNCTION arth_i(first,increment,n)
INTEGER(I4B), INTENT(IN) :: first,increment,n
INTEGER(I4B), DIMENSION(n) :: arth_i
INTEGER(I4B) :: k,k2,temp
if (n > 0) arth_i(1)=first
if (n <= NPAR_ARTH) then
    do k=2,n
        arth_i(k)=arth_i(k-1)+increment
    end do
else
    do k=2,NPAR2_ARTH
        arth_i(k)=arth_i(k-1)+increment
    end do
    temp=increment*NPAR2_ARTH
    k=NPAR2_ARTH
    do
        if (k >= n) exit
        k2=k+k
        arth_i(k+1:min(k2,n))=temp+arth_i(1:min(k,n-k))
        temp=temp+temp
        k=k2
    end do
end if
END FUNCTION arth_i
!BL
!BL
FUNCTION geop_r(first,factor,n)
REAL(SP), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(n) :: geop_r
INTEGER(I4B) :: k,k2
REAL(SP) :: temp
if (n > 0) geop_r(1)=first
if (n <= NPAR_GEOP) then
    do k=2,n
        geop_r(k)=geop_r(k-1)*factor
    end do
else
    do k=2,NPAR2_GEOP
        geop_r(k)=geop_r(k-1)*factor
    end do
    temp=factor**NPAR2_GEOP
    k=NPAR2_GEOP
    do
        if (k >= n) exit
        k2=k+k
        geop_r(k+1:min(k2,n))=temp*geop_r(1:min(k,n-k))
        temp=temp*temp
        k=k2
    end do

```



```

end if
END FUNCTION geop_r
!BL
FUNCTION geop_d(first,factor,n)
REAL(DP), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(n) :: geop_d
INTEGER(I4B) :: k,k2
REAL(DP) :: temp
if (n > 0) geop_d(1)=first
if (n <= NPAR_GEOP) then
do k=2,n
geop_d(k)=geop_d(k-1)*factor
end do
else
do k=2,NPAR2_GEOP
geop_d(k)=geop_d(k-1)*factor
end do
temp=factor**NPAR2_GEOP
k=NPAR2_GEOP
do
if (k >= n) exit
k2=k+k
geop_d(k+1:min(k2,n))=temp*geop_d(1:min(k,n-k))
temp=temp*temp
k=k2
end do
end if
END FUNCTION geop_d
!BL
FUNCTION geop_i(first,factor,n)
INTEGER(I4B), INTENT(IN) :: first,factor,n
INTEGER(I4B), DIMENSION(n) :: geop_i
INTEGER(I4B) :: k,k2,temp
if (n > 0) geop_i(1)=first
if (n <= NPAR_GEOP) then
do k=2,n
geop_i(k)=geop_i(k-1)*factor
end do
else
do k=2,NPAR2_GEOP
geop_i(k)=geop_i(k-1)*factor
end do
temp=factor**NPAR2_GEOP
k=NPAR2_GEOP
do
if (k >= n) exit
k2=k+k
geop_i(k+1:min(k2,n))=temp*geop_i(1:min(k,n-k))
temp=temp*temp
k=k2
end do
end if
END FUNCTION geop_i

```

```

!BL
FUNCTION geop_c(first,factor,n)
COMPLEX(SP), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
COMPLEX(SP), DIMENSION(n) :: geop_c
INTEGER(I4B) :: k,k2
COMPLEX(SP) :: temp
if (n > 0) geop_c(1)=first
if (n <= NPAR_GEOP) then
  do k=2,n
    geop_c(k)=geop_c(k-1)*factor
  end do
else
  do k=2,NPAR2_GEOP
    geop_c(k)=geop_c(k-1)*factor
  end do
  temp=factor**NPAR2_GEOP
  k=NPAR2_GEOP
  do
    if (k >= n) exit
    k2=k+k
    geop_c(k+1:min(k2,n))=temp*geop_c(1:min(k,n-k))
    temp=temp*temp
    k=k2
  end do
end if
END FUNCTION geop_c
!BL
FUNCTION geop_dv(first,factor,n)
REAL(DP), DIMENSION(:), INTENT(IN) :: first,factor
INTEGER(I4B), INTENT(IN) :: n
REAL(DP), DIMENSION(size(first),n) :: geop_dv
INTEGER(I4B) :: k,k2
REAL(DP), DIMENSION(size(first)) :: temp
if (n > 0) geop_dv(:,1)=first(:)
if (n <= NPAR_GEOP) then
  do k=2,n
    geop_dv(:,k)=geop_dv(:,k-1)*factor(:)
  end do
else
  do k=2,NPAR2_GEOP
    geop_dv(:,k)=geop_dv(:,k-1)*factor(:)
  end do
  temp=factor**NPAR2_GEOP
  k=NPAR2_GEOP
  do
    if (k >= n) exit
    k2=k+k
    geop_dv(:,k+1:min(k2,n))=geop_dv(:,1:min(k,n-k))*&
      spread(temp,2,size(geop_dv(:,1:min(k,n-k)),2))
    temp=temp*temp
    k=k2
  end do
end if

```

```

END FUNCTION geop_dv
!BL
!BL
RECURSIVE FUNCTION cumsum_r(arr,seed) RESULT(ans)
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
REAL(SP), OPTIONAL, INTENT(IN) :: seed
REAL(SP), DIMENSION(size(arr)) :: ans
INTEGER(I4B) :: n,j
REAL(SP) :: sd
n=size(arr)
if (n == 0_i4b) RETURN
sd=0.0_sp
if (present(seed)) sd=seed
ans(1)=arr(1)+sd
if (n < NPAR_CUMSUM) then
  do j=2,n
    ans(j)=ans(j-1)+arr(j)
  end do
else
  ans(2:n:2)=cumsum_r(arr(2:n:2)+arr(1:n-1:2),sd)
  ans(3:n:2)=ans(2:n-1:2)+arr(3:n:2)
end if
END FUNCTION cumsum_r
!BL
RECURSIVE FUNCTION cumsum_i(arr,seed) RESULT(ans)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B), OPTIONAL, INTENT(IN) :: seed
INTEGER(I4B), DIMENSION(size(arr)) :: ans
INTEGER(I4B) :: n,j,sd
n=size(arr)
if (n == 0_i4b) RETURN
sd=0_i4b
if (present(seed)) sd=seed
ans(1)=arr(1)+sd
if (n < NPAR_CUMSUM) then
  do j=2,n
    ans(j)=ans(j-1)+arr(j)
  end do
else
  ans(2:n:2)=cumsum_i(arr(2:n:2)+arr(1:n-1:2),sd)
  ans(3:n:2)=ans(2:n-1:2)+arr(3:n:2)
end if
END FUNCTION cumsum_i
!BL
!BL
RECURSIVE FUNCTION cumprod(arr,seed) RESULT(ans)
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
REAL(SP), OPTIONAL, INTENT(IN) :: seed
REAL(SP), DIMENSION(size(arr)) :: ans
INTEGER(I4B) :: n,j
REAL(SP) :: sd
n=size(arr)
if (n == 0_i4b) RETURN
sd=1.0_sp

```

```

if (present(seed)) sd=seed
ans(1)=arr(1)*sd
if (n < NPAR_CUMPROD) then
  do j=2,n
    ans(j)=ans(j-1)*arr(j)
  end do
else
  ans(2:n:2)=cumprod(arr(2:n:2)*arr(1:n-1:2),sd)
  ans(3:n:2)=ans(2:n-1:2)*arr(3:n:2)
end if
END FUNCTION cumprod
!BL
!BL
FUNCTION poly_rr(x,coeffs)
REAL(SP), INTENT(IN) :: x
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs
REAL(SP) :: poly_rr
REAL(SP) :: pow
REAL(SP), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n <= 0) then
  poly_rr=0.0_sp
else if (n < NPAR_POLY) then
  poly_rr=coeffs(n)
  do i=n-1,1,-1
    poly_rr=x*poly_rr+coeffs(i)
  end do
else
  allocate(vec(n+1))
  pow=x
  vec(1:n)=coeffs
  do
    vec(n+1)=0.0_sp
    nn=ishft(n+1,-1)
    vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
    if (nn == 1) exit
    pow=pow*pow
    n=nn
  end do
  poly_rr=vec(1)
  deallocate(vec)
end if
END FUNCTION poly_rr
!BL
FUNCTION poly_dd(x,coeffs)
REAL(DP), INTENT(IN) :: x
REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs
REAL(DP) :: poly_dd
REAL(DP) :: pow
REAL(DP), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n <= 0) then

```

```

        poly_dd=0.0_dp
    else if (n < NPAR_POLY) then
        poly_dd=coeffs(n)
        do i=n-1,1,-1
            poly_dd=x*poly_dd+coeffs(i)
        end do
    else
        allocate(vec(n+1))
        pow=x
        vec(1:n)=coeffs
        do
            vec(n+1)=0.0_dp
            nn=ishft(n+1,-1)
            vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
            if (nn == 1) exit
            pow=pow*pow
            n=nn
        end do
        poly_dd=vec(1)
        deallocate(vec)
    end if
END FUNCTION poly_dd
!BL
FUNCTION poly_rc(x,coeffs)
COMPLEX(SPC), INTENT(IN) :: x
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs
COMPLEX(SPC) :: poly_rc
COMPLEX(SPC) :: pow
COMPLEX(SPC), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n <= 0) then
    poly_rc=0.0_sp
else if (n < NPAR_POLY) then
    poly_rc=coeffs(n)
    do i=n-1,1,-1
        poly_rc=x*poly_rc+coeffs(i)
    end do
else
    allocate(vec(n+1))
    pow=x
    vec(1:n)=coeffs
    do
        vec(n+1)=0.0_sp
        nn=ishft(n+1,-1)
        vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
        if (nn == 1) exit
        pow=pow*pow
        n=nn
    end do
    poly_rc=vec(1)
    deallocate(vec)
end if
END FUNCTION poly_rc

```

```

!BL
FUNCTION poly_cc(x,coeffs)
COMPLEX(SPC), INTENT(IN) :: x
COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: coeffs
COMPLEX(SPC) :: poly_cc
COMPLEX(SPC) :: pow
COMPLEX(SPC), DIMENSION(:), ALLOCATABLE :: vec
INTEGER(I4B) :: i,n,nn
n=size(coeffs)
if (n <= 0) then
  poly_cc=0.0_sp
else if (n < NPAR_POLY) then
  poly_cc=coeffs(n)
  do i=n-1,1,-1
    poly_cc=x*poly_cc+coeffs(i)
  end do
else
  allocate(vec(n+1))
  pow=x
  vec(1:n)=coeffs
  do
    vec(n+1)=0.0_sp
    nn=ishft(n+1,-1)
    vec(1:nn)=vec(1:n:2)+pow*vec(2:n+1:2)
    if (nn == 1) exit
    pow=pow*pow
    n=nn
  end do
  poly_cc=vec(1)
  deallocate(vec)
end if
END FUNCTION poly_cc
!BL
FUNCTION poly_rrv(x,coeffs)
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs,x
REAL(SP), DIMENSION(size(x)) :: poly_rrv
INTEGER(I4B) :: i,n,m
m=size(coeffs)
n=size(x)
if (m <= 0) then
  poly_rrv=0.0_sp
else if (m < n .or. m < NPAR_POLY) then
  poly_rrv=coeffs(m)
  do i=m-1,1,-1
    poly_rrv=x*poly_rrv+coeffs(i)
  end do
else
  do i=1,n
    poly_rrv(i)=poly_rr(x(i),coeffs)
  end do
end if
END FUNCTION poly_rrv
!BL
FUNCTION poly_ddv(x,coeffs)

```

```

REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs,x
REAL(DP), DIMENSION(size(x)) :: poly_ddv
INTEGER(I4B) :: i,n,m
m=size(coeffs)
n=size(x)
if (m <= 0) then
    poly_ddv=0.0_dp
else if (m < n .or. m < NPAR_POLY) then
    poly_ddv=coeffs(m)
    do i=m-1,1,-1
        poly_ddv=x*poly_ddv+coeffs(i)
    end do
else
    do i=1,n
        poly_ddv(i)=poly_dd(x(i),coeffs)
    end do
end if
END FUNCTION poly_ddv
!BL
FUNCTION poly_msk_rrv(x,coeffs,mask)
REAL(SP), DIMENSION(:), INTENT(IN) :: coeffs,x
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
REAL(SP), DIMENSION(size(x)) :: poly_msk_rrv
poly_msk_rrv=unpack(poly_rrv(pack(x,mask),coeffs),mask,0.0_sp)
END FUNCTION poly_msk_rrv
!BL
FUNCTION poly_msk_ddv(x,coeffs,mask)
REAL(DP), DIMENSION(:), INTENT(IN) :: coeffs,x
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: mask
REAL(DP), DIMENSION(size(x)) :: poly_msk_ddv
poly_msk_ddv=unpack(poly_ddv(pack(x,mask),coeffs),mask,0.0_dp)
END FUNCTION poly_msk_ddv
!BL
!BL
RECURSIVE FUNCTION poly_term_rr(a,b) RESULT(u)
REAL(SP), DIMENSION(:), INTENT(IN) :: a
REAL(SP), INTENT(IN) :: b
REAL(SP), DIMENSION(size(a)) :: u
INTEGER(I4B) :: n,j
n=size(a)
if (n <= 0) RETURN
u(1)=a(1)
if (n < NPAR_POLYTERM) then
    do j=2,n
        u(j)=a(j)+b*u(j-1)
    end do
else
    u(2:n:2)=poly_term_rr(a(2:n:2)+a(1:n-1:2)*b,b*b)
    u(3:n:2)=a(3:n:2)+b*u(2:n-1:2)
end if
END FUNCTION poly_term_rr
!BL
RECURSIVE FUNCTION poly_term_cc(a,b) RESULT(u)
COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: a

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```

COMPLEX(SPC), INTENT(IN) :: b
COMPLEX(SPC), DIMENSION(size(a)) :: u
INTEGER(I4B) :: n,j
n=size(a)
if (n <= 0) RETURN
u(1)=a(1)
if (n < NPAR_POLYTERM) then
  do j=2,n
    u(j)=a(j)+b*u(j-1)
  end do
else
  u(2:n:2)=poly_term_cc(a(2:n:2)+a(1:n-1:2)*b,b*b)
  u(3:n:2)=a(3:n:2)+b*u(2:n-1:2)
end if
END FUNCTION poly_term_cc
!BL
!BL
FUNCTION zroots_unity(n,nn)
INTEGER(I4B), INTENT(IN) :: n,nn
COMPLEX(SPC), DIMENSION(nn) :: zroots_unity
INTEGER(I4B) :: k
REAL(SP) :: theta
zroots_unity(1)=1.0
theta=TWOPI/n
k=1
do
  if (k >= nn) exit
  zroots_unity(k+1)=cmplx(cos(k*theta),sin(k*theta),SPC)
  zroots_unity(k+2:min(2*k,nn))=zroots_unity(k+1)*&
    zroots_unity(2:min(k,nn-k))
  k=2*k
end do
END FUNCTION zroots_unity
!BL
FUNCTION outerprod_r(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outerprod_r
outerprod_r = spread(a,dim=2,ncopies=size(b)) * &
  spread(b,dim=1,ncopies=size(a))
END FUNCTION outerprod_r
!BL
FUNCTION outerprod_d(a,b)
REAL(DP), DIMENSION(:), INTENT(IN) :: a,b
REAL(DP), DIMENSION(size(a),size(b)) :: outerprod_d
outerprod_d = spread(a,dim=2,ncopies=size(b)) * &
  spread(b,dim=1,ncopies=size(a))
END FUNCTION outerprod_d
!BL
FUNCTION outerdiv(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outerdiv
outerdiv = spread(a,dim=2,ncopies=size(b)) / &
  spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiv

```



```

!BL
FUNCTION outersum(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outersum
outersum = spread(a,dim=2,ncopies=size(b)) + &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outersum
!BL
FUNCTION outerdiff_r(a,b)
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
REAL(SP), DIMENSION(size(a),size(b)) :: outerdiff_r
outerdiff_r = spread(a,dim=2,ncopies=size(b)) - &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_r
!BL
FUNCTION outerdiff_d(a,b)
REAL(DP), DIMENSION(:), INTENT(IN) :: a,b
REAL(DP), DIMENSION(size(a),size(b)) :: outerdiff_d
outerdiff_d = spread(a,dim=2,ncopies=size(b)) - &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_d
!BL
FUNCTION outerdiff_i(a,b)
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: a,b
INTEGER(I4B), DIMENSION(size(a),size(b)) :: outerdiff_i
outerdiff_i = spread(a,dim=2,ncopies=size(b)) - &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerdiff_i
!BL
FUNCTION outerand(a,b)
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: a,b
LOGICAL(LGT), DIMENSION(size(a),size(b)) :: outerand
outerand = spread(a,dim=2,ncopies=size(b)) .and. &
    spread(b,dim=1,ncopies=size(a))
END FUNCTION outerand
!BL
SUBROUTINE scatter_add_r(dest,source,dest_index)
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
REAL(SP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source),size(dest_index),'scatter_add_r')
m=size(dest)
do j=1,n
    i=dest_index(j)
    if (i > 0 .and. i <= m) dest(i)=dest(i)+source(j)
end do
END SUBROUTINE scatter_add_r
SUBROUTINE scatter_add_d(dest,source,dest_index)
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
REAL(DP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source),size(dest_index),'scatter_add_d')

```

```

m=size(dest)
do j=1,n
  i=dest_index(j)
  if (i > 0 .and. i <= m) dest(i)=dest(i)+source(j)
end do
END SUBROUTINE scatter_add_d
SUBROUTINE scatter_max_r(dest,source,dest_index)
REAL(SP), DIMENSION(:), INTENT(OUT) :: dest
REAL(SP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source),size(dest_index),'scatter_max_r')
m=size(dest)
do j=1,n
  i=dest_index(j)
  if (i > 0 .and. i <= m) dest(i)=max(dest(i),source(j))
end do
END SUBROUTINE scatter_max_r
SUBROUTINE scatter_max_d(dest,source,dest_index)
REAL(DP), DIMENSION(:), INTENT(OUT) :: dest
REAL(DP), DIMENSION(:), INTENT(IN) :: source
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: dest_index
INTEGER(I4B) :: m,n,j,i
n=assert_eq2(size(source),size(dest_index),'scatter_max_d')
m=size(dest)
do j=1,n
  i=dest_index(j)
  if (i > 0 .and. i <= m) dest(i)=max(dest(i),source(j))
end do
END SUBROUTINE scatter_max_d
!BL
SUBROUTINE diagadd_rv(mat,diag)
REAL(SP), DIMENSION(:,,:), INTENT(INOUT) :: mat
REAL(SP), DIMENSION(:), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = assert_eq2(size(diag),min(size(mat,1),size(mat,2)),'diagadd_rv')
do j=1,n
  mat(j,j)=mat(j,j)+diag(j)
end do
END SUBROUTINE diagadd_rv
!BL
SUBROUTINE diagadd_r(mat,diag)
REAL(SP), DIMENSION(:,,:), INTENT(INOUT) :: mat
REAL(SP), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
  mat(j,j)=mat(j,j)+diag
end do
END SUBROUTINE diagadd_r
!BL
SUBROUTINE diagmult_rv(mat,diag)
REAL(SP), DIMENSION(:,,:), INTENT(INOUT) :: mat
REAL(SP), DIMENSION(:), INTENT(IN) :: diag

```

```

    INTEGER(I4B) :: j,n
    n = assert_eq2(size(diag),min(size(mat,1),size(mat,2)),'diagmult_rv')
    do j=1,n
        mat(j,j)=mat(j,j)*diag(j)
    end do
END SUBROUTINE diagmult_rv
!BL
SUBROUTINE diagmult_r(mat,diag)
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
REAL(SP), INTENT(IN) :: diag
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
    mat(j,j)=mat(j,j)*diag
end do
END SUBROUTINE diagmult_r
!BL
FUNCTION get_diag_rv(mat)
REAL(SP), DIMENSION(:,:), INTENT(IN) :: mat
REAL(SP), DIMENSION(size(mat,1)) :: get_diag_rv
INTEGER(I4B) :: j
j=assert_eq2(size(mat,1),size(mat,2),'get_diag_rv')
do j=1,size(mat,1)
    get_diag_rv(j)=mat(j,j)
end do
END FUNCTION get_diag_rv
!BL
FUNCTION get_diag_dv(mat)
REAL(DP), DIMENSION(:,:), INTENT(IN) :: mat
REAL(DP), DIMENSION(size(mat,1)) :: get_diag_dv
INTEGER(I4B) :: j
j=assert_eq2(size(mat,1),size(mat,2),'get_diag_dv')
do j=1,size(mat,1)
    get_diag_dv(j)=mat(j,j)
end do
END FUNCTION get_diag_dv
!BL
SUBROUTINE put_diag_rv(diagv,mat)
REAL(SP), DIMENSION(:), INTENT(IN) :: diagv
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
INTEGER(I4B) :: j,n
n=assert_eq2(size(diagv),min(size(mat,1),size(mat,2)),'put_diag_rv')
do j=1,n
    mat(j,j)=diagv(j)
end do
END SUBROUTINE put_diag_rv
!BL
SUBROUTINE put_diag_r(scal,mat)
REAL(SP), INTENT(IN) :: scal
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: mat
INTEGER(I4B) :: j,n
n = min(size(mat,1),size(mat,2))
do j=1,n
    mat(j,j)=scal

```

```

        end do
    END SUBROUTINE put_diag_r
!BL
    SUBROUTINE unit_matrix(mat)
    REAL(SP), DIMENSION(:, :), INTENT(OUT) :: mat
    INTEGER(I4B) :: i,n
    n=min(size(mat,1),size(mat,2))
    mat(:, :)=0.0_sp
    do i=1,n
        mat(i,i)=1.0_sp
    end do
    END SUBROUTINE unit_matrix
!BL
    FUNCTION upper_triangle(j,k,extra)
    INTEGER(I4B), INTENT(IN) :: j,k
    INTEGER(I4B), OPTIONAL, INTENT(IN) :: extra
    LOGICAL(LGT), DIMENSION(j,k) :: upper_triangle
    INTEGER(I4B) :: n
    n=0
    if (present(extra)) n=extra
    upper_triangle=(outerdiff(arth_i(1,1,j),arth_i(1,1,k)) < n)
    END FUNCTION upper_triangle
!BL
    FUNCTION lower_triangle(j,k,extra)
    INTEGER(I4B), INTENT(IN) :: j,k
    INTEGER(I4B), OPTIONAL, INTENT(IN) :: extra
    LOGICAL(LGT), DIMENSION(j,k) :: lower_triangle
    INTEGER(I4B) :: n
    n=0
    if (present(extra)) n=extra
    lower_triangle=(outerdiff(arth_i(1,1,j),arth_i(1,1,k)) > -n)
    END FUNCTION lower_triangle
!BL
    FUNCTION vabs(v)
    REAL(SP), DIMENSION(:), INTENT(IN) :: v
    REAL(SP) :: vabs
    vabs=sqrt(dot_product(v,v))
    END FUNCTION vabs
!BL
END MODULE nrutil

MODULE ode_path
    USE nrtype
    INTEGER(I4B) :: nok,nbad,kount
    LOGICAL(LGT), SAVE :: save_steps=.false.
    REAL(SP) :: dxsav
    REAL(SP), DIMENSION(:), POINTER :: xp
    REAL(SP), DIMENSION(:, :), POINTER :: yp
END MODULE ode_path

MODULE hypgeo_info
    USE nrtype
    COMPLEX(SPC) :: hypgeo_aa,hypgeo_bb,hypgeo_cc,hypgeo_dz,hypgeo_z0
END MODULE hypgeo_info

```

```

MODULE nr
  INTERFACE
    SUBROUTINE airy(x,ai,bi,aip,bip)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), INTENT(OUT) :: ai,bi,aip,bip
    END SUBROUTINE airy
  END INTERFACE
  INTERFACE
    SUBROUTINE amebsa(p,y,pb,yb,ftol,func,iter,temptr)
    USE nrtype
    INTEGER(I4B), INTENT(INOUT) :: iter
    REAL(SP), INTENT(INOUT) :: yb
    REAL(SP), INTENT(IN) :: ftol,temptr
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: y,pb
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: p
    INTERFACE
      FUNCTION func(x)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x
      REAL(SP) :: func
      END FUNCTION func
    END INTERFACE
  END SUBROUTINE amebsa
END INTERFACE
  INTERFACE
    SUBROUTINE amoeba(p,y,ftol,func,iter)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: iter
    REAL(SP), INTENT(IN) :: ftol
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: p
    INTERFACE
      FUNCTION func(x)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x
      REAL(SP) :: func
      END FUNCTION func
    END INTERFACE
  END SUBROUTINE amoeba
END INTERFACE
  INTERFACE
    SUBROUTINE anneal(x,y,iorder)
    USE nrtype
    INTEGER(I4B), DIMENSION(:), INTENT(INOUT) :: iorder
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    END SUBROUTINE anneal
  END INTERFACE
  INTERFACE
    SUBROUTINE asolve(b,x,itrnsp)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: b
    REAL(DP), DIMENSION(:), INTENT(OUT) :: x
  END INTERFACE

```

```

        INTEGER(I4B), INTENT(IN) :: itrnsp
    END SUBROUTINE asolve
END INTERFACE
INTERFACE
    SUBROUTINE atimes(x,r,itrnsp)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: x
    REAL(DP), DIMENSION(:), INTENT(OUT) :: r
    INTEGER(I4B), INTENT(IN) :: itrnsp
    END SUBROUTINE atimes
END INTERFACE
INTERFACE
    SUBROUTINE avevar(data,ave,var)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data
    REAL(SP), INTENT(OUT) :: ave,var
    END SUBROUTINE avevar
END INTERFACE
INTERFACE
    SUBROUTINE balanc(a)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    END SUBROUTINE balanc
END INTERFACE
INTERFACE
    SUBROUTINE banbks(a,m1,m2,al,indx,b)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: m1,m2
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indx
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a,al
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: b
    END SUBROUTINE banbks
END INTERFACE
INTERFACE
    SUBROUTINE bandec(a,m1,m2,al,indx,d)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: m1,m2
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: indx
    REAL(SP), INTENT(OUT) :: d
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: al
    END SUBROUTINE bandec
END INTERFACE
INTERFACE
    SUBROUTINE banmul(a,m1,m2,x,b)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: m1,m2
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(OUT) :: b
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    END SUBROUTINE banmul
END INTERFACE
INTERFACE
    SUBROUTINE bcucof(y,y1,y2,y12,d1,d2,c)

```

```

        USE nrtype
        REAL(SP), INTENT(IN) :: d1,d2
        REAL(SP), DIMENSION(4), INTENT(IN) :: y,y1,y2,y12
        REAL(SP), DIMENSION(4,4), INTENT(OUT) :: c
        END SUBROUTINE bcucof
    END INTERFACE
INTERFACE
    SUBROUTINE bcuint(y,y1,y2,y12,x1l,x1u,x2l,x2u,x1,x2,ansy,&
        ansy1,ansy2)
        USE nrtype
        REAL(SP), DIMENSION(4), INTENT(IN) :: y,y1,y2,y12
        REAL(SP), INTENT(IN) :: x1l,x1u,x2l,x2u,x1,x2
        REAL(SP), INTENT(OUT) :: ansy,ansy1,ansy2
    END SUBROUTINE bcuint
END INTERFACE
INTERFACE beschb
    SUBROUTINE beschb_s(x,gam1,gam2,gampl,gammi)
        USE nrtype
        REAL(DP), INTENT(IN) :: x
        REAL(DP), INTENT(OUT) :: gam1,gam2,gampl,gammi
    END SUBROUTINE beschb_s
!BL
    SUBROUTINE beschb_v(x,gam1,gam2,gampl,gammi)
        USE nrtype
        REAL(DP), DIMENSION(:), INTENT(IN) :: x
        REAL(DP), DIMENSION(:), INTENT(OUT) :: gam1,gam2,gampl,gammi
    END SUBROUTINE beschb_v
END INTERFACE
INTERFACE bessi
    FUNCTION bessi_s(n,x)
        USE nrtype
        INTEGER(I4B), INTENT(IN) :: n
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: bessi_s
    END FUNCTION bessi_s
!BL
    FUNCTION bessi_v(n,x)
        USE nrtype
        INTEGER(I4B), INTENT(IN) :: n
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: bessi_v
    END FUNCTION bessi_v
END INTERFACE
INTERFACE bessio
    FUNCTION bessio_s(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: bessio_s
    END FUNCTION bessio_s
!BL
    FUNCTION bessio_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: bessio_v

```

```

        END FUNCTION bessj0_v
    END INTERFACE
    INTERFACE bessj1
        FUNCTION bessj1_s(x)
            USE nrtype
            REAL(SP), INTENT(IN) :: x
            REAL(SP) :: bessj1_s
        END FUNCTION bessj1_s
    !BL
        FUNCTION bessj1_v(x)
            USE nrtype
            REAL(SP), DIMENSION(:), INTENT(IN) :: x
            REAL(SP), DIMENSION(size(x)) :: bessj1_v
        END FUNCTION bessj1_v
    END INTERFACE
    INTERFACE
        SUBROUTINE bessik(x,xnu,ri,rk,rip,rkp)
            USE nrtype
            REAL(SP), INTENT(IN) :: x,xnu
            REAL(SP), INTENT(OUT) :: ri,rk,rip,rkp
        END SUBROUTINE bessik
    END INTERFACE
    INTERFACE bessj
        FUNCTION bessj_s(n,x)
            USE nrtype
            INTEGER(I4B), INTENT(IN) :: n
            REAL(SP), INTENT(IN) :: x
            REAL(SP) :: bessj_s
        END FUNCTION bessj_s
    !BL
        FUNCTION bessj_v(n,x)
            USE nrtype
            INTEGER(I4B), INTENT(IN) :: n
            REAL(SP), DIMENSION(:), INTENT(IN) :: x
            REAL(SP), DIMENSION(size(x)) :: bessj_v
        END FUNCTION bessj_v
    END INTERFACE
    INTERFACE bessj0
        FUNCTION bessj0_s(x)
            USE nrtype
            REAL(SP), INTENT(IN) :: x
            REAL(SP) :: bessj0_s
        END FUNCTION bessj0_s
    !BL
        FUNCTION bessj0_v(x)
            USE nrtype
            REAL(SP), DIMENSION(:), INTENT(IN) :: x
            REAL(SP), DIMENSION(size(x)) :: bessj0_v
        END FUNCTION bessj0_v
    END INTERFACE
    INTERFACE bessj1
        FUNCTION bessj1_s(x)
            USE nrtype
            REAL(SP), INTENT(IN) :: x

```



```

      REAL(SP) :: bessj1_s
    END FUNCTION bessj1_s
!BL
    FUNCTION bessj1_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessj1_v
    END FUNCTION bessj1_v
  END INTERFACE
  INTERFACE bessjy
    SUBROUTINE bessjy_s(x,xnu,rj,ry,rjp,ryp)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,xnu
    REAL(SP), INTENT(OUT) :: rj,ry,rjp,ryp
    END SUBROUTINE bessjy_s
!BL
    SUBROUTINE bessjy_v(x,xnu,rj,ry,rjp,ryp)
    USE nrtype
    REAL(SP), INTENT(IN) :: xnu
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(OUT) :: rj,rjp,ry,ryp
    END SUBROUTINE bessjy_v
  END INTERFACE
  INTERFACE bessk
    FUNCTION bessk_s(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessk_s
    END FUNCTION bessk_s
!BL
    FUNCTION bessk_v(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessk_v
    END FUNCTION bessk_v
  END INTERFACE
  INTERFACE bessk0
    FUNCTION bessk0_s(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessk0_s
    END FUNCTION bessk0_s
!BL
    FUNCTION bessk0_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessk0_v
    END FUNCTION bessk0_v
  END INTERFACE
  INTERFACE bessk1
    FUNCTION bessk1_s(x)
    USE nrtype

```

```

    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessk1_s
    END FUNCTION bessk1_s
!BL
    FUNCTION bessk1_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessk1_v
    END FUNCTION bessk1_v
END INTERFACE
INTERFACE bessy
    FUNCTION bessy_s(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessy_s
    END FUNCTION bessy_s
!BL
    FUNCTION bessy_v(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessy_v
    END FUNCTION bessy_v
END INTERFACE
INTERFACE bessy0
    FUNCTION bessy0_s(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessy0_s
    END FUNCTION bessy0_s
!BL
    FUNCTION bessy0_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessy0_v
    END FUNCTION bessy0_v
END INTERFACE
INTERFACE bessy1
    FUNCTION bessy1_s(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: bessy1_s
    END FUNCTION bessy1_s
!BL
    FUNCTION bessy1_v(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: bessy1_v
    END FUNCTION bessy1_v
END INTERFACE
INTERFACE beta
    FUNCTION beta_s(z,w)
    USE nrtype

```

```

      REAL(SP), INTENT(IN) :: z,w
      REAL(SP) :: beta_s
      END FUNCTION beta_s
!BL
      FUNCTION beta_v(z,w)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: z,w
      REAL(SP), DIMENSION(size(z)) :: beta_v
      END FUNCTION beta_v
END INTERFACE
INTERFACE betacf
      FUNCTION betacf_s(a,b,x)
      USE nrtype
      REAL(SP), INTENT(IN) :: a,b,x
      REAL(SP) :: betacf_s
      END FUNCTION betacf_s
!BL
      FUNCTION betacf_v(a,b,x)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,x
      REAL(SP), DIMENSION(size(x)) :: betacf_v
      END FUNCTION betacf_v
END INTERFACE
INTERFACE betai
      FUNCTION betai_s(a,b,x)
      USE nrtype
      REAL(SP), INTENT(IN) :: a,b,x
      REAL(SP) :: betai_s
      END FUNCTION betai_s
!BL
      FUNCTION betai_v(a,b,x)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,x
      REAL(SP), DIMENSION(size(a)) :: betai_v
      END FUNCTION betai_v
END INTERFACE
INTERFACE bico
      FUNCTION bico_s(n,k)
      USE nrtype
      INTEGER(I4B), INTENT(IN) :: n,k
      REAL(SP) :: bico_s
      END FUNCTION bico_s
!BL
      FUNCTION bico_v(n,k)
      USE nrtype
      INTEGER(I4B), DIMENSION(:), INTENT(IN) :: n,k
      REAL(SP), DIMENSION(size(n)) :: bico_v
      END FUNCTION bico_v
END INTERFACE
INTERFACE
      FUNCTION bnldev(pp,n)
      USE nrtype
      REAL(SP), INTENT(IN) :: pp
      INTEGER(I4B), INTENT(IN) :: n

```

```

      REAL(SP) :: bnldev
    END FUNCTION bnldev
  END INTERFACE
INTERFACE
    FUNCTION brent(ax,bx,cx,func,tol,xmin)
    USE nrtype
    REAL(SP), INTENT(IN) :: ax,bx,cx,tol
    REAL(SP), INTENT(OUT) :: xmin
    REAL(SP) :: brent
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION brent
END INTERFACE
INTERFACE
    SUBROUTINE broydn(x,check)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
    LOGICAL(LGT), INTENT(OUT) :: check
    END SUBROUTINE broydn
END INTERFACE
INTERFACE
    SUBROUTINE bsstep(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
    REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
    REAL(SP), INTENT(INOUT) :: x
    REAL(SP), INTENT(IN) :: htry,eps
    REAL(SP), INTENT(OUT) :: hdid,hnext
    INTERFACE
        SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
        END SUBROUTINE derivs
    END INTERFACE
    END SUBROUTINE bsstep
END INTERFACE
INTERFACE
    SUBROUTINE caldat(julian,mm,id,iyyy)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: julian
    INTEGER(I4B), INTENT(OUT) :: mm,id,iyyy
    END SUBROUTINE caldat
END INTERFACE
INTERFACE
    FUNCTION chder(a,b,c)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b

```

```

REAL(SP), DIMENSION(:), INTENT(IN) :: c
REAL(SP), DIMENSION(size(c)) :: chder
END FUNCTION chder
END INTERFACE
INTERFACE chebev
  FUNCTION chebev_s(a,b,c,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b,x
    REAL(SP), DIMENSION(:), INTENT(IN) :: c
    REAL(SP) :: chebev_s
  END FUNCTION chebev_s
!BL
  FUNCTION chebev_v(a,b,c,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(:), INTENT(IN) :: c,x
    REAL(SP), DIMENSION(size(x)) :: chebev_v
  END FUNCTION chebev_v
END INTERFACE
INTERFACE
  FUNCTION chebft(a,b,n,func)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(n) :: chebft
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x
      REAL(SP), DIMENSION(size(x)) :: func
    END FUNCTION func
  END INTERFACE
END FUNCTION chebft
END INTERFACE
INTERFACE
  FUNCTION chebpc(c)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: c
    REAL(SP), DIMENSION(size(c)) :: chebpc
  END FUNCTION chebpc
END INTERFACE
INTERFACE
  FUNCTION chint(a,b,c)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(:), INTENT(IN) :: c
    REAL(SP), DIMENSION(size(c)) :: chint
  END FUNCTION chint
END INTERFACE
INTERFACE
  SUBROUTINE choldc(a,p)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: p

```

```

        END SUBROUTINE choldc
    END INTERFACE
INTERFACE
    SUBROUTINE chols1(a,p,b,x)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    REAL(SP), DIMENSION(:), INTENT(IN) :: p,b
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
    END SUBROUTINE chols1
END INTERFACE
INTERFACE
    SUBROUTINE chsone(bins,ebins,knstrn,df,chsq,prob)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: knstrn
    REAL(SP), INTENT(OUT) :: df,chsq,prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: bins,ebins
    END SUBROUTINE chsone
END INTERFACE
INTERFACE
    SUBROUTINE chstwo(bins1,bins2,knstrn,df,chsq,prob)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: knstrn
    REAL(SP), INTENT(OUT) :: df,chsq,prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: bins1,bins2
    END SUBROUTINE chstwo
END INTERFACE
INTERFACE
    SUBROUTINE cisi(x,ci,si)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), INTENT(OUT) :: ci,si
    END SUBROUTINE cisi
END INTERFACE
INTERFACE
    SUBROUTINE cntab1(nn,chisq,df,prob,cramrv,ccc)
    USE nrtype
    INTEGER(I4B), DIMENSION(:,:), INTENT(IN) :: nn
    REAL(SP), INTENT(OUT) :: chisq,df,prob,cramrv,ccc
    END SUBROUTINE cntab1
END INTERFACE
INTERFACE
    SUBROUTINE cntab2(nn,h,hx,hy,hygx,hxgy,uygx,uxgy,uxy)
    USE nrtype
    INTEGER(I4B), DIMENSION(:,:), INTENT(IN) :: nn
    REAL(SP), INTENT(OUT) :: h,hx,hy,hygx,hxgy,uygx,uxgy,uxy
    END SUBROUTINE cntab2
END INTERFACE
INTERFACE
    FUNCTION convlv(data,respns,isign)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data
    REAL(SP), DIMENSION(:), INTENT(IN) :: respns
    INTEGER(I4B), INTENT(IN) :: isign
    REAL(SP), DIMENSION(size(data)) :: convlv

```

```

        END FUNCTION convlv
    END INTERFACE
INTERFACE
    FUNCTION correl(data1,data2)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
        REAL(SP), DIMENSION(size(data1)) :: correl
    END FUNCTION correl
END INTERFACE
INTERFACE
    SUBROUTINE cosft1(y)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
    END SUBROUTINE cosft1
END INTERFACE
INTERFACE
    SUBROUTINE cosft2(y,isign)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
        INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE cosft2
END INTERFACE
INTERFACE
    SUBROUTINE covsrt(covar,maska)
        USE nrtype
        REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: covar
        LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: maska
    END SUBROUTINE covsrt
END INTERFACE
INTERFACE
    SUBROUTINE cyclic(a,b,c,alpha,beta,r,x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN):: a,b,c,r
        REAL(SP), INTENT(IN) :: alpha,beta
        REAL(SP), DIMENSION(:), INTENT(OUT):: x
    END SUBROUTINE cyclic
END INTERFACE
INTERFACE
    SUBROUTINE daub4(a,isign)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
        INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE daub4
END INTERFACE
INTERFACE dawson
    FUNCTION dawson_s(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: dawson_s
    END FUNCTION dawson_s
!BL
    FUNCTION dawson_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x

```

```

REAL(SP), DIMENSION(size(x)) :: dawson_v
END FUNCTION dawson_v
END INTERFACE
INTERFACE
  FUNCTION dbrent(ax,bx,cx,func,dbrent_dfunc,tol,xmin)
  USE nrtype
  REAL(SP), INTENT(IN) :: ax,bx,cx,tol
  REAL(SP), INTENT(OUT) :: xmin
  REAL(SP) :: dbrent
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: func
  END FUNCTION func
!BL
  FUNCTION dbrent_dfunc(x)
  USE nrtype
  REAL(SP), INTENT(IN) :: x
  REAL(SP) :: dbrent_dfunc
  END FUNCTION dbrent_dfunc
END INTERFACE
END FUNCTION dbrent
END INTERFACE
INTERFACE
  SUBROUTINE ddpoly(c,x,pd)
  USE nrtype
  REAL(SP), INTENT(IN) :: x
  REAL(SP), DIMENSION(:), INTENT(IN) :: c
  REAL(SP), DIMENSION(:), INTENT(OUT) :: pd
  END SUBROUTINE ddpoly
END INTERFACE
INTERFACE
  FUNCTION decchk(string,ch)
  USE nrtype
  CHARACTER(1), DIMENSION(:), INTENT(IN) :: string
  CHARACTER(1), INTENT(OUT) :: ch
  LOGICAL(LGT) :: decchk
  END FUNCTION decchk
END INTERFACE
INTERFACE
  SUBROUTINE dfpmin(p,gtol,iter,fret,func,dfunc)
  USE nrtype
  INTEGER(I4B), INTENT(OUT) :: iter
  REAL(SP), INTENT(IN) :: gtol
  REAL(SP), INTENT(OUT) :: fret
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: p
  INTERFACE
    FUNCTION func(p)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: p
    REAL(SP) :: func
  END FUNCTION func
!BL

```



```

        FUNCTION dfunc(p)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: p
        REAL(SP), DIMENSION(size(p)) :: dfunc
        END FUNCTION dfunc
    END INTERFACE
    END SUBROUTINE dfpmin
END INTERFACE
INTERFACE
    FUNCTION dfidr(func,x,h,err)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,h
    REAL(SP), INTENT(OUT) :: err
    REAL(SP) :: dfidr
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION dfidr
END INTERFACE
INTERFACE
    SUBROUTINE dftcor(w,delta,a,b,endpts,corre,corim,corfac)
    USE nrtype
    REAL(SP), INTENT(IN) :: w,delta,a,b
    REAL(SP), INTENT(OUT) :: corre,corim,corfac
    REAL(SP), DIMENSION(:), INTENT(IN) :: endpts
    END SUBROUTINE dftcor
END INTERFACE
INTERFACE
    SUBROUTINE dftint(func,a,b,w,cosint,sinint)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b,w
    REAL(SP), INTENT(OUT) :: cosint,sinint
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE
    END SUBROUTINE dftint
END INTERFACE
INTERFACE
    SUBROUTINE difeq(k,k1,k2,jsf,is1,isf,indexv,s,y)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: is1,isf,jsf,k,k1,k2
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indexv
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: s
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: y
    END SUBROUTINE difeq
END INTERFACE

```

```

INTERFACE
  FUNCTION eclass(lista,listb,n)
  USE nrtype
  INTEGER(I4B), DIMENSION(:), INTENT(IN) :: lista,listb
  INTEGER(I4B), INTENT(IN) :: n
  INTEGER(I4B), DIMENSION(n) :: eclass
  END FUNCTION eclass
END INTERFACE
INTERFACE
  FUNCTION eclazz(equiv,n)
  USE nrtype
  INTERFACE
    FUNCTION equiv(i,j)
    USE nrtype
    LOGICAL(LGT) :: equiv
    INTEGER(I4B), INTENT(IN) :: i,j
    END FUNCTION equiv
  END INTERFACE
  INTEGER(I4B), INTENT(IN) :: n
  INTEGER(I4B), DIMENSION(n) :: eclazz
  END FUNCTION eclazz
END INTERFACE
INTERFACE
  FUNCTION ei(x)
  USE nrtype
  REAL(SP), INTENT(IN) :: x
  REAL(SP) :: ei
  END FUNCTION ei
END INTERFACE
INTERFACE
  SUBROUTINE eigsrt(d,v)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: d
  REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: v
  END SUBROUTINE eigsrt
END INTERFACE
INTERFACE elle
  FUNCTION elle_s(phi,ak)
  USE nrtype
  REAL(SP), INTENT(IN) :: phi,ak
  REAL(SP) :: elle_s
  END FUNCTION elle_s
!BL
  FUNCTION elle_v(phi,ak)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: phi,ak
  REAL(SP), DIMENSION(size(phi)) :: elle_v
  END FUNCTION elle_v
END INTERFACE
INTERFACE ellf
  FUNCTION ellf_s(phi,ak)
  USE nrtype
  REAL(SP), INTENT(IN) :: phi,ak
  REAL(SP) :: ellf_s

```

```

        END FUNCTION ellf_s
!BL
        FUNCTION ellf_v(phi,ak)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: phi,ak
        REAL(SP), DIMENSION(size(phi)) :: ellf_v
        END FUNCTION ellf_v
    END INTERFACE
    INTERFACE ellpi
        FUNCTION ellpi_s(phi,en,ak)
        USE nrtype
        REAL(SP), INTENT(IN) :: phi,en,ak
        REAL(SP) :: ellpi_s
        END FUNCTION ellpi_s
!BL
        FUNCTION ellpi_v(phi,en,ak)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: phi,en,ak
        REAL(SP), DIMENSION(size(phi)) :: ellpi_v
        END FUNCTION ellpi_v
    END INTERFACE
    INTERFACE
        SUBROUTINE elmhes(a)
        USE nrtype
        REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
        END SUBROUTINE elmhes
    END INTERFACE
    INTERFACE erf
        FUNCTION erf_s(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: erf_s
        END FUNCTION erf_s
!BL
        FUNCTION erf_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: erf_v
        END FUNCTION erf_v
    END INTERFACE
    INTERFACE erfc
        FUNCTION erfc_s(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: erfc_s
        END FUNCTION erfc_s
!BL
        FUNCTION erfc_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: erfc_v
        END FUNCTION erfc_v
    END INTERFACE
    INTERFACE erfcc

```

```

        FUNCTION erfcc_s(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: erfcc_s
        END FUNCTION erfcc_s
!BL
        FUNCTION erfcc_v(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: erfcc_v
        END FUNCTION erfcc_v
END INTERFACE
INTERFACE
    SUBROUTINE eulsum(sum,term,jterm)
    USE nrtype
    REAL(SP), INTENT(INOUT) :: sum
    REAL(SP), INTENT(IN) :: term
    INTEGER(I4B), INTENT(IN) :: jterm
    END SUBROUTINE eulsum
END INTERFACE
INTERFACE
    FUNCTION evlmem(fdt,d,xms)
    USE nrtype
    REAL(SP), INTENT(IN) :: fdt,xms
    REAL(SP), DIMENSION(:), INTENT(IN) :: d
    REAL(SP) :: evlmem
    END FUNCTION evlmem
END INTERFACE
INTERFACE expdev
    SUBROUTINE expdev_s(harvest)
    USE nrtype
    REAL(SP), INTENT(OUT) :: harvest
    END SUBROUTINE expdev_s
!BL
    SUBROUTINE expdev_v(harvest)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
    END SUBROUTINE expdev_v
END INTERFACE
INTERFACE
    FUNCTION expint(n,x)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: expint
    END FUNCTION expint
END INTERFACE
INTERFACE factln
    FUNCTION factln_s(n)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP) :: factln_s
    END FUNCTION factln_s
!BL

```

```

        FUNCTION factln_v(n)
        USE nrtype
        INTEGER(I4B), DIMENSION(:), INTENT(IN) :: n
        REAL(SP), DIMENSION(size(n)) :: factln_v
        END FUNCTION factln_v
    END INTERFACE
    INTERFACE factrl
        FUNCTION factrl_s(n)
        USE nrtype
        INTEGER(I4B), INTENT(IN) :: n
        REAL(SP) :: factrl_s
        END FUNCTION factrl_s
!BL
        FUNCTION factrl_v(n)
        USE nrtype
        INTEGER(I4B), DIMENSION(:), INTENT(IN) :: n
        REAL(SP), DIMENSION(size(n)) :: factrl_v
        END FUNCTION factrl_v
    END INTERFACE
    INTERFACE
        SUBROUTINE fasper(x,y,ofac,hifac,px,py,jmax,prob)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
        REAL(SP), INTENT(IN) :: ofac,hifac
        INTEGER(I4B), INTENT(OUT) :: jmax
        REAL(SP), INTENT(OUT) :: prob
        REAL(SP), DIMENSION(:), POINTER :: px,py
        END SUBROUTINE fasper
    END INTERFACE
    INTERFACE
        SUBROUTINE fdjac(x,fvec,df)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: fvec
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
        REAL(SP), DIMENSION(:,:), INTENT(OUT) :: df
        END SUBROUTINE fdjac
    END INTERFACE
    INTERFACE
        SUBROUTINE fgauss(x,a,y,dyda)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x,a
        REAL(SP), DIMENSION(:), INTENT(OUT) :: y
        REAL(SP), DIMENSION(:,:), INTENT(OUT) :: dyda
        END SUBROUTINE fgauss
    END INTERFACE
    INTERFACE
        SUBROUTINE fit(x,y,a,b,siga,sigb,chi2,q,sig)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
        REAL(SP), INTENT(OUT) :: a,b,siga,sigb,chi2,q
        REAL(SP), DIMENSION(:), OPTIONAL, INTENT(IN) :: sig
        END SUBROUTINE fit
    END INTERFACE
    INTERFACE

```

```

SUBROUTINE fitexy(x,y,sigx,sigy,a,b,siga,sigb,chi2,q)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,sigx,sigy
REAL(SP), INTENT(OUT) :: a,b,siga,sigb,chi2,q
END SUBROUTINE fitexy
END INTERFACE
INTERFACE
SUBROUTINE fixrts(d)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: d
END SUBROUTINE fixrts
END INTERFACE
INTERFACE
FUNCTION fleg(x,n)
USE nrtype
REAL(SP), INTENT(IN) :: x
INTEGER(I4B), INTENT(IN) :: n
REAL(SP), DIMENSION(n) :: fleg
END FUNCTION fleg
END INTERFACE
INTERFACE
SUBROUTINE flmoon(n,nph,jd,frac)
USE nrtype
INTEGER(I4B), INTENT(IN) :: n,nph
INTEGER(I4B), INTENT(OUT) :: jd
REAL(SP), INTENT(OUT) :: frac
END SUBROUTINE flmoon
END INTERFACE
INTERFACE four1
SUBROUTINE four1_dp(data,isign)
USE nrtype
COMPLEX(DPC), DIMENSION(:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE four1_dp
!BL
SUBROUTINE four1_sp(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE four1_sp
END INTERFACE
INTERFACE
SUBROUTINE four1_alt(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE four1_alt
END INTERFACE
INTERFACE
SUBROUTINE four1_gather(data,isign)
USE nrtype
COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: data
INTEGER(I4B), INTENT(IN) :: isign
END SUBROUTINE four1_gather

```

```

END INTERFACE
INTERFACE
  SUBROUTINE four2(data, isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE four2
END INTERFACE
INTERFACE
  SUBROUTINE four2_alt(data, isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE four2_alt
END INTERFACE
INTERFACE
  SUBROUTINE four3(data, isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE four3
END INTERFACE
INTERFACE
  SUBROUTINE four3_alt(data, isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE four3_alt
END INTERFACE
INTERFACE
  SUBROUTINE fourcol(data, isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE fourcol
END INTERFACE
INTERFACE
  SUBROUTINE fourcol_3d(data, isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE fourcol_3d
END INTERFACE
INTERFACE
  SUBROUTINE fourn_gather(data, nn, isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:), INTENT(INOUT) :: data
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: nn
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE fourn_gather
END INTERFACE
INTERFACE fourrow
  SUBROUTINE fourrow_dp(data, isign)
    USE nrtype

```

```

        COMPLEX(DPC), DIMENSION(:,:), INTENT(INOUT) :: data
        INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE fourrow_dp
!BL
    SUBROUTINE fourrow_sp(data,isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE fourrow_sp
END INTERFACE
INTERFACE
    SUBROUTINE fourrow_3d(data,isign)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:,:,:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE fourrow_3d
END INTERFACE
INTERFACE
    FUNCTION fpoly(x,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(n) :: fpoly
    END FUNCTION fpoly
END INTERFACE
INTERFACE
    SUBROUTINE fred2(a,b,t,f,w,g,ak)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(:), INTENT(OUT) :: t,f,w
    INTERFACE
        FUNCTION g(t)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: t
        REAL(SP), DIMENSION(size(t)) :: g
        END FUNCTION g
!BL
        FUNCTION ak(t,s)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: t,s
        REAL(SP), DIMENSION(size(t),size(s)) :: ak
        END FUNCTION ak
    END INTERFACE
END SUBROUTINE fred2
END INTERFACE
INTERFACE
    FUNCTION fredin(x,a,b,t,f,w,g,ak)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,t,f,w
    REAL(SP), DIMENSION(size(x)) :: fredin
    INTERFACE
        FUNCTION g(t)
        USE nrtype

```



```

        REAL(SP), DIMENSION(:), INTENT(IN) :: t
        REAL(SP), DIMENSION(size(t)) :: g
    END FUNCTION g
!BL
    FUNCTION ak(t,s)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: t,s
    REAL(SP), DIMENSION(size(t),size(s)) :: ak
    END FUNCTION ak
    END INTERFACE
    END FUNCTION fredin
END INTERFACE
INTERFACE
    SUBROUTINE frenel(x,s,c)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), INTENT(OUT) :: s,c
    END SUBROUTINE frenel
END INTERFACE
INTERFACE
    SUBROUTINE frprmn(p,ftol,iter,fret)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: iter
    REAL(SP), INTENT(IN) :: ftol
    REAL(SP), INTENT(OUT) :: fret
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: p
    END SUBROUTINE frprmn
END INTERFACE
INTERFACE
    SUBROUTINE ftest(data1,data2,f,prob)
    USE nrtype
    REAL(SP), INTENT(OUT) :: f,prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    END SUBROUTINE ftest
END INTERFACE
INTERFACE
    FUNCTION gamdev(ia)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: ia
    REAL(SP) :: gamdev
    END FUNCTION gamdev
END INTERFACE
INTERFACE gammln
    FUNCTION gammln_s(xx)
    USE nrtype
    REAL(SP), INTENT(IN) :: xx
    REAL(SP) :: gammln_s
    END FUNCTION gammln_s
!BL
    FUNCTION gammln_v(xx)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: xx
    REAL(SP), DIMENSION(size(xx)) :: gammln_v
    END FUNCTION gammln_v

```

```

END INTERFACE
INTERFACE gammp
  FUNCTION gammp_s(a,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,x
    REAL(SP) :: gammp_s
  END FUNCTION gammp_s
!BL
  FUNCTION gammp_v(a,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,x
    REAL(SP), DIMENSION(size(a)) :: gammp_v
  END FUNCTION gammp_v
END INTERFACE
INTERFACE gammq
  FUNCTION gammq_s(a,x)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,x
    REAL(SP) :: gammq_s
  END FUNCTION gammq_s
!BL
  FUNCTION gammq_v(a,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,x
    REAL(SP), DIMENSION(size(a)) :: gammq_v
  END FUNCTION gammq_v
END INTERFACE
INTERFACE gasdev
  SUBROUTINE gasdev_s(harvest)
    USE nrtype
    REAL(SP), INTENT(OUT) :: harvest
  END SUBROUTINE gasdev_s
!BL
  SUBROUTINE gasdev_v(harvest)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
  END SUBROUTINE gasdev_v
END INTERFACE
INTERFACE
  SUBROUTINE gaucof(a,b,amu0,x,w)
    USE nrtype
    REAL(SP), INTENT(IN) :: amu0
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: a,b
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
  END SUBROUTINE gaucof
END INTERFACE
INTERFACE
  SUBROUTINE gauher(x,w)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
  END SUBROUTINE gauher
END INTERFACE
INTERFACE
  SUBROUTINE gaujac(x,w,alf,bet)

```

```

        USE nrtype
        REAL(SP), INTENT(IN) :: alf,bet
        REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
        END SUBROUTINE gaujac
    END INTERFACE
INTERFACE
    SUBROUTINE gaulag(x,w,alf)
    USE nrtype
    REAL(SP), INTENT(IN) :: alf
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
    END SUBROUTINE gaulag
END INTERFACE
INTERFACE
    SUBROUTINE gauleg(x1,x2,x,w)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x,w
    END SUBROUTINE gauleg
END INTERFACE
INTERFACE
    SUBROUTINE gaussj(a,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a,b
    END SUBROUTINE gaussj
END INTERFACE
INTERFACE gcf
    FUNCTION gcf_s(a,x,gln)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,x
    REAL(SP), OPTIONAL, INTENT(OUT) :: gln
    REAL(SP) :: gcf_s
    END FUNCTION gcf_s
!BL
    FUNCTION gcf_v(a,x,gln)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,x
    REAL(SP), DIMENSION(:), OPTIONAL, INTENT(OUT) :: gln
    REAL(SP), DIMENSION(size(a)) :: gcf_v
    END FUNCTION gcf_v
END INTERFACE
INTERFACE
    FUNCTION golden(ax,bx,cx,func,tol,xmin)
    USE nrtype
    REAL(SP), INTENT(IN) :: ax,bx,cx,tol
    REAL(SP), INTENT(OUT) :: xmin
    REAL(SP) :: golden
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION golden

```

```

END INTERFACE
INTERFACE gser
  FUNCTION gser_s(a,x,gln)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,x
    REAL(SP), OPTIONAL, INTENT(OUT) :: gln
    REAL(SP) :: gser_s
  END FUNCTION gser_s
!BL
  FUNCTION gser_v(a,x,gln)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,x
    REAL(SP), DIMENSION(:), OPTIONAL, INTENT(OUT) :: gln
    REAL(SP), DIMENSION(size(a)) :: gser_v
  END FUNCTION gser_v
END INTERFACE
INTERFACE
  SUBROUTINE hqr(a,wr,wi)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: wr,wi
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
  END SUBROUTINE hqr
END INTERFACE
INTERFACE
  SUBROUTINE hunt(xx,x,jlo)
    USE nrtype
    INTEGER(I4B), INTENT(INOUT) :: jlo
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: xx
  END SUBROUTINE hunt
END INTERFACE
INTERFACE
  SUBROUTINE hypdrv(s,ry,rdyds)
    USE nrtype
    REAL(SP), INTENT(IN) :: s
    REAL(SP), DIMENSION(:), INTENT(IN) :: ry
    REAL(SP), DIMENSION(:), INTENT(OUT) :: rdyds
  END SUBROUTINE hypdrv
END INTERFACE
INTERFACE
  FUNCTION hypgeo(a,b,c,z)
    USE nrtype
    COMPLEX(SPC), INTENT(IN) :: a,b,c,z
    COMPLEX(SPC) :: hypgeo
  END FUNCTION hypgeo
END INTERFACE
INTERFACE
  SUBROUTINE hypser(a,b,c,z,series,deriv)
    USE nrtype
    COMPLEX(SPC), INTENT(IN) :: a,b,c,z
    COMPLEX(SPC), INTENT(OUT) :: series,deriv
  END SUBROUTINE hypser
END INTERFACE
INTERFACE

```

```

FUNCTION icrc(crc,buf,jinit,jrev)
USE nrtype
CHARACTER(1), DIMENSION(:), INTENT(IN) :: buf
INTEGER(I2B), INTENT(IN) :: crc,jinit
INTEGER(I4B), INTENT(IN) :: jrev
INTEGER(I2B) :: icrc
END FUNCTION icrc
END INTERFACE
INTERFACE
FUNCTION igray(n,is)
USE nrtype
INTEGER(I4B), INTENT(IN) :: n,is
INTEGER(I4B) :: igray
END FUNCTION igray
END INTERFACE
INTERFACE
RECURSIVE SUBROUTINE index_bypack(arr,index,partial)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B), DIMENSION(:), INTENT(INOUT) :: index
INTEGER, OPTIONAL, INTENT(IN) :: partial
END SUBROUTINE index_bypack
END INTERFACE
INTERFACE indexx
SUBROUTINE indexx_sp(arr,index)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: arr
INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: index
END SUBROUTINE indexx_sp
SUBROUTINE indexx_i4b(iarr,index)
USE nrtype
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: iarr
INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: index
END SUBROUTINE indexx_i4b
END INTERFACE
INTERFACE
FUNCTION interp(uc)
USE nrtype
REAL(DP), DIMENSION(:,:), INTENT(IN) :: uc
REAL(DP), DIMENSION(2*size(uc,1)-1,2*size(uc,1)-1) :: interp
END FUNCTION interp
END INTERFACE
INTERFACE
FUNCTION rank(indx)
USE nrtype
INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indx
INTEGER(I4B), DIMENSION(size(indx)) :: rank
END FUNCTION rank
END INTERFACE
INTERFACE
FUNCTION irbit1(iseed)
USE nrtype
INTEGER(I4B), INTENT(INOUT) :: iseed
INTEGER(I4B) :: irbit1

```

```

        END FUNCTION irbit1
    END INTERFACE
INTERFACE
    FUNCTION irbit2(iseed)
        USE nrtype
        INTEGER(I4B), INTENT(INOUT) :: iseed
        INTEGER(I4B) :: irbit2
    END FUNCTION irbit2
END INTERFACE
INTERFACE
    SUBROUTINE jacobi(a,d,v,nrot)
        USE nrtype
        INTEGER(I4B), INTENT(OUT) :: nrot
        REAL(SP), DIMENSION(:), INTENT(OUT) :: d
        REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
        REAL(SP), DIMENSION(:,:), INTENT(OUT) :: v
    END SUBROUTINE jacobi
END INTERFACE
INTERFACE
    SUBROUTINE jacobn(x,y,dfdx,dfdy)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dfdx
        REAL(SP), DIMENSION(:,:), INTENT(OUT) :: dfdy
    END SUBROUTINE jacobn
END INTERFACE
INTERFACE
    FUNCTION julday(mm,id,iyyy)
        USE nrtype
        INTEGER(I4B), INTENT(IN) :: mm,id,iyyy
        INTEGER(I4B) :: julday
    END FUNCTION julday
END INTERFACE
INTERFACE
    SUBROUTINE kendl1(data1,data2,tau,z,prob)
        USE nrtype
        REAL(SP), INTENT(OUT) :: tau,z,prob
        REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    END SUBROUTINE kendl1
END INTERFACE
INTERFACE
    SUBROUTINE kendl2(tab,tau,z,prob)
        USE nrtype
        REAL(SP), DIMENSION(:,:), INTENT(IN) :: tab
        REAL(SP), INTENT(OUT) :: tau,z,prob
    END SUBROUTINE kendl2
END INTERFACE
INTERFACE
    FUNCTION kermom(y,m)
        USE nrtype
        REAL(DP), INTENT(IN) :: y
        INTEGER(I4B), INTENT(IN) :: m
        REAL(DP), DIMENSION(m) :: kermom

```

```

        END FUNCTION kermom
    END INTERFACE
INTERFACE
    SUBROUTINE ks2d1s(x1,y1,quadv1,d1,prob)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x1,y1
    REAL(SP), INTENT(OUT) :: d1,prob
    INTERFACE
        SUBROUTINE quadv1(x,y,fa,fb,fc,fd)
        USE nrtype
        REAL(SP), INTENT(IN) :: x,y
        REAL(SP), INTENT(OUT) :: fa,fb,fc,fd
        END SUBROUTINE quadv1
    END INTERFACE
    END SUBROUTINE ks2d1s
END INTERFACE
INTERFACE
    SUBROUTINE ks2d2s(x1,y1,x2,y2,d,prob)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x1,y1,x2,y2
    REAL(SP), INTENT(OUT) :: d,prob
    END SUBROUTINE ks2d2s
END INTERFACE
INTERFACE
    SUBROUTINE ksone(data,func,d,prob)
    USE nrtype
    REAL(SP), INTENT(OUT) :: d,prob
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: data
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE
    END SUBROUTINE ksone
END INTERFACE
INTERFACE
    SUBROUTINE kstwo(data1,data2,d,prob)
    USE nrtype
    REAL(SP), INTENT(OUT) :: d,prob
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    END SUBROUTINE kstwo
END INTERFACE
INTERFACE
    SUBROUTINE laguer(a,x,its)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: its
    COMPLEX(SPC), INTENT(INOUT) :: x
    COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: a
    END SUBROUTINE laguer
END INTERFACE
INTERFACE
    SUBROUTINE lfit(x,y,sig,a,maska,covar,chisq,funcs)

```

```

USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,sig
REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: maska
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: covar
REAL(SP), INTENT(OUT) :: chisq
INTERFACE
  SUBROUTINE funcs(x,arr)
    USE nrtype
    REAL(SP),INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(OUT) :: arr
  END SUBROUTINE funcs
END INTERFACE
END SUBROUTINE lfit
END INTERFACE
INTERFACE
  SUBROUTINE linbcg(b,x,itol,tol,itmax,iter,err)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: b
    REAL(DP), DIMENSION(:), INTENT(INOUT) :: x
    INTEGER(I4B), INTENT(IN) :: itol,itmax
    REAL(DP), INTENT(IN) :: tol
    INTEGER(I4B), INTENT(OUT) :: iter
    REAL(DP), INTENT(OUT) :: err
  END SUBROUTINE linbcg
END INTERFACE
INTERFACE
  SUBROUTINE linmin(p,xi,fret)
    USE nrtype
    REAL(SP), INTENT(OUT) :: fret
    REAL(SP), DIMENSION(:), TARGET, INTENT(INOUT) :: p,xi
  END SUBROUTINE linmin
END INTERFACE
INTERFACE
  SUBROUTINE lnsrch(xold,fold,g,p,x,f,stpmax,check,func)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: xold,g
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: p
    REAL(SP), INTENT(IN) :: fold,stpmax
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x
    REAL(SP), INTENT(OUT) :: f
    LOGICAL(LGT), INTENT(OUT) :: check
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP) :: func
      REAL(SP), DIMENSION(:), INTENT(IN) :: x
    END FUNCTION func
  END INTERFACE
END SUBROUTINE lnsrch
END INTERFACE
INTERFACE
  FUNCTION locatenr(xx,x)
    USE nrtype

```



```

REAL(SP), DIMENSION(:), INTENT(IN) :: xx
REAL(SP), INTENT(IN) :: x
INTEGER(I4B) :: locatenr
END FUNCTION locatenr
END INTERFACE
INTERFACE
  FUNCTION lop(u)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: u
    REAL(DP), DIMENSION(size(u,1),size(u,1)) :: lop
  END FUNCTION lop
END INTERFACE
INTERFACE
  SUBROUTINE lubksb(a,indx,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indx
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: b
  END SUBROUTINE lubksb
END INTERFACE
INTERFACE
  SUBROUTINE ludcmp(a,indx,d)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: indx
    REAL(SP), INTENT(OUT) :: d
  END SUBROUTINE ludcmp
END INTERFACE
INTERFACE
  SUBROUTINE machar(ibeta,it,irnd,ngrd,machep,negep,iexp,minexp,&
    maxexp,eps,epsneg,xmin,xmax)
    USE nrtype
    INTEGER(I4B), INTENT(OUT) :: ibeta,iexp,irnd,it,machep,maxexp,&
    minexp,negep,ngrd
    REAL(SP), INTENT(OUT) :: eps,epsneg,xmax,xmin
  END SUBROUTINE machar
END INTERFACE
INTERFACE
  SUBROUTINE medfit(x,y,a,b,abdev)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), INTENT(OUT) :: a,b,abdev
  END SUBROUTINE medfit
END INTERFACE
INTERFACE
  SUBROUTINE memcof(data,xms,d)
    USE nrtype
    REAL(SP), INTENT(OUT) :: xms
    REAL(SP), DIMENSION(:), INTENT(IN) :: data
    REAL(SP), DIMENSION(:), INTENT(OUT) :: d
  END SUBROUTINE memcof
END INTERFACE
INTERFACE
  SUBROUTINE mgfas(u,maxcyc)

```

```

    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    INTEGER(I4B), INTENT(IN) :: maxcyc
    END SUBROUTINE mgfas
END INTERFACE
INTERFACE
    SUBROUTINE mglin(u,ncycle)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    INTEGER(I4B), INTENT(IN) :: ncycle
    END SUBROUTINE mglin
END INTERFACE
INTERFACE
    SUBROUTINE midexp(funk,aa,bb,s,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: aa,bb
    REAL(SP), INTENT(INOUT) :: s
    INTEGER(I4B), INTENT(IN) :: n
    INTERFACE
        FUNCTION funk(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: funk
        END FUNCTION funk
    END INTERFACE
    END SUBROUTINE midexp
END INTERFACE
INTERFACE
    SUBROUTINE midinf(funk,aa,bb,s,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: aa,bb
    REAL(SP), INTENT(INOUT) :: s
    INTEGER(I4B), INTENT(IN) :: n
    INTERFACE
        FUNCTION funk(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: funk
        END FUNCTION funk
    END INTERFACE
    END SUBROUTINE midinf
END INTERFACE
INTERFACE
    SUBROUTINE midpnt(func,a,b,s,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP), INTENT(INOUT) :: s
    INTEGER(I4B), INTENT(IN) :: n
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE

```

```

END INTERFACE
END SUBROUTINE midpnt
END INTERFACE
INTERFACE
  SUBROUTINE midsql(funk,aa,bb,s,n)
  USE nrtype
  REAL(SP), INTENT(IN) :: aa,bb
  REAL(SP), INTENT(INOUT) :: s
  INTEGER(I4B), INTENT(IN) :: n
  INTERFACE
    FUNCTION funk(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: funk
    END FUNCTION funk
  END INTERFACE
END SUBROUTINE midsql
END INTERFACE
INTERFACE
  SUBROUTINE midsqu(funk,aa,bb,s,n)
  USE nrtype
  REAL(SP), INTENT(IN) :: aa,bb
  REAL(SP), INTENT(INOUT) :: s
  INTEGER(I4B), INTENT(IN) :: n
  INTERFACE
    FUNCTION funk(x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(size(x)) :: funk
    END FUNCTION funk
  END INTERFACE
END SUBROUTINE midsqu
END INTERFACE
INTERFACE
  RECURSIVE SUBROUTINE miser(func,regn,ndim,npts,dith,ave,var)
  USE nrtype
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP) :: func
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    END FUNCTION func
  END INTERFACE
  REAL(SP), DIMENSION(:), INTENT(IN) :: regn
  INTEGER(I4B), INTENT(IN) :: ndim,npts
  REAL(SP), INTENT(IN) :: dith
  REAL(SP), INTENT(OUT) :: ave,var
END SUBROUTINE miser
END INTERFACE
INTERFACE
  SUBROUTINE mmid(y,dydx,xs,htot,nstep,yout,derivs)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: nstep
  REAL(SP), INTENT(IN) :: xs,htot

```

```

REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
INTERFACE
  SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
  END SUBROUTINE derivs
END INTERFACE
END SUBROUTINE mmid
END INTERFACE
INTERFACE
  SUBROUTINE mnbrak(ax,bx,cx,fa,fb,fc,func)
    USE nrtype
    REAL(SP), INTENT(INOUT) :: ax,bx
    REAL(SP), INTENT(OUT) :: cx,fa,fb,fc
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP), INTENT(IN) :: x
      REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END SUBROUTINE mnbrak
END INTERFACE
INTERFACE
  SUBROUTINE mnewt(ntrial,x,tolx,tolf,usrfun)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: ntrial
    REAL(SP), INTENT(IN) :: tolx,tolf
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
  INTERFACE
    SUBROUTINE usrfun(x,fvec,fjac)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x
      REAL(SP), DIMENSION(:), INTENT(OUT) :: fvec
      REAL(SP), DIMENSION(:,:), INTENT(OUT) :: fjac
    END SUBROUTINE usrfun
  END INTERFACE
END SUBROUTINE mnewt
END INTERFACE
INTERFACE
  SUBROUTINE moment(data,ave,adev,sdev,var,skew,curt)
    USE nrtype
    REAL(SP), INTENT(OUT) :: ave,adev,sdev,var,skew,curt
    REAL(SP), DIMENSION(:), INTENT(IN) :: data
  END SUBROUTINE moment
END INTERFACE
INTERFACE
  SUBROUTINE mp2dfr(a,s,n,m)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    INTEGER(I4B), INTENT(OUT) :: m

```

```

    CHARACTER(1), DIMENSION(:), INTENT(INOUT) :: a
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: s
    END SUBROUTINE mp2dfr
END INTERFACE
INTERFACE
    SUBROUTINE mpdiv(q,r,u,v,n,m)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: q,r
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: u,v
    INTEGER(I4B), INTENT(IN) :: n,m
    END SUBROUTINE mpdiv
END INTERFACE
INTERFACE
    SUBROUTINE mpinv(u,v,n,m)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: u
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: v
    INTEGER(I4B), INTENT(IN) :: n,m
    END SUBROUTINE mpinv
END INTERFACE
INTERFACE
    SUBROUTINE mpmul(w,u,v,n,m)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: u,v
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: w
    INTEGER(I4B), INTENT(IN) :: n,m
    END SUBROUTINE mpmul
END INTERFACE
INTERFACE
    SUBROUTINE mppi(n)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    END SUBROUTINE mppi
END INTERFACE
INTERFACE
    SUBROUTINE mprove(a,alud,indx,b,x)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a,alud
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indx
    REAL(SP), DIMENSION(:), INTENT(IN) :: b
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
    END SUBROUTINE mprove
END INTERFACE
INTERFACE
    SUBROUTINE mpsqrt(w,u,v,n,m)
    USE nrtype
    CHARACTER(1), DIMENSION(:), INTENT(OUT) :: w,u
    CHARACTER(1), DIMENSION(:), INTENT(IN) :: v
    INTEGER(I4B), INTENT(IN) :: n,m
    END SUBROUTINE mpsqrt
END INTERFACE
INTERFACE
    SUBROUTINE mrqcof(x,y,sig,a,maska,alpha,beta,chisq,funcs)
    USE nrtype

```

```

REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,a,sig
REAL(SP), DIMENSION(:), INTENT(OUT) :: beta
REAL(SP), DIMENSION(:,:), INTENT(OUT) :: alpha
REAL(SP), INTENT(OUT) :: chisq
LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: maska
INTERFACE
  SUBROUTINE funcs(x,a,yfit,dyda)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: x,a
  REAL(SP), DIMENSION(:), INTENT(OUT) :: yfit
  REAL(SP), DIMENSION(:,:), INTENT(OUT) :: dyda
  END SUBROUTINE funcs
END INTERFACE
END SUBROUTINE mrqcof
END INTERFACE
INTERFACE
  SUBROUTINE mrqmin(x,y,sig,a,maska,covar,alpha,chisq,funcs,alamda)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,sig
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
  REAL(SP), DIMENSION(:,:), INTENT(OUT) :: covar,alpha
  REAL(SP), INTENT(OUT) :: chisq
  REAL(SP), INTENT(INOUT) :: alamda
  LOGICAL(LGT), DIMENSION(:), INTENT(IN) :: maska
  INTERFACE
    SUBROUTINE funcs(x,a,yfit,dyda)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: yfit
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: dyda
    END SUBROUTINE funcs
  END INTERFACE
  END SUBROUTINE mrqmin
END INTERFACE
INTERFACE
  SUBROUTINE newt(x,check)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: x
  LOGICAL(LGT), INTENT(OUT) :: check
  END SUBROUTINE newt
END INTERFACE
INTERFACE
  SUBROUTINE odeint(ystart,x1,x2,eps,h1,hmin,derivs,rkqs)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: ystart
  REAL(SP), INTENT(IN) :: x1,x2,eps,h1,hmin
  INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
  END INTERFACE
END INTERFACE
!BL

```

```

SUBROUTINE rkqs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
REAL(SP), INTENT(INOUT) :: x
REAL(SP), INTENT(IN) :: htry,eps
REAL(SP), INTENT(OUT) :: hdid,hnext
INTERFACE
SUBROUTINE derivs(x,y,dydx)
USE nrtype
REAL(SP), INTENT(IN) :: x
REAL(SP), DIMENSION(:), INTENT(IN) :: y
REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
END SUBROUTINE derivs
END INTERFACE
END SUBROUTINE rkqs
END INTERFACE
END SUBROUTINE odeint
END INTERFACE
INTERFACE
SUBROUTINE orthog(anu,alpha,beta,a,b)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: anu,alpha,beta
REAL(SP), DIMENSION(:), INTENT(OUT) :: a,b
END SUBROUTINE orthog
END INTERFACE
INTERFACE
SUBROUTINE pade(cof,resid)
USE nrtype
REAL(DP), DIMENSION(:), INTENT(INOUT) :: cof
REAL(SP), INTENT(OUT) :: resid
END SUBROUTINE pade
END INTERFACE
INTERFACE
FUNCTION pccheb(d)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: d
REAL(SP), DIMENSION(size(d)) :: pccheb
END FUNCTION pccheb
END INTERFACE
INTERFACE
SUBROUTINE pcshft(a,b,d)
USE nrtype
REAL(SP), INTENT(IN) :: a,b
REAL(SP), DIMENSION(:), INTENT(INOUT) :: d
END SUBROUTINE pcshft
END INTERFACE
INTERFACE
SUBROUTINE pearsn(x,y,r,prob,z)
USE nrtype
REAL(SP), INTENT(OUT) :: r,prob,z
REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
END SUBROUTINE pearsn
END INTERFACE

```

```

INTERFACE
  SUBROUTINE period(x,y,ofac,hifac,px,py,jmax,prob)
  USE nrtype
  INTEGER(I4B), INTENT(OUT) :: jmax
  REAL(SP), INTENT(IN) :: ofac,hifac
  REAL(SP), INTENT(OUT) :: prob
  REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
  REAL(SP), DIMENSION(:), POINTER :: px,py
  END SUBROUTINE period
END INTERFACE
INTERFACE plgndr
  FUNCTION plgndr_s(l,m,x)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: l,m
  REAL(SP), INTENT(IN) :: x
  REAL(SP) :: plgndr_s
  END FUNCTION plgndr_s
!BL
  FUNCTION plgndr_v(l,m,x)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: l,m
  REAL(SP), DIMENSION(:), INTENT(IN) :: x
  REAL(SP), DIMENSION(size(x)) :: plgndr_v
  END FUNCTION plgndr_v
END INTERFACE
INTERFACE
  FUNCTION poidev(xm)
  USE nrtype
  REAL(SP), INTENT(IN) :: xm
  REAL(SP) :: poidev
  END FUNCTION poidev
END INTERFACE
INTERFACE
  FUNCTION polcoe(x,y)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
  REAL(SP), DIMENSION(size(x)) :: polcoe
  END FUNCTION polcoe
END INTERFACE
INTERFACE
  FUNCTION polcof(xa,ya)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya
  REAL(SP), DIMENSION(size(xa)) :: polcof
  END FUNCTION polcof
END INTERFACE
INTERFACE
  SUBROUTINE poldiv(u,v,q,r)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: u,v
  REAL(SP), DIMENSION(:), INTENT(OUT) :: q,r
  END SUBROUTINE poldiv
END INTERFACE
INTERFACE

```



```

SUBROUTINE polin2(x1a,x2a,ya,x1,x2,y,dy)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x1a,x2a
REAL(SP), DIMENSION(:,:), INTENT(IN) :: ya
REAL(SP), INTENT(IN) :: x1,x2
REAL(SP), INTENT(OUT) :: y,dy
END SUBROUTINE polin2
END INTERFACE
INTERFACE
SUBROUTINE polint(xa,ya,x,y,dy)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya
REAL(SP), INTENT(IN) :: x
REAL(SP), INTENT(OUT) :: y,dy
END SUBROUTINE polint
END INTERFACE
INTERFACE
SUBROUTINE powell(p,xi,ftol,iter,fret)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: p
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: xi
INTEGER(I4B), INTENT(OUT) :: iter
REAL(SP), INTENT(IN) :: ftol
REAL(SP), INTENT(OUT) :: fret
END SUBROUTINE powell
END INTERFACE
INTERFACE
FUNCTION predic(data,d,nfut)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: data,d
INTEGER(I4B), INTENT(IN) :: nfut
REAL(SP), DIMENSION(nfut) :: predic
END FUNCTION predic
END INTERFACE
INTERFACE
FUNCTION probks(alam)
USE nrtype
REAL(SP), INTENT(IN) :: alam
REAL(SP) :: probks
END FUNCTION probks
END INTERFACE
INTERFACE psdes
SUBROUTINE psdes_s(lword,rword)
USE nrtype
INTEGER(I4B), INTENT(INOUT) :: lword,rword
END SUBROUTINE psdes_s
!BL
SUBROUTINE psdes_v(lword,rword)
USE nrtype
INTEGER(I4B), DIMENSION(:), INTENT(INOUT) :: lword,rword
END SUBROUTINE psdes_v
END INTERFACE
INTERFACE
SUBROUTINE pwt(a,isign)

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```

        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
        INTEGER(I4B), INTENT(IN) :: isign
        END SUBROUTINE pwt
    END INTERFACE
INTERFACE
    SUBROUTINE pwtset(n)
        USE nrtype
        INTEGER(I4B), INTENT(IN) :: n
        END SUBROUTINE pwtset
END INTERFACE
INTERFACE pythag
    FUNCTION pythag_dp(a,b)
        USE nrtype
        REAL(DP), INTENT(IN) :: a,b
        REAL(DP) :: pythag_dp
    END FUNCTION pythag_dp
!BL
    FUNCTION pythag_sp(a,b)
        USE nrtype
        REAL(SP), INTENT(IN) :: a,b
        REAL(SP) :: pythag_sp
    END FUNCTION pythag_sp
END INTERFACE
INTERFACE
    SUBROUTINE pzextr(iest,xest,yest,yz,dy)
        USE nrtype
        INTEGER(I4B), INTENT(IN) :: iest
        REAL(SP), INTENT(IN) :: xest
        REAL(SP), DIMENSION(:), INTENT(IN) :: yest
        REAL(SP), DIMENSION(:), INTENT(OUT) :: yz,dy
    END SUBROUTINE pzextr
END INTERFACE
!!! FB:
!   INTERFACE
!       FUNCTION qgaus(func,a,b)
!           USE nrtype
!           REAL(SP), INTENT(IN) :: a,b
!           REAL(SP) :: qgaus
!           INTERFACE
!               FUNCTION func(x)
!                   USE nrtype
!                   REAL(SP), DIMENSION(:), INTENT(IN) :: x
!                   REAL(SP), DIMENSION(size(x)) :: func
!               END FUNCTION func
!           END INTERFACE
!       END FUNCTION qgaus
!   END INTERFACE
!!! /FB
INTERFACE
    SUBROUTINE qrdcmp(a,c,d,sing)
        USE nrtype
        REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
        REAL(SP), DIMENSION(:), INTENT(OUT) :: c,d

```

```

    LOGICAL(LGT), INTENT(OUT) :: sing
    END SUBROUTINE qrdcmp
END INTERFACE
INTERFACE
    FUNCTION qromb(func,a,b)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP) :: qromb
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION qromb
END INTERFACE
INTERFACE
    FUNCTION qromo(func,a,b,choose)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP) :: qromo
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: func
        END FUNCTION func
    END INTERFACE
END INTERFACE
INTERFACE
    SUBROUTINE choose(funk,aa,bb,s,n)
    USE nrtype
    REAL(SP), INTENT(IN) :: aa,bb
    REAL(SP), INTENT(INOUT) :: s
    INTEGER(I4B), INTENT(IN) :: n
    INTERFACE
        FUNCTION funk(x)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x
        REAL(SP), DIMENSION(size(x)) :: funk
        END FUNCTION funk
    END INTERFACE
    END SUBROUTINE choose
END INTERFACE
END FUNCTION qromo
END INTERFACE
INTERFACE
    SUBROUTINE qroot(p,b,c,eps)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: p
    REAL(SP), INTENT(INOUT) :: b,c
    REAL(SP), INTENT(IN) :: eps
    END SUBROUTINE qroot
END INTERFACE

```

```

INTERFACE
  SUBROUTINE qrsolv(a,c,d,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    REAL(SP), DIMENSION(:), INTENT(IN) :: c,d
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: b
  END SUBROUTINE qrsolv
END INTERFACE
INTERFACE
  SUBROUTINE grupdt(r,qt,u,v)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: r,qt
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: u
    REAL(SP), DIMENSION(:), INTENT(IN) :: v
  END SUBROUTINE grupdt
END INTERFACE
INTERFACE
  FUNCTION qsimp(func,a,b)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP) :: qsimp
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x
      REAL(SP), DIMENSION(size(x)) :: func
    END FUNCTION func
  END INTERFACE
END FUNCTION qsimp
END INTERFACE
INTERFACE
  FUNCTION qtrap(func,a,b)
    USE nrtype
    REAL(SP), INTENT(IN) :: a,b
    REAL(SP) :: qtrap
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: x
      REAL(SP), DIMENSION(size(x)) :: func
    END FUNCTION func
  END INTERFACE
END FUNCTION qtrap
END INTERFACE
INTERFACE
  SUBROUTINE quadct(x,y,xx,yy,fa,fb,fc,fd)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,y
    REAL(SP), DIMENSION(:), INTENT(IN) :: xx,yy
    REAL(SP), INTENT(OUT) :: fa,fb,fc,fd
  END SUBROUTINE quadct
END INTERFACE
INTERFACE
  SUBROUTINE quadmx(a)

```

```

        USE nrtype
        REAL(SP), DIMENSION(:,:), INTENT(OUT) :: a
    END SUBROUTINE quadmx
END INTERFACE
INTERFACE
    SUBROUTINE quadv1(x,y,fa,fb,fc,fd)
        USE nrtype
        REAL(SP), INTENT(IN) :: x,y
        REAL(SP), INTENT(OUT) :: fa,fb,fc,fd
    END SUBROUTINE quadv1
END INTERFACE
INTERFACE
    FUNCTION ran(idum)
        INTEGER(selected_int_kind(9)), INTENT(INOUT) :: idum
        REAL :: ran
    END FUNCTION ran
END INTERFACE
INTERFACE ran0
    SUBROUTINE ran0_s(harvest)
        USE nrtype
        REAL(SP), INTENT(OUT) :: harvest
    END SUBROUTINE ran0_s
!BL
    SUBROUTINE ran0_v(harvest)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
    END SUBROUTINE ran0_v
END INTERFACE
INTERFACE ran1
    SUBROUTINE ran1_s(harvest)
        USE nrtype
        REAL(SP), INTENT(OUT) :: harvest
    END SUBROUTINE ran1_s
!BL
    SUBROUTINE ran1_v(harvest)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
    END SUBROUTINE ran1_v
END INTERFACE
INTERFACE ran2
    SUBROUTINE ran2_s(harvest)
        USE nrtype
        REAL(SP), INTENT(OUT) :: harvest
    END SUBROUTINE ran2_s
!BL
    SUBROUTINE ran2_v(harvest)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
    END SUBROUTINE ran2_v
END INTERFACE
INTERFACE ran3
    SUBROUTINE ran3_s(harvest)
        USE nrtype
        REAL(SP), INTENT(OUT) :: harvest

```

```

      END SUBROUTINE ran3_s
!BL
      SUBROUTINE ran3_v(harvest)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(OUT) :: harvest
      END SUBROUTINE ran3_v
END INTERFACE
INTERFACE
      SUBROUTINE ratint(xa,ya,x,y,dy)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya
      REAL(SP), INTENT(IN) :: x
      REAL(SP), INTENT(OUT) :: y,dy
      END SUBROUTINE ratint
END INTERFACE
INTERFACE
      SUBROUTINE ratlsq(func,a,b,mm,kk,cof,dev)
      USE nrtype
      REAL(DP), INTENT(IN) :: a,b
      INTEGER(I4B), INTENT(IN) :: mm,kk
      REAL(DP), DIMENSION(:), INTENT(OUT) :: cof
      REAL(DP), INTENT(OUT) :: dev
      INTERFACE
            FUNCTION func(x)
            USE nrtype
            REAL(DP), DIMENSION(:), INTENT(IN) :: x
            REAL(DP), DIMENSION(size(x)) :: func
            END FUNCTION func
      END INTERFACE
      END SUBROUTINE ratlsq
END INTERFACE
INTERFACE ratval
      FUNCTION ratval_s(x,cof,mm,kk)
      USE nrtype
      REAL(DP), INTENT(IN) :: x
      INTEGER(I4B), INTENT(IN) :: mm,kk
      REAL(DP), DIMENSION(mm+kk+1), INTENT(IN) :: cof
      REAL(DP) :: ratval_s
      END FUNCTION ratval_s
!BL
      FUNCTION ratval_v(x,cof,mm,kk)
      USE nrtype
      REAL(DP), DIMENSION(:), INTENT(IN) :: x
      INTEGER(I4B), INTENT(IN) :: mm,kk
      REAL(DP), DIMENSION(mm+kk+1), INTENT(IN) :: cof
      REAL(DP), DIMENSION(size(x)) :: ratval_v
      END FUNCTION ratval_v
END INTERFACE
INTERFACE rc
      FUNCTION rc_s(x,y)
      USE nrtype
      REAL(SP), INTENT(IN) :: x,y
      REAL(SP) :: rc_s
      END FUNCTION rc_s

```

```

!BL
  FUNCTION rc_v(x,y)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), DIMENSION(size(x)) :: rc_v
  END FUNCTION rc_v
END INTERFACE
INTERFACE rd
  FUNCTION rd_s(x,y,z)
    USE nrtype
    REAL(SP), INTENT(IN) :: x,y,z
    REAL(SP) :: rd_s
  END FUNCTION rd_s
!BL
  FUNCTION rd_v(x,y,z)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,z
    REAL(SP), DIMENSION(size(x)) :: rd_v
  END FUNCTION rd_v
END INTERFACE
INTERFACE realft
  SUBROUTINE realft_dp(data,isign,zdata)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
    COMPLEX(DPC), DIMENSION(:), OPTIONAL, TARGET :: zdata
  END SUBROUTINE realft_dp
!BL
  SUBROUTINE realft_sp(data,isign,zdata)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: data
    INTEGER(I4B), INTENT(IN) :: isign
    COMPLEX(SPC), DIMENSION(:), OPTIONAL, TARGET :: zdata
  END SUBROUTINE realft_sp
END INTERFACE
INTERFACE
  RECURSIVE FUNCTION recur1(a,b) RESULT(u)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b
    REAL(SP), DIMENSION(size(a)) :: u
  END FUNCTION recur1
END INTERFACE
INTERFACE
  FUNCTION recur2(a,b,c)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c
    REAL(SP), DIMENSION(size(a)) :: recur2
  END FUNCTION recur2
END INTERFACE
INTERFACE
  SUBROUTINE relax(u,rhs)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: rhs

```

```

        END SUBROUTINE relax
    END INTERFACE
INTERFACE
    SUBROUTINE relax2(u,rhs)
        USE nrtype
        REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
        REAL(DP), DIMENSION(:,:), INTENT(IN) :: rhs
    END SUBROUTINE relax2
END INTERFACE
INTERFACE
    FUNCTION resid(u,rhs)
        USE nrtype
        REAL(DP), DIMENSION(:,:), INTENT(IN) :: u,rhs
        REAL(DP), DIMENSION(size(u,1),size(u,1)) :: resid
    END FUNCTION resid
END INTERFACE
INTERFACE rf
    FUNCTION rf_s(x,y,z)
        USE nrtype
        REAL(SP), INTENT(IN) :: x,y,z
        REAL(SP) :: rf_s
    END FUNCTION rf_s
!BL
    FUNCTION rf_v(x,y,z)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,z
        REAL(SP), DIMENSION(size(x)) :: rf_v
    END FUNCTION rf_v
END INTERFACE
INTERFACE rj
    FUNCTION rj_s(x,y,z,p)
        USE nrtype
        REAL(SP), INTENT(IN) :: x,y,z,p
        REAL(SP) :: rj_s
    END FUNCTION rj_s
!BL
    FUNCTION rj_v(x,y,z,p)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,z,p
        REAL(SP), DIMENSION(size(x)) :: rj_v
    END FUNCTION rj_v
END INTERFACE
INTERFACE
    SUBROUTINE rk4(y,dydx,x,h,yout,derivs)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
        REAL(SP), INTENT(IN) :: x,h
        REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
    INTERFACE
        SUBROUTINE derivs(x,y,dydx)
            USE nrtype
            REAL(SP), INTENT(IN) :: x
            REAL(SP), DIMENSION(:), INTENT(IN) :: y
            REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx

```



```

        END SUBROUTINE derivs
    END INTERFACE
    END SUBROUTINE rk4
END INTERFACE
INTERFACE
    SUBROUTINE rkck(y,dydx,x,h,yout,yerr,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
    REAL(SP), INTENT(IN) :: x,h
    REAL(SP), DIMENSION(:), INTENT(OUT) :: yout,yerr
    INTERFACE
        SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
        END SUBROUTINE derivs
    END INTERFACE
    END SUBROUTINE rkck
END INTERFACE
INTERFACE
    SUBROUTINE rkdump(vstart,x1,x2,nstep,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: vstart
    REAL(SP), INTENT(IN) :: x1,x2
    INTEGER(I4B), INTENT(IN) :: nstep
    INTERFACE
        SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
        END SUBROUTINE derivs
    END INTERFACE
    END SUBROUTINE rkdump
END INTERFACE
INTERFACE
    SUBROUTINE rkqs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
    REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
    REAL(SP), INTENT(INOUT) :: x
    REAL(SP), INTENT(IN) :: htry,eps
    REAL(SP), INTENT(OUT) :: hdid,hnext
    INTERFACE
        SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
        END SUBROUTINE derivs
    END INTERFACE
    END SUBROUTINE rkqs
END INTERFACE

```

```

INTERFACE
  SUBROUTINE rlft2(data,spec,speq,isign)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: data
    COMPLEX(SPC), DIMENSION(:,:), INTENT(OUT) :: spec
    COMPLEX(SPC), DIMENSION(:), INTENT(OUT) :: speq
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE rlft2
END INTERFACE
INTERFACE
  SUBROUTINE rlft3(data,spec,speq,isign)
    USE nrtype
    REAL(SP), DIMENSION(:,:,:), INTENT(INOUT) :: data
    COMPLEX(SPC), DIMENSION(:,:,:), INTENT(OUT) :: spec
    COMPLEX(SPC), DIMENSION(:,:), INTENT(OUT) :: speq
    INTEGER(I4B), INTENT(IN) :: isign
  END SUBROUTINE rlft3
END INTERFACE
INTERFACE
  SUBROUTINE rotate(r,qt,i,a,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), TARGET, INTENT(INOUT) :: r,qt
    INTEGER(I4B), INTENT(IN) :: i
    REAL(SP), INTENT(IN) :: a,b
  END SUBROUTINE rotate
END INTERFACE
INTERFACE
  SUBROUTINE rsolv(a,d,b)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: a
    REAL(SP), DIMENSION(:), INTENT(IN) :: d
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: b
  END SUBROUTINE rsolv
END INTERFACE
INTERFACE
  FUNCTION rstrct(uf)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: uf
    REAL(DP), DIMENSION((size(uf,1)+1)/2,(size(uf,1)+1)/2) :: rstrct
  END FUNCTION rstrct
END INTERFACE
INTERFACE
  FUNCTION rtbis(func,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtbis
  INTERFACE
    FUNCTION func(x)
      USE nrtype
      REAL(SP), INTENT(IN) :: x
      REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END FUNCTION rtbis

```

```

END INTERFACE
INTERFACE
  FUNCTION rtflsp(func,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtflsp
    INTERFACE
      FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
      END FUNCTION func
    END INTERFACE
  END FUNCTION rtflsp
END INTERFACE
INTERFACE
  FUNCTION rtnewt(funcd,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtnewt
    INTERFACE
      SUBROUTINE funcd(x,fval,fderiv)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), INTENT(OUT) :: fval,fderiv
      END SUBROUTINE funcd
    END INTERFACE
  END FUNCTION rtnewt
END INTERFACE
INTERFACE
  FUNCTION rtsafe(funcd,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtsafe
    INTERFACE
      SUBROUTINE funcd(x,fval,fderiv)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP), INTENT(OUT) :: fval,fderiv
      END SUBROUTINE funcd
    END INTERFACE
  END FUNCTION rtsafe
END INTERFACE
INTERFACE
  FUNCTION rtsec(func,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: rtsec
    INTERFACE
      FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
      END FUNCTION func
    END INTERFACE
  END FUNCTION rtsec
END INTERFACE

```

```

END INTERFACE
END FUNCTION rtsec
END INTERFACE
INTERFACE
  SUBROUTINE rzextr(iest,xest,yest,yz,dy)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: iest
  REAL(SP), INTENT(IN) :: xest
  REAL(SP), DIMENSION(:), INTENT(IN) :: yest
  REAL(SP), DIMENSION(:), INTENT(OUT) :: yz,dy
  END SUBROUTINE rzextr
END INTERFACE
INTERFACE
  FUNCTION savgol(nl,nrr,ld,m)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: nl,nrr,ld,m
  REAL(SP), DIMENSION(nl+nrr+1) :: savgol
  END FUNCTION savgol
END INTERFACE
INTERFACE
  SUBROUTINE scrsho(func)
  USE nrtype
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
  END SUBROUTINE scrsho
END INTERFACE
INTERFACE
  FUNCTION select(k,arr)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: k
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
  REAL(SP) :: select
  END FUNCTION select
END INTERFACE
INTERFACE
  FUNCTION select_bypack(k,arr)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: k
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
  REAL(SP) :: select_bypack
  END FUNCTION select_bypack
END INTERFACE
INTERFACE
  SUBROUTINE select_heap(arr,heap)
  USE nrtype
  REAL(SP), DIMENSION(:), INTENT(IN) :: arr
  REAL(SP), DIMENSION(:), INTENT(OUT) :: heap
  END SUBROUTINE select_heap
END INTERFACE

```

```

INTERFACE
  FUNCTION select_inplace(k,arr)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: k
    REAL(SP), DIMENSION(:), INTENT(IN) :: arr
    REAL(SP) :: select_inplace
  END FUNCTION select_inplace
END INTERFACE
INTERFACE
  SUBROUTINE simplx(a,m1,m2,m3,icase,izrov,iposv)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    INTEGER(I4B), INTENT(IN) :: m1,m2,m3
    INTEGER(I4B), INTENT(OUT) :: icase
    INTEGER(I4B), DIMENSION(:), INTENT(OUT) :: izrov,iposv
  END SUBROUTINE simplx
END INTERFACE
INTERFACE
  SUBROUTINE simpr(y,dydx,dfdx,dfdy,xs,htot,nstep,yout,derivs)
    USE nrtype
    REAL(SP), INTENT(IN) :: xs,htot
    REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx,dfdx
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: dfdy
    INTEGER(I4B), INTENT(IN) :: nstep
    REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
  INTERFACE
    SUBROUTINE derivs(x,y,dydx)
      USE nrtype
      REAL(SP), INTENT(IN) :: x
      REAL(SP), DIMENSION(:), INTENT(IN) :: y
      REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
  END INTERFACE
END SUBROUTINE simpr
END INTERFACE
INTERFACE
  SUBROUTINE sinft(y)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
  END SUBROUTINE sinft
END INTERFACE
INTERFACE
  SUBROUTINE slvsm2(u,rhs)
    USE nrtype
    REAL(DP), DIMENSION(3,3), INTENT(OUT) :: u
    REAL(DP), DIMENSION(3,3), INTENT(IN) :: rhs
  END SUBROUTINE slvsm2
END INTERFACE
INTERFACE
  SUBROUTINE slvsml(u,rhs)
    USE nrtype
    REAL(DP), DIMENSION(3,3), INTENT(OUT) :: u
    REAL(DP), DIMENSION(3,3), INTENT(IN) :: rhs
  END SUBROUTINE slvsml

```

```

END INTERFACE
INTERFACE
  SUBROUTINE sncndn(uu,emmc,sn,cn,dn)
    USE nrtype
    REAL(SP), INTENT(IN) :: uu,emmc
    REAL(SP), INTENT(OUT) :: sn,cn,dn
  END SUBROUTINE sncndn
END INTERFACE
INTERFACE
  FUNCTION snrm(sx,itol)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: sx
    INTEGER(I4B), INTENT(IN) :: itol
    REAL(DP) :: snrm
  END FUNCTION snrm
END INTERFACE
INTERFACE
  SUBROUTINE sobseq(x,init)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x
    INTEGER(I4B), OPTIONAL, INTENT(IN) :: init
  END SUBROUTINE sobseq
END INTERFACE
INTERFACE
  SUBROUTINE solvde(itmax,conv,slowc,scalv,indexv,nb,y)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: itmax,nb
    REAL(SP), INTENT(IN) :: conv,slowc
    REAL(SP), DIMENSION(:), INTENT(IN) :: scalv
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: indexv
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: y
  END SUBROUTINE solvde
END INTERFACE
INTERFACE
  SUBROUTINE sor(a,b,c,d,e,f,u,rjac)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: a,b,c,d,e,f
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: u
    REAL(DP), INTENT(IN) :: rjac
  END SUBROUTINE sor
END INTERFACE
INTERFACE
  SUBROUTINE sort(arr)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
  END SUBROUTINE sort
END INTERFACE
INTERFACE
  SUBROUTINE sort2(arr,slave)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr,slave
  END SUBROUTINE sort2
END INTERFACE
INTERFACE

```

```

SUBROUTINE sort3(arr,slave1,slave2)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr,slave1,slave2
END SUBROUTINE sort3
END INTERFACE
INTERFACE
SUBROUTINE sort_bypack(arr)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
END SUBROUTINE sort_bypack
END INTERFACE
INTERFACE
SUBROUTINE sort_byreshape(arr)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
END SUBROUTINE sort_byreshape
END INTERFACE
INTERFACE
SUBROUTINE sort_heap(arr)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
END SUBROUTINE sort_heap
END INTERFACE
INTERFACE
SUBROUTINE sort_pick(arr)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
END SUBROUTINE sort_pick
END INTERFACE
INTERFACE
SUBROUTINE sort_radix(arr)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
END SUBROUTINE sort_radix
END INTERFACE
INTERFACE
SUBROUTINE sort_shell(arr)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
END SUBROUTINE sort_shell
END INTERFACE
INTERFACE
SUBROUTINE spctrm(p,k,ovrlap,unit,n_window)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(OUT) :: p
INTEGER(I4B), INTENT(IN) :: k
LOGICAL(LGT), INTENT(IN) :: ovrlap
INTEGER(I4B), OPTIONAL, INTENT(IN) :: n_window,unit
END SUBROUTINE spctrm
END INTERFACE
INTERFACE
SUBROUTINE spear(data1,data2,d,zd,probd,rs,probrs)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2

```

```

      REAL(SP), INTENT(OUT) :: d,zd,probd,rs,probrs
    END SUBROUTINE spear
  END INTERFACE
INTERFACE sphbes
  SUBROUTINE sphbes_s(n,x,sj,sy,sjp,syp)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), INTENT(IN) :: x
    REAL(SP), INTENT(OUT) :: sj,sy,sjp,syp
  END SUBROUTINE sphbes_s
!BL
  SUBROUTINE sphbes_v(n,x,sj,sy,sjp,syp)
    USE nrtype
    INTEGER(I4B), INTENT(IN) :: n
    REAL(SP), DIMENSION(:), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(OUT) :: sj,sy,sjp,syp
  END SUBROUTINE sphbes_v
END INTERFACE
INTERFACE
  SUBROUTINE splie2(x1a,x2a,ya,y2a)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x1a,x2a
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: ya
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: y2a
  END SUBROUTINE splie2
END INTERFACE
INTERFACE
  FUNCTION splin2(x1a,x2a,ya,y2a,x1,x2)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x1a,x2a
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: ya,y2a
    REAL(SP), INTENT(IN) :: x1,x2
    REAL(SP) :: splin2
  END FUNCTION splin2
END INTERFACE
INTERFACE
  SUBROUTINE spline(x,y,yp1,ypn,y2)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
    REAL(SP), INTENT(IN) :: yp1,ypn
    REAL(SP), DIMENSION(:), INTENT(OUT) :: y2
  END SUBROUTINE spline
END INTERFACE
INTERFACE
  FUNCTION splint(xa,ya,y2a,x)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya,y2a
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: splint
  END FUNCTION splint
END INTERFACE
INTERFACE sprsax
  SUBROUTINE sprsax_dp(sa,x,b)
    USE nrtype

```



```

        TYPE(sprs2_dp), INTENT(IN) :: sa
        REAL(DP), DIMENSION (:), INTENT(IN) :: x
        REAL(DP), DIMENSION (:), INTENT(OUT) :: b
    END SUBROUTINE sprsax_dp
!BL
    SUBROUTINE sprsax_sp(sa,x,b)
    USE nrtype
    TYPE(sprs2_sp), INTENT(IN) :: sa
    REAL(SP), DIMENSION (:), INTENT(IN) :: x
    REAL(SP), DIMENSION (:), INTENT(OUT) :: b
    END SUBROUTINE sprsax_sp
END INTERFACE
INTERFACE sprsdiag
    SUBROUTINE sprsdiag_dp(sa,b)
    USE nrtype
    TYPE(sprs2_dp), INTENT(IN) :: sa
    REAL(DP), DIMENSION (:), INTENT(OUT) :: b
    END SUBROUTINE sprsdiag_dp
!BL
    SUBROUTINE sprsdiag_sp(sa,b)
    USE nrtype
    TYPE(sprs2_sp), INTENT(IN) :: sa
    REAL(SP), DIMENSION (:), INTENT(OUT) :: b
    END SUBROUTINE sprsdiag_sp
END INTERFACE
INTERFACE sprsin
    SUBROUTINE sprsin_sp(a,thresh,sa)
    USE nrtype
    REAL(SP), DIMENSION (:,:), INTENT(IN) :: a
    REAL(SP), INTENT(IN) :: thresh
    TYPE(sprs2_sp), INTENT(OUT) :: sa
    END SUBROUTINE sprsin_sp
!BL
    SUBROUTINE sprsin_dp(a,thresh,sa)
    USE nrtype
    REAL(DP), DIMENSION (:,:), INTENT(IN) :: a
    REAL(DP), INTENT(IN) :: thresh
    TYPE(sprs2_dp), INTENT(OUT) :: sa
    END SUBROUTINE sprsin_dp
END INTERFACE
INTERFACE
    SUBROUTINE sprstp(sa)
    USE nrtype
    TYPE(sprs2_sp), INTENT(INOUT) :: sa
    END SUBROUTINE sprstp
END INTERFACE
INTERFACE sprstx
    SUBROUTINE sprstx_dp(sa,x,b)
    USE nrtype
    TYPE(sprs2_dp), INTENT(IN) :: sa
    REAL(DP), DIMENSION (:), INTENT(IN) :: x
    REAL(DP), DIMENSION (:), INTENT(OUT) :: b
    END SUBROUTINE sprstx_dp
!BL

```

```

SUBROUTINE sprstx_sp(sa,x,b)
USE nrtype
TYPE(sprs2_sp), INTENT(IN) :: sa
REAL(SP), DIMENSION (:), INTENT(IN) :: x
REAL(SP), DIMENSION (:), INTENT(OUT) :: b
END SUBROUTINE sprstx_sp
END INTERFACE
INTERFACE
SUBROUTINE stifbs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
USE nrtype
REAL(SP), DIMENSION (:), INTENT(INOUT) :: y
REAL(SP), DIMENSION (:), INTENT(IN) :: dydx,yscal
REAL(SP), INTENT(IN) :: htry,eps
REAL(SP), INTENT(INOUT) :: x
REAL(SP), INTENT(OUT) :: hdid,hnext
INTERFACE
SUBROUTINE derivs(x,y,dydx)
USE nrtype
REAL(SP), INTENT(IN) :: x
REAL(SP), DIMENSION (:), INTENT(IN) :: y
REAL(SP), DIMENSION (:), INTENT(OUT) :: dydx
END SUBROUTINE derivs
END INTERFACE
END SUBROUTINE stifbs
END INTERFACE
INTERFACE
SUBROUTINE stiff(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
USE nrtype
REAL(SP), DIMENSION (:), INTENT(INOUT) :: y
REAL(SP), DIMENSION (:), INTENT(IN) :: dydx,yscal
REAL(SP), INTENT(INOUT) :: x
REAL(SP), INTENT(IN) :: htry,eps
REAL(SP), INTENT(OUT) :: hdid,hnext
INTERFACE
SUBROUTINE derivs(x,y,dydx)
USE nrtype
REAL(SP), INTENT(IN) :: x
REAL(SP), DIMENSION (:), INTENT(IN) :: y
REAL(SP), DIMENSION (:), INTENT(OUT) :: dydx
END SUBROUTINE derivs
END INTERFACE
END SUBROUTINE stiff
END INTERFACE
INTERFACE
SUBROUTINE stoerm(y,d2y,xs,htot,nstep,yout,derivs)
USE nrtype
REAL(SP), DIMENSION (:), INTENT(IN) :: y,d2y
REAL(SP), INTENT(IN) :: xs,htot
INTEGER(I4B), INTENT(IN) :: nstep
REAL(SP), DIMENSION (:), INTENT(OUT) :: yout
INTERFACE
SUBROUTINE derivs(x,y,dydx)
USE nrtype
REAL(SP), INTENT(IN) :: x

```

```

        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
END INTERFACE
END SUBROUTINE stoerm
END INTERFACE
INTERFACE svbksb
    SUBROUTINE svbksb_dp(u,w,v,b,x)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(IN) :: u,v
    REAL(DP), DIMENSION(:), INTENT(IN) :: w,b
    REAL(DP), DIMENSION(:), INTENT(OUT) :: x
    END SUBROUTINE svbksb_dp
!BL
    SUBROUTINE svbksb_sp(u,w,v,b,x)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(IN) :: u,v
    REAL(SP), DIMENSION(:), INTENT(IN) :: w,b
    REAL(SP), DIMENSION(:), INTENT(OUT) :: x
    END SUBROUTINE svbksb_sp
END INTERFACE
INTERFACE svdcmp
    SUBROUTINE svdcmp_dp(a,w,v)
    USE nrtype
    REAL(DP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(DP), DIMENSION(:), INTENT(OUT) :: w
    REAL(DP), DIMENSION(:,:), INTENT(OUT) :: v
    END SUBROUTINE svdcmp_dp
!BL
    SUBROUTINE svdcmp_sp(a,w,v)
    USE nrtype
    REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: w
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: v
    END SUBROUTINE svdcmp_sp
END INTERFACE
INTERFACE
    SUBROUTINE svdfit(x,y,sig,a,v,w,chisq,funcs)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: x,y,sig
    REAL(SP), DIMENSION(:), INTENT(OUT) :: a,w
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: v
    REAL(SP), INTENT(OUT) :: chisq
    INTERFACE
        FUNCTION funcs(x,n)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        INTEGER(I4B), INTENT(IN) :: n
        REAL(SP), DIMENSION(n) :: funcs
        END FUNCTION funcs
    END INTERFACE
END SUBROUTINE svdfit
END INTERFACE
INTERFACE

```

```

SUBROUTINE svdvar(v,w,cvm)
USE nrtype
REAL(SP), DIMENSION(:,:), INTENT(IN) :: v
REAL(SP), DIMENSION(:), INTENT(IN) :: w
REAL(SP), DIMENSION(:,:), INTENT(OUT) :: cvm
END SUBROUTINE svdvar
END INTERFACE
INTERFACE
FUNCTION toeplz(r,y)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: r,y
REAL(SP), DIMENSION(size(y)) :: toeplz
END FUNCTION toeplz
END INTERFACE
INTERFACE
SUBROUTINE tpctest(data1,data2,t,prob)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
REAL(SP), INTENT(OUT) :: t,prob
END SUBROUTINE tpctest
END INTERFACE
INTERFACE
SUBROUTINE tqli(d,e,z)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(INOUT) :: d,e
REAL(SP), DIMENSION(:,:), OPTIONAL, INTENT(INOUT) :: z
END SUBROUTINE tqli
END INTERFACE
INTERFACE
SUBROUTINE trapzd(func,a,b,s,n)
USE nrtype
REAL(SP), INTENT(IN) :: a,b
REAL(SP), INTENT(INOUT) :: s
INTEGER(I4B), INTENT(IN) :: n
INTERFACE
FUNCTION func(x)
USE nrtype
REAL(SP), DIMENSION(:), INTENT(IN) :: x
REAL(SP), DIMENSION(size(x)) :: func
END FUNCTION func
END INTERFACE
END SUBROUTINE trapzd
END INTERFACE
INTERFACE
SUBROUTINE tred2(a,d,e,novectors)
USE nrtype
REAL(SP), DIMENSION(:,:), INTENT(INOUT) :: a
REAL(SP), DIMENSION(:), INTENT(OUT) :: d,e
LOGICAL(LGT), OPTIONAL, INTENT(IN) :: novectors
END SUBROUTINE tred2
END INTERFACE
! On a purely serial machine, for greater efficiency, remove
! the generic name tridag from the following interface,
! and put it on the next one after that.

```

```

INTERFACE tridag
  RECURSIVE SUBROUTINE tridag_par(a,b,c,r,u)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c,r
    REAL(SP), DIMENSION(:), INTENT(OUT) :: u
  END SUBROUTINE tridag_par
END INTERFACE
INTERFACE
  SUBROUTINE tridag_ser(a,b,c,r,u)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c,r
    REAL(SP), DIMENSION(:), INTENT(OUT) :: u
  END SUBROUTINE tridag_ser
END INTERFACE
INTERFACE
  SUBROUTINE ttest(data1,data2,t,prob)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    REAL(SP), INTENT(OUT) :: t,prob
  END SUBROUTINE ttest
END INTERFACE
INTERFACE
  SUBROUTINE tutest(data1,data2,t,prob)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    REAL(SP), INTENT(OUT) :: t,prob
  END SUBROUTINE tutest
END INTERFACE
INTERFACE
  SUBROUTINE twofft(data1,data2,fft1,fft2)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: data1,data2
    COMPLEX(SPC), DIMENSION(:), INTENT(OUT) :: fft1,fft2
  END SUBROUTINE twofft
END INTERFACE
INTERFACE
  FUNCTION vander(x,q)
    USE nrtype
    REAL(DP), DIMENSION(:), INTENT(IN) :: x,q
    REAL(DP), DIMENSION(size(x)) :: vander
  END FUNCTION vander
END INTERFACE
INTERFACE
  SUBROUTINE vegas(region,func,init,ncall,itmx,nprn,tgral,sd,chi2a)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: region
    INTEGER(I4B), INTENT(IN) :: init,ncall,itmx,nprn
    REAL(SP), INTENT(OUT) :: tgral,sd,chi2a
  INTERFACE
    FUNCTION func(pt,wgt)
      USE nrtype
      REAL(SP), DIMENSION(:), INTENT(IN) :: pt
      REAL(SP), INTENT(IN) :: wgt
      REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END INTERFACE

```

```

        END FUNCTION func
    END INTERFACE
    END SUBROUTINE vegas
END INTERFACE
INTERFACE
    SUBROUTINE voltra(t0,h,t,f,g,ak)
    USE nrtype
    REAL(SP), INTENT(IN) :: t0,h
    REAL(SP), DIMENSION(:), INTENT(OUT) :: t
    REAL(SP), DIMENSION(:,:), INTENT(OUT) :: f
    INTERFACE
        FUNCTION g(t)
        USE nrtype
        REAL(SP), INTENT(IN) :: t
        REAL(SP), DIMENSION(:), POINTER :: g
    END FUNCTION g
!BL
    FUNCTION ak(t,s)
    USE nrtype
    REAL(SP), INTENT(IN) :: t,s
    REAL(SP), DIMENSION(:,:), POINTER :: ak
    END FUNCTION ak
    END INTERFACE
    END SUBROUTINE voltra
END INTERFACE
INTERFACE
    SUBROUTINE wt1(a,isign,wtstep)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
    INTEGER(I4B), INTENT(IN) :: isign
    INTERFACE
        SUBROUTINE wtstep(a,isign)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
        INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE wtstep
    END INTERFACE
    END SUBROUTINE wt1
END INTERFACE
INTERFACE
    SUBROUTINE wtn(a,nn,isign,wtstep)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
    INTEGER(I4B), DIMENSION(:), INTENT(IN) :: nn
    INTEGER(I4B), INTENT(IN) :: isign
    INTERFACE
        SUBROUTINE wtstep(a,isign)
        USE nrtype
        REAL(SP), DIMENSION(:), INTENT(INOUT) :: a
        INTEGER(I4B), INTENT(IN) :: isign
    END SUBROUTINE wtstep
    END INTERFACE
    END SUBROUTINE wtn
END INTERFACE

```

```

INTERFACE
  FUNCTION wwghts(n,h,kermom)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: n
  REAL(SP), INTENT(IN) :: h
  REAL(SP), DIMENSION(n) :: wwghts
  INTERFACE
    FUNCTION kermom(y,m)
    USE nrtype
    REAL(DP), INTENT(IN) :: y
    INTEGER(I4B), INTENT(IN) :: m
    REAL(DP), DIMENSION(m) :: kermom
    END FUNCTION kermom
  END INTERFACE
END FUNCTION wwghts
END INTERFACE
INTERFACE
  SUBROUTINE zbrac(func,x1,x2,succes)
  USE nrtype
  REAL(SP), INTENT(INOUT) :: x1,x2
  LOGICAL(LGT), INTENT(OUT) :: succes
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END SUBROUTINE zbrac
END INTERFACE
INTERFACE
  SUBROUTINE zbrak(func,x1,x2,n,xb1,xb2,nb)
  USE nrtype
  INTEGER(I4B), INTENT(IN) :: n
  INTEGER(I4B), INTENT(OUT) :: nb
  REAL(SP), INTENT(IN) :: x1,x2
  REAL(SP), DIMENSION(:), POINTER :: xb1,xb2
  INTERFACE
    FUNCTION func(x)
    USE nrtype
    REAL(SP), INTENT(IN) :: x
    REAL(SP) :: func
    END FUNCTION func
  END INTERFACE
END SUBROUTINE zbrak
END INTERFACE
INTERFACE
  FUNCTION zbrent(func,x1,x2,tol)
  USE nrtype
  REAL(SP), INTENT(IN) :: x1,x2,tol
  REAL(SP) :: zbrent
  INTERFACE
    FUNCTION func(x)
    USE nrtype

```

```

        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
    END FUNCTION func
END INTERFACE
END FUNCTION zbrent
END INTERFACE
INTERFACE
    SUBROUTINE zrhqr(a,rtr,rti)
    USE nrtype
    REAL(SP), DIMENSION(:), INTENT(IN) :: a
    REAL(SP), DIMENSION(:), INTENT(OUT) :: rtr,rti
    END SUBROUTINE zrhqr
END INTERFACE
INTERFACE
    FUNCTION zriddr(func,x1,x2,xacc)
    USE nrtype
    REAL(SP), INTENT(IN) :: x1,x2,xacc
    REAL(SP) :: zriddr
    INTERFACE
        FUNCTION func(x)
        USE nrtype
        REAL(SP), INTENT(IN) :: x
        REAL(SP) :: func
        END FUNCTION func
    END INTERFACE
    END FUNCTION zriddr
END INTERFACE
INTERFACE
    SUBROUTINE zroots(a,roots,polish)
    USE nrtype
    COMPLEX(SPC), DIMENSION(:), INTENT(IN) :: a
    COMPLEX(SPC), DIMENSION(:), INTENT(OUT) :: roots
    LOGICAL(LGT), INTENT(IN) :: polish
    END SUBROUTINE zroots
END INTERFACE
END MODULE nr

```

```

SUBROUTINE rkck(y,dydx,x,h,yout,yerr,derivs)
USE nrtype; USE nrutil, ONLY : assert_eq
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
REAL(SP), INTENT(IN) :: x,h
REAL(SP), DIMENSION(:), INTENT(OUT) :: yout,yerr
INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
END INTERFACE

```



```

INTEGER(I4B) :: ndum
REAL(SP), DIMENSION(size(y)) :: ak2,ak3,ak4,ak5,ak6,ytemp
REAL(SP), PARAMETER :: A2=0.2_sp,A3=0.3_sp,A4=0.6_sp,A5=1.0_sp,&
    A6=0.875_sp,B21=0.2_sp,B31=3.0_sp/40.0_sp,B32=9.0_sp/40.0_sp,&
    B41=0.3_sp,B42=-0.9_sp,B43=1.2_sp,B51=-11.0_sp/54.0_sp,&
    B52=2.5_sp,B53=-70.0_sp/27.0_sp,B54=35.0_sp/27.0_sp,&
    B61=1631.0_sp/55296.0_sp,B62=175.0_sp/512.0_sp,&
    B63=575.0_sp/13824.0_sp,B64=44275.0_sp/110592.0_sp,&
    B65=253.0_sp/4096.0_sp,C1=37.0_sp/378.0_sp,&
    C3=250.0_sp/621.0_sp,C4=125.0_sp/594.0_sp,&
    C6=512.0_sp/1771.0_sp,DC1=C1-2825.0_sp/27648.0_sp,&
    DC3=C3-18575.0_sp/48384.0_sp,DC4=C4-13525.0_sp/55296.0_sp,&
    DC5=-277.0_sp/14336.0_sp,DC6=C6-0.25_sp
ndum=assert_eq(size(y),size(dydx),size(yout),size(yerr),'rkck')
ytemp=y+B21*h*dydx
call derivs(x+A2*h,ytemp,ak2)
ytemp=y+h*(B31*dydx+B32*ak2)
call derivs(x+A3*h,ytemp,ak3)
ytemp=y+h*(B41*dydx+B42*ak2+B43*ak3)
call derivs(x+A4*h,ytemp,ak4)
ytemp=y+h*(B51*dydx+B52*ak2+B53*ak3+B54*ak4)
call derivs(x+A5*h,ytemp,ak5)
ytemp=y+h*(B61*dydx+B62*ak2+B63*ak3+B64*ak4+B65*ak5)
call derivs(x+A6*h,ytemp,ak6)
yout=y+h*(C1*dydx+C3*ak3+C4*ak4+C6*ak6)
yerr=h*(DC1*dydx+DC3*ak3+DC4*ak4+DC5*ak5+DC6*ak6)
END SUBROUTINE rkck

SUBROUTINE rkqs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
USE nr, ONLY : rkck
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
REAL(SP), INTENT(INOUT) :: x
REAL(SP), INTENT(IN) :: htry,eps
REAL(SP), INTENT(OUT) :: hdid,hnext
INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
END INTERFACE
INTEGER(I4B) :: ndum
REAL(SP) :: errmax,h,htemp,xnew
REAL(SP), DIMENSION(size(y)) :: yerr,ytemp
REAL(SP), PARAMETER :: SAFETY=0.9_sp,PGROW=-0.2_sp,PSHRNK=-0.25_sp,&
    ERRCON=1.89e-4
ndum=assert_eq(size(y),size(dydx),size(yscal),'rkqs')
h=htry
do

```

```

        call rkck(y,dydx,x,h,ytemp,yerr,derivs)
        errmax=maxval(abs(yerr(:)/yscal(:)))/eps
        if (errmax <= 1.0) exit
        htemp=SAFETY*h*(errmax**PSHRNK)
        h=sign(max(abs(htemp),0.1_sp*abs(h)),h)
        xnew=x+h
        if (xnew == x) call nrerror('stepsize underflow in rkqs')
    end do
    if (errmax > ERRCON) then
        hnext=SAFETY*h*(errmax**PGROW)
    else
        hnext=5.0_sp*h
    end if
    hdid=h
    x=x+h
    y(:)=ytemp(:)
END SUBROUTINE rkqs

SUBROUTINE mmid(y,dydx,xs,htot,nstep,yout,derivs)
USE nrtype; USE nrutil, ONLY : assert_eq,swap
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: nstep
REAL(SP), INTENT(IN) :: xs,htot
REAL(SP), DIMENSION(:), INTENT(IN) :: y,dydx
REAL(SP), DIMENSION(:), INTENT(OUT) :: yout
INTERFACE
    SUBROUTINE derivs(x,y,dydx)
        USE nrtype
        IMPLICIT NONE
        REAL(SP), INTENT(IN) :: x
        REAL(SP), DIMENSION(:), INTENT(IN) :: y
        REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
END INTERFACE
INTEGER(I4B) :: n,ndum
REAL(SP) :: h,h2,x
REAL(SP), DIMENSION(size(y)) :: ym,yn
ndum=assert_eq(size(y),size(dydx),size(yout),'mmid')
h=htot/nstep
ym=y
yn=y+h*dydx
x=xs+h
call derivs(x,yn,yout)
h2=2.0_sp*h
do n=2,nstep
    call swap(ym,yn)
    yn=yn+h2*yout
    x=x+h
    call derivs(x,yn,yout)
end do
yout=0.5_sp*(ym+yn+h*yout)
END SUBROUTINE mmid

SUBROUTINE pzextr(iest,xest,yest,yz,dy)

```

```

USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
IMPLICIT NONE
INTEGER(I4B), INTENT(IN) :: iest
REAL(SP), INTENT(IN) :: xest
REAL(SP), DIMENSION(:), INTENT(IN) :: yest
REAL(SP), DIMENSION(:), INTENT(OUT) :: yz,dy
INTEGER(I4B), PARAMETER :: IEST_MAX=16
INTEGER(I4B) :: j,nv
INTEGER(I4B), SAVE :: nvold=-1
REAL(SP) :: delta,f1,f2
REAL(SP), DIMENSION(size(yz)) :: d,tmp,q
REAL(SP), DIMENSION(IEST_MAX), SAVE :: x
REAL(SP), DIMENSION(:,:), ALLOCATABLE, SAVE :: qcol
nv=assert_eq(size(yz),size(yest),size(dy),'pzextr')
if (iest > IEST_MAX) call &
    nrerror('pzextr: probable misuse, too much extrapolation')
if (nv /= nvold) then
    if (allocated(qcol)) deallocate(qcol)
    allocate(qcol(nv,IEST_MAX))
    nvold=nv
end if
x(iest)=xest
dy(:)=yest(:)
yz(:)=yest(:)
if (iest == 1) then
    qcol(:,1)=yest(:)
else
    d(:)=yest(:)
    do j=1,iest-1
        delta=1.0_sp/(x(iest-j)-xest)
        f1=xest*delta
        f2=x(iest-j)*delta
        q(:)=qcol(:,j)
        qcol(:,j)=dy(:)
        tmp(:)=d(:)-q(:)
        dy(:)=f1*tmp(:)
        d(:)=f2*tmp(:)
        yz(:)=yz(:)+dy(:)
    end do
    qcol(:,iest)=dy(:)
end if
END SUBROUTINE pzextr

SUBROUTINE bsstep(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
USE nrtype; USE nrutil, ONLY : arth,assert_eq,cumsum,iminloc,nrerror,&
    outerdiff,outerprod,upper_triangle
USE nr, ONLY : mmid,pzextr
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
REAL(SP), INTENT(INOUT) :: x
REAL(SP), INTENT(IN) :: htry,eps
REAL(SP), INTENT(OUT) :: hdid,hnext
INTERFACE

```

```

SUBROUTINE derivs(x,y,dydx)
USE nrtype
IMPLICIT NONE
REAL(SP), INTENT(IN) :: x
REAL(SP), DIMENSION(:), INTENT(IN) :: y
REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
END SUBROUTINE derivs
END INTERFACE
INTEGER(I4B), PARAMETER :: IMAX=9, KMAXX=IMAX-1
REAL(SP), PARAMETER :: SAFE1=0.25_sp,SAFE2=0.7_sp,REDMAX=1.0e-5_sp,&
  REDMIN=0.7_sp,TINY=1.0e-30_sp,SCALMX=0.1_sp
INTEGER(I4B) :: k,km,ndum
INTEGER(I4B), DIMENSION(IMAX) :: nseq = (/ 2,4,6,8,10,12,14,16,18 /)
INTEGER(I4B), SAVE :: kopt,kmax
REAL(SP), DIMENSION(KMAXX,KMAXX), SAVE :: alf
REAL(SP), DIMENSION(KMAXX) :: err
REAL(SP), DIMENSION(IMAX), SAVE :: a
REAL(SP), SAVE :: epsold = -1.0_sp,xnew
REAL(SP) :: eps1,errmax,fact,h,red,scale,wrkmin,xest
REAL(SP), DIMENSION(size(y)) :: yerr,ysav,yseq
LOGICAL(LGT) :: reduct
LOGICAL(LGT), SAVE :: first=.true.
ndum=assert_eq(size(y),size(dydx),size(yscal),'bsstep')
if (eps /= epsold) then
  hnext=-1.0e29_sp
  xnew=-1.0e29_sp
  eps1=SAFE1*eps
  a(:)=cumsum(nseq,1)
  where (upper_triangle(KMAXX,KMAXX)) alf=eps1** &
    (outerdiff(a(2:),a(2:))/outerprod(arth( &
      3.0_sp,2.0_sp,KMAXX),(a(2:)-a(1)+1.0_sp)))
  epsold=eps
  do kopt=2,KMAXX-1
    if (a(kopt+1) > a(kopt)*alf(kopt-1,kopt)) exit
  end do
  kmax=kopt
end if
h=htry
ysav(:)=y(:)
if (h /= hnext .or. x /= xnew) then
  first=.true.
  kopt=kmax
end if
reduct=.false.
main_loop: do
  do k=1,kmax
    xnew=x+h
    if (xnew == x) call nrerror('step size underflow in bsstep')
    call mmid(ysav,dydx,x,h,nseq(k),yseq,derivs)
    xest=(h/nseq(k))**2
    call pzextr(k,xest,yseq,y,yerr)
    if (k /= 1) then
      errmax=maxval(abs(yerr(:)/yscal(:)))
      errmax=max(TINY,errmax)/eps
    end if
  end do
end if

```

```

        km=k-1
        err(km)=(errmax/SAFE1)**(1.0_sp/(2*km+1))
    end if
    if (k /= 1 .and. (k >= kopt-1 .or. first)) then
        if (errmax < 1.0) exit main_loop
        if (k == kmax .or. k == kopt+1) then
            red=SAFE2/err(km)
            exit
        else if (k == kopt) then
            if (alf(kopt-1,kopt) < err(km)) then
                red=1.0_sp/err(km)
                exit
            end if
        else if (kopt == kmax) then
            if (alf(km,kmax-1) < err(km)) then
                red=alf(km,kmax-1)*SAFE2/err(km)
                exit
            end if
        else if (alf(km,kopt) < err(km)) then
            red=alf(km,kopt-1)/err(km)
            exit
        end if
    end if
end do
red=max(min(red,REDMIN),REDMAX)
h=h*red
reduct=.true.
end do main_loop
x=xnew
hdid=h
first=.false.
kopt=1+iminloc(a(2:km+1)*max(err(1:km),SCALMX))
scale=max(err(kopt-1),SCALMX)
wrkmin=scale*a(kopt)
hnext=h/scale
if (kopt >= k .and. kopt /= kmax .and. .not. reduct) then
    fact=max(scale/alf(kopt-1,kopt),SCALMX)
    if (a(kopt+1)*fact <= wrkmin) then
        hnext=h/fact
        kopt=kopt+1
    end if
end if
end if
END SUBROUTINE bsstep

FUNCTION hypgeo(a,b,c,z)
USE nrtype
USE hypgeo_info
USE nr, ONLY : bsstep,hypdrv,hypser,odeint
IMPLICIT NONE
COMPLEX(SPC), INTENT(IN) :: a,b,c,z
COMPLEX(SPC) :: hypgeo
REAL(SP), PARAMETER :: EPS=1.0e-6_sp
COMPLEX(SPC), DIMENSION(2) :: y
REAL(SP), DIMENSION(4) :: ry

```

```

if (real(z)**2+aimag(z)**2 <= 0.25) then
  call hypser(a,b,c,z,hypgeo,y(2))
  RETURN
else if (real(z) < 0.0) then
  hypgeo_z0=cplx(-0.5_sp,0.0_sp,kind=spc)
else if (real(z) <= 1.0) then
  hypgeo_z0=cplx(0.5_sp,0.0_sp,kind=spc)
else
  hypgeo_z0=cplx(0.0_sp,sign(0.5_sp,aimag(z)),kind=spc)
end if
hypgeo_aa=a
hypgeo_bb=b
hypgeo_cc=c
hypgeo_dz=z-hypgeo_z0
call hypser(hypgeo_aa,hypgeo_bb,hypgeo_cc,hypgeo_z0,y(1),y(2))
ry(1:4:2)=real(y)
ry(2:4:2)=aimag(y)
! call odeint(ry,0.0_sp,1.0_sp,EPS,0.1_sp,0.0001_sp,hypdrv,bsstep)
call odeint(ry,0.0_sp,1.0_sp,EPS,0.1_sp,0.000001_sp,hypdrv,bsstep) !!! FB
y=cplx(ry(1:4:2),ry(2:4:2),kind=spc)
hypgeo=y(1)
END FUNCTION hypgeo

SUBROUTINE hypdrv(s,ry,rdyds)
USE nrtype
USE hypgeo_info
IMPLICIT NONE
REAL(SP), INTENT(IN) :: s
REAL(SP), DIMENSION(:), INTENT(IN) :: ry
REAL(SP), DIMENSION(:), INTENT(OUT) :: rdyds
COMPLEX(SPC), DIMENSION(2) :: y,dyds
COMPLEX(SPC) :: z
y=cplx(ry(1:4:2),ry(2:4:2),kind=spc)
z=hypgeo_z0+s*hypgeo_dz
dyds(1)=y(2)*hypgeo_dz
dyds(2)=((hypgeo_aa*hypgeo_bb)*y(1)-(hypgeo_cc-&
((hypgeo_aa+hypgeo_bb)+1.0_sp)*z)*y(2))*hypgeo_dz/(z*(1.0_sp-z))
rdyds(1:4:2)=real(dyds)
rdyds(2:4:2)=aimag(dyds)
END SUBROUTINE hypdrv

SUBROUTINE hypser(a,b,c,z,series,deriv)
USE nrtype; USE nrutil, ONLY : nrerror
IMPLICIT NONE
COMPLEX(SPC), INTENT(IN) :: a,b,c,z
COMPLEX(SPC), INTENT(OUT) :: series,deriv
INTEGER(I4B) :: n
INTEGER(I4B), PARAMETER :: MAXIT=1000
COMPLEX(SPC) :: aa,bb,cc,fac,temp
deriv=cplx(0.0_sp,0.0_sp,kind=spc)
fac=cplx(1.0_sp,0.0_sp,kind=spc)
temp=fac
aa=a
bb=b

```

```

cc=c
do n=1,MAXIT
  fac=((aa*bb)/cc)*fac
  deriv=deriv+fac
  fac=fac*z/n
  series=temp+fac
  if (series == temp) RETURN
  temp=series
  aa=aa+1.0
  bb=bb+1.0
  cc=cc+1.0
end do
call nrerror('hypser: convergence failure')
END SUBROUTINE hypser

SUBROUTINE odeint(ystart,x1,x2,eps,h1,hmin,derivs,rkqs)
USE nrtype; USE nrutil, ONLY : nrerror,reallocate
USE ode_path
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(INOUT) :: ystart
REAL(SP), INTENT(IN) :: x1,x2,eps,h1,hmin
INTERFACE
  SUBROUTINE derivs(x,y,dydx)
  USE nrtype
  IMPLICIT NONE
  REAL(SP), INTENT(IN) :: x
  REAL(SP), DIMENSION(:), INTENT(IN) :: y
  REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
  END SUBROUTINE derivs
!BL
  SUBROUTINE rkqs(y,dydx,x,htry,eps,yscal,hdid,hnext,derivs)
  USE nrtype
  IMPLICIT NONE
  REAL(SP), DIMENSION(:), INTENT(INOUT) :: y
  REAL(SP), DIMENSION(:), INTENT(IN) :: dydx,yscal
  REAL(SP), INTENT(INOUT) :: x
  REAL(SP), INTENT(IN) :: htry,eps
  REAL(SP), INTENT(OUT) :: hdid,hnext
  INTERFACE
    SUBROUTINE derivs(x,y,dydx)
    USE nrtype
    IMPLICIT NONE
    REAL(SP), INTENT(IN) :: x
    REAL(SP), DIMENSION(:), INTENT(IN) :: y
    REAL(SP), DIMENSION(:), INTENT(OUT) :: dydx
    END SUBROUTINE derivs
  END INTERFACE
  END SUBROUTINE rkqs
END INTERFACE
REAL(SP), PARAMETER :: TINY=1.0e-30_sp
INTEGER(I4B), PARAMETER :: MAXSTP=10000
INTEGER(I4B) :: nstp
REAL(SP) :: h,hdid,hnext,x,xsav
REAL(SP), DIMENSION(size(ystart)) :: dydx,y,yscal

```

```

x=x1
h=sign(h1,x2-x1)
nok=0
nbad=0
kount=0
y(:)=ystart(:)
nullify(xp,yp)
if (save_steps) then
  xsav=x-2.0_sp*dxsav
  allocate(xp(256))
  allocate(yp(size(ystart),size(xp)))
end if
do nstp=1,MAXSTP
  call derivs(x,y,dydx)
  yscal(:)=abs(y(:))+abs(h*dydx(:))+TINY
  if (save_steps .and. (abs(x-xsav) > abs(dxsav))) &
    call save_a_step
  if ((x+h-x2)*(x+h-x1) > 0.0) h=x2-x
  call rkqs(y,dydx,x,h,eps,yscal,hdid,hnext,derivs)
  if (hdid == h) then
    nok=nok+1
  else
    nbad=nbad+1
  end if
  if ((x-x2)*(x2-x1) >= 0.0) then
    ystart(:)=y(:)
    if (save_steps) call save_a_step
    RETURN
  end if
  if (abs(hnext) < hmin) then
print *, "abs(hnext) = ", abs(hnext)
print *, "hmin = ", hmin
    call nrerror('stepsize smaller than minimum in odeint')
  end if
  h=hnext
end do
call nrerror('too many steps in odeint')
CONTAINS
!BL
SUBROUTINE save_a_step
kount=kount+1
if (kount > size(xp)) then
  xp=>reallocate(xp,2*size(xp))
  yp=>reallocate(yp,size(yp,1),size(xp))
end if
xp(kount)=x
yp(:,kount)=y(:)
xsav=x
END SUBROUTINE save_a_step
END SUBROUTINE odeint

FUNCTION gammln_s(xx)
USE nrtype; USE nrutil, ONLY : arth,assert
IMPLICIT NONE

```



```

REAL(SP), INTENT(IN) :: xx
REAL(SP) :: gammln_s
REAL(DP) :: tmp,x
REAL(DP) :: stp = 2.5066282746310005_dp
REAL(DP), DIMENSION(6) :: coef = (/76.18009172947146_dp,&
-86.50532032941677_dp,24.01409824083091_dp,&
-1.231739572450155_dp,0.1208650973866179e-2_dp,&
-0.5395239384953e-5_dp/)
call assert(xx > 0.0, 'gammln_s arg')
x=xx
tmp=x+5.5_dp
tmp=(x+0.5_dp)*log(tmp)-tmp
gammln_s=tmp+log(stp*(1.000000000190015_dp+&
sum(coef(:)/arth(x+1.0_dp,1.0_dp,size(coef))))/x)
END FUNCTION gammln_s

FUNCTION gammln_v(xx)
USE nrtype; USE nrutil, ONLY: assert
IMPLICIT NONE
INTEGER(I4B) :: i
REAL(SP), DIMENSION(:), INTENT(IN) :: xx
REAL(SP), DIMENSION(size(xx)) :: gammln_v
REAL(DP), DIMENSION(size(xx)) :: ser,tmp,x,y
REAL(DP) :: stp = 2.5066282746310005_dp
REAL(DP), DIMENSION(6) :: coef = (/76.18009172947146_dp,&
-86.50532032941677_dp,24.01409824083091_dp,&
-1.231739572450155_dp,0.1208650973866179e-2_dp,&
-0.5395239384953e-5_dp/)
if (size(xx) == 0) RETURN
call assert(all(xx > 0.0), 'gammln_v arg')
x=xx
tmp=x+5.5_dp
tmp=(x+0.5_dp)*log(tmp)-tmp
ser=1.000000000190015_dp
y=x
do i=1,size(coef)
    y=y+1.0_dp
    ser=ser+coef(i)/y
end do
gammln_v=tmp+log(stp*ser/x)
END FUNCTION gammln_v

! FUNCTION qgaus(func,a,b)
! USE nrtype
! REAL(SP), INTENT(IN) :: a,b
! REAL(SP) :: qgaus
! INTERFACE
!     FUNCTION func(x)
!     USE nrtype
!     REAL(SP), DIMENSION(:), INTENT(IN) :: x
!     REAL(SP), DIMENSION(size(x)) :: func
!     END FUNCTION func
! END INTERFACE
! REAL(SP) :: xm,xr

```

```

!   REAL(SP), DIMENSION(5) :: dx, w = (/ 0.2955242247_sp,0.2692667193_sp,&
!       0.2190863625_sp,0.1494513491_sp,0.0666713443_sp /),&
!       x = (/ 0.1488743389_sp,0.4333953941_sp,0.6794095682_sp,&
!       0.8650633666_sp,0.9739065285_sp /)
!   xm=0.5_sp*(b+a)
!   xr=0.5_sp*(b-a)
!   dx(:)=xr*x(:)
!   qgaus=xr*sum(w(:)*(func(xm+dx)+func(xm-dx)))
!   END FUNCTION qgaus

```

```

FUNCTION locatenr(xx,x)
USE nrtype
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: xx
REAL(SP), INTENT(IN) :: x
INTEGER(I4B) :: locatenr
INTEGER(I4B) :: n,jl,jm,ju
LOGICAL :: ascnd
n=size(xx)
ascnd = (xx(n) >= xx(1))
jl=0
ju=n+1
do
  if (ju-jl <= 1) exit
  jm=(ju+jl)/2
  if (ascnd .eqv. (x >= xx(jm))) then
    jl=jm
  else
    ju=jm
  end if
end do
if (x == xx(1)) then
  locatenr=1
else if (x == xx(n)) then
  locatenr=n-1
else
  locatenr=jl
end if
END FUNCTION locatenr

```

```

SUBROUTINE tridag_ser(a,b,c,r,u)
USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c,r
REAL(SP), DIMENSION(:), INTENT(OUT) :: u
REAL(SP), DIMENSION(size(b)) :: gam
INTEGER(I4B) :: n,j
REAL(SP) :: bet
n=assert_eq((/size(a)+1,size(b),size(c)+1,size(r),size(u)/),'tridag_ser')
bet=b(1)
if (bet == 0.0) call nrerror('tridag_ser: Error at code stage 1')
u(1)=r(1)/bet
do j=2,n
  gam(j)=c(j-1)/bet

```

```

        bet=b(j)-a(j-1)*gam(j)
        if (bet == 0.0) &
            call nrerror('tridag_ser: Error at code stage 2')
        u(j)=(r(j)-a(j-1)*u(j-1))/bet
    end do
do j=n-1,1,-1
    u(j)=u(j)-gam(j+1)*u(j+1)
end do
END SUBROUTINE tridag_ser

RECURSIVE SUBROUTINE tridag_par(a,b,c,r,u)
USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
USE nr, ONLY : tridag_ser
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: a,b,c,r
REAL(SP), DIMENSION(:), INTENT(OUT) :: u
INTEGER(I4B), PARAMETER :: NPAR_TRIDAG=4
INTEGER(I4B) :: n,n2,nm,nx
REAL(SP), DIMENSION(size(b)/2) :: y,q,piva
REAL(SP), DIMENSION(size(b)/2-1) :: x,z
REAL(SP), DIMENSION(size(a)/2) :: pivc
n=assert_eq((/size(a)+1,size(b),size(c)+1,size(r),size(u)/),'tridag_par')
if (n < NPAR_TRIDAG) then
    call tridag_ser(a,b,c,r,u)
else
    if (maxval(abs(b(1:n))) == 0.0) &
        call nrerror('tridag_par: possible singular matrix')
    n2=size(y)
    nm=size(pivc)
    nx=size(x)
    piva = a(1:n-1:2)/b(1:n-1:2)
    pivc = c(2:n-1:2)/b(3:n:2)
    y(1:nm) = b(2:n-1:2)-piva(1:nm)*c(1:n-2:2)-pivc*a(2:n-1:2)
    q(1:nm) = r(2:n-1:2)-piva(1:nm)*r(1:n-2:2)-pivc*r(3:n:2)
    if (nm < n2) then
        y(n2) = b(n)-piva(n2)*c(n-1)
        q(n2) = r(n)-piva(n2)*r(n-1)
    end if
    x = -piva(2:n2)*a(2:n-2:2)
    z = -pivc(1:nx)*c(3:n-1:2)
    call tridag_par(x,y,z,q,u(2:n:2))
    u(1) = (r(1)-c(1)*u(2))/b(1)
    u(3:n-1:2) = (r(3:n-1:2)-a(2:n-2:2)*u(2:n-2:2) &
        -c(3:n-1:2)*u(4:n:2))/b(3:n-1:2)
    if (nm == n2) u(n)=(r(n)-a(n-1)*u(n-1))/b(n)
end if
END SUBROUTINE tridag_par

SUBROUTINE spline(x,y,yp1,ypn,y2)
USE nrtype; USE nrutil, ONLY : assert_eq
USE nr, ONLY : tridag
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: x,y
REAL(SP), INTENT(IN) :: yp1,ypn

```

```

REAL(SP), DIMENSION(:), INTENT(OUT) :: y2
INTEGER(I4B) :: n
REAL(SP), DIMENSION(size(x)) :: a,b,c,r
n=assert_eq(size(x),size(y),size(y2),'spline')
c(1:n-1)=x(2:n)-x(1:n-1)
r(1:n-1)=6.0_sp*((y(2:n)-y(1:n-1))/c(1:n-1))
r(2:n-1)=r(2:n-1)-r(1:n-2)
a(2:n-1)=c(1:n-2)
b(2:n-1)=2.0_sp*(c(2:n-1)+a(2:n-1))
b(1)=1.0
b(n)=1.0
if (yp1 > 0.99e30_sp) then
  r(1)=0.0
  c(1)=0.0
else
  r(1)=(3.0_sp/(x(2)-x(1)))*((y(2)-y(1))/(x(2)-x(1))-yp1)
  c(1)=0.5
end if
if (ypn > 0.99e30_sp) then
  r(n)=0.0
  a(n)=0.0
else
  r(n)=(-3.0_sp/(x(n)-x(n-1)))*((y(n)-y(n-1))/(x(n)-x(n-1))-ypn)
  a(n)=0.5
end if
call tridag(a(2:n),b(1:n),c(1:n-1),r(1:n),y2(1:n))
END SUBROUTINE spline

FUNCTION splint(xa,ya,y2a,x)
USE nrtype; USE nrutil, ONLY : assert_eq,nrerror
USE nr, ONLY: locatenr
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(IN) :: xa,ya,y2a
REAL(SP), INTENT(IN) :: x
REAL(SP) :: splint
INTEGER(I4B) :: khi,klo,n
REAL(SP) :: a,b,h
n=assert_eq(size(xa),size(ya),size(y2a),'splint')
klo=max(min(locatenr(xa,x),n-1),1)
khi=klo+1
h=xa(khi)-xa(klo)
if (h == 0.0) call nrerror('bad xa input in splint')
a=(xa(khi)-x)/h
b=(x-xa(klo))/h
splint=a*ya(klo)+b*ya(khi)+((a**3-a)*y2a(klo)+(b**3-b)*y2a(khi))*(h**2)/6.0_sp
END FUNCTION splint

SUBROUTINE sort(arr)
USE nrtype; USE nrutil, ONLY : swap,nrerror
IMPLICIT NONE
REAL(SP), DIMENSION(:), INTENT(INOUT) :: arr
INTEGER(I4B), PARAMETER :: NN=15, NSTACK=50
REAL(SP) :: a
INTEGER(I4B) :: n,k,i,j,jstack,l,r

```

```

INTEGER(I4B), DIMENSION(NSTACK) :: istack
n=size(arr)
jstack=0
l=1
r=n
do
  if (r-l < NN) then
    do j=l+1,r
      a=arr(j)
      do i=j-1,l,-1
        if (arr(i) <= a) exit
        arr(i+1)=arr(i)
      end do
      arr(i+1)=a
    end do
    if (jstack == 0) RETURN
    r=istack(jstack)
    l=istack(jstack-1)
    jstack=jstack-2
  else
    k=(l+r)/2
    call swap(arr(k),arr(l+1))
    call swap(arr(l),arr(r),arr(l)>arr(r))
    call swap(arr(l+1),arr(r),arr(l+1)>arr(r))
    call swap(arr(l),arr(l+1),arr(l)>arr(l+1))
    i=l+1
    j=r
    a=arr(l+1)
    do
      do
        i=i+1
        if (arr(i) >= a) exit
      end do
      do
        j=j-1
        if (arr(j) <= a) exit
      end do
      if (j < i) exit
      call swap(arr(i),arr(j))
    end do
    arr(l+1)=arr(j)
    arr(j)=a
    jstack=jstack+2
    if (jstack > NSTACK) call nrerror('sort: NSTACK too small')
    if (r-i+1 >= j-1) then
      istack(jstack)=r
      istack(jstack-1)=i
      r=j-1
    else
      istack(jstack)=j-1
      istack(jstack-1)=l
      l=i
    end if
  end if
end if

```

```

end do
END SUBROUTINE sort

!!! Whizard wrapper for NR tools
module nr_tools
  use kinds, only: default !NODEP!
  use nrtype, only: i4b, sp, spc !NODEP!
  use nr, only: gammln, hypgeo, locatenr, sort, spline, splint !NODEP!
  implicit none
  save
  private

  public :: nr_hypgeo, nr_gamma, nr_locate, nr_sort, nr_spline_t

  type :: nr_spline_t
    real(sp), dimension(:), allocatable :: xa, ya_re, ya_im, y2a_re, y2a_im
  contains
    procedure :: init => nr_spline_init
    procedure :: interpolate => nr_spline_interpolate
    procedure :: dealloc => nr_spline_dealloc
  end type nr_spline_t

contains

  function nr_hypgeo (a, b, c, d) result (h)
    complex(default), intent(in) :: a, b, c, d
    complex(default) :: h
    complex(spc) :: a_sp, b_sp, c_sp, d_sp
    a_sp = cmplx(a,kind=sp)
    b_sp = cmplx(b,kind=sp)
    c_sp = cmplx(c,kind=sp)
    d_sp = cmplx(d,kind=sp)
    h = cmplx( hypgeo (a_sp, b_sp, c_sp, d_sp) , kind=default )
  end function nr_hypgeo

  function nr_gamma (x) result (y)
    real(default), intent(in) :: x
    real(default) :: y
    y = real( exp(gammln(real(x,kind=sp))) , kind=default )
  end function nr_gamma

  function nr_locate (xa, x) result (pos)
    real(default), dimension(:), intent(in) :: xa
    real(default), intent(in) :: x
    integer :: pos
    pos = locatenr (real(xa,kind=sp), real(x,kind=sp))
  end function

  ! function nr_qgaus (fun, pts) result (res)
  !   real(default), dimension(:), intent(in) :: pts
  !   complex(default) :: res
  !   integer :: i_pts

```

```

!      real(sp) :: lo, hi, re, im
!      interface
!          function fun (x)
!              use kinds, only: default !NODEP!
!              real(default), intent(in) :: x
!              complex(default) :: fun
!          end function fun
!      end interface
!      res = 0.0_default
!      if ( size(pts) < 2 ) return
!      do i_pts=1, size(pts)-1
!          lo = real(pts(i_pts ),kind=sp)
!          hi = real(pts(i_pts+1),kind=sp)
!          re = qgaus (fun_re, lo, hi)
!          im = qgaus (fun_im, lo, hi)
!          res = res + cmplx(re,im,kind=default)
!      end do
!      contains
!          function fun_re (xa_sp)
!              use kinds, only: default !NODEP!
!              use nrtype, only: sp !NODEP!
!              real(sp), dimension(:), intent(in) :: xa_sp
!              real(sp), dimension(size(xa_sp)) :: fun_re
!              real(default), dimension(size(xa_sp)) :: xa
!              integer :: ix
!              xa = real(xa_sp,kind=default)
!              fun_re = (/ (real(fun(xa(ix))),kind=sp), ix=1, size(xa)) /)
!          end function fun_re
!          function fun_im (xa_sp)
!              use kinds, only: default !NODEP!
!              use nrtype, only: sp !NODEP!
!              real(sp), dimension(:), intent(in) :: xa_sp
!              real(sp), dimension(size(xa_sp)) :: fun_im
!              real(default), dimension(size(xa_sp)) :: xa
!              integer :: ix
!              xa = real(xa_sp,kind=default)
!              fun_im = (/ (real(aimag(fun(xa(ix)))),kind=sp), ix=1, size(xa)) /)
!          end function fun_im
!      end function nr_qgaus

subroutine nr_sort (array)
    real(default), dimension(:), intent(inout) :: array
    real(sp), dimension(size(array)) :: array_sp
    array_sp = real(array,kind=sp)
    call sort (array_sp)
    array = real(array_sp,kind=default)
end subroutine nr_sort

subroutine nr_spline_init (spl, xa_in, ya_in)
    class(nr_spline_t), intent(inout) :: spl
    real(default), dimension(:), intent(in) :: xa_in
    complex(default), dimension(:), intent(in) :: ya_in
    integer :: n
    if ( allocated(spl%xa) ) then

```

```

        print *, "ERROR: nr_spline: init: already initialized!"
        stop
    end if
    n = size(xa_in)
    allocate( spl%xa(n) )
    allocate( spl%ya_re(n) )
    allocate( spl%ya_im(n) )
    allocate( spl%y2a_re(n) )
    allocate( spl%y2a_im(n) )
    spl%xa = real(xa_in,kind=sp)
    spl%ya_re = real(ya_in,kind=sp)
    spl%ya_im = real(aimag(ya_in),kind=sp)
    call spline (spl%xa, spl%ya_re, 1.e30, 1.e30, spl%y2a_re)
    call spline (spl%xa, spl%ya_im, 1.e30, 1.e30, spl%y2a_im)
end subroutine nr_spline_init

function nr_spline_interpolate (spl, x) result (y)
    complex(default) :: y
    class(nr_spline_t), intent(in) :: spl
    real(default), intent(in) :: x
    real(sp) :: y_re, y_im
    if ( .not.allocated(spl%xa) ) then
        print *, "ERROR: nr_spline: interpolate: not initialized!"
        stop
    end if
    y_re = splint (spl%xa, spl%ya_re, spl%y2a_re, real(x,kind=sp))
    y_im = splint (spl%xa, spl%ya_im, spl%y2a_im, real(x,kind=sp))
    y = cmplx(y_re,y_im,kind=default)
end function nr_spline_interpolate

subroutine nr_spline_dealloc (spl)
    class(nr_spline_t), intent(inout) :: spl
    if ( .not.allocated(spl%xa) ) then
        print *, "ERROR: nr_spline: dealloc: not initialized!"
        stop
    end if
    deallocate( spl%xa )
    deallocate( spl%ya_re )
    deallocate( spl%ya_im )
    deallocate( spl%y2a_re )
    deallocate( spl%y2a_im )
end subroutine nr_spline_dealloc
end module nr_tools

<toppiik.f>≡
! WHIZARD <Version> <Date>

! TOPPIK code by M. Jezabek, T. Teubner (v1.1, 1992), T. Teubner (1998)
!
! FB: -commented out numerical recipes code for hypergeometric 2F1
!      included in hypgeo.f90;
!      -commented out unused function 'ZAPVQ1';
!      -replaced function 'cdabs' by 'abs';
!      -replaced function 'dimag' by 'aimag';
!      -replaced function 'dcmplx(,)' by 'cmplx(,kind=kind(0d0))';

```



```

!      -replaced function 'dreal' by 'real';
!      -replaced function 'cdlog' by 'log';
!      -replaced PAUSE by PRINT statement to avoid compiler warning;
!      -initialized 'idum' explicitly as real to avoid compiler warning.
!      -modified 'adglg1', 'adglg2' and 'tttoppik' to catch unstable runs.
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

C *****
C
C Working version with all the different original potentials
C like (p^2+q^2)/|p-q|^2, not transformed in terms of delta and 1/r^2;
C accuracy eps=1.d-3 possible (only), but should be save, 13.8.'98, tt.
C
C *****
C
C      subroutine tttoppik(xenergy,xtm,xtg,xalphas,xscale,xcutn,xcutv,
C      u      xc0,xc1,xc2,xcdeltc,xcdelctl,xcfullc,xcfulll,xcrm2,
C      u      xkincm,xkinca,jknflg,jgcflg,
C      u      xkincv,jvflg,xim,xdi,np,xpp,xww,xsdsp,zvfct)
C
C *****
C
C !! THIS IS NOT A PUBLIC VERSION !!
C
C -- Calculation of the Green function in momentum space by solving the
C Lippmann-Schwinger equation
C  $G(p) = G_0(p) + G_0(p) \int_0^{xcutn} V(p,q) G(q) dq$ 
C
C -- Written by Thomas Teubner, Hamburg, November 1998
C * Based on TOPPIK Version 1.1
C from M. Jezabek and TT, Karlsruhe, June 1992
C * Version originally for non-constant top-width
C * Constant width supplied here
C * No generator included
C
C -- Use of double precision everywhere
C
C -- All masses, momenta, energies, widths in GeV
C
C -- Input parameters:
C
C xenergy : E=Sqrt[s]-2*topmass
C xtm     : topmass (in the Pole scheme)
C xtg     : top-width
C xalphas : alpha_s^{MSbar,n_f=5}(xscale)
C xscale  : soft scale mu_{soft}
C xcutn   : numerical UV cutoff on all momenta
C          (UV cutoff of the Gauss-Legendre grid)
C xcutv   : renormalization cutoff on the
C          delta-, the (p^2+q^2)/(p-q)^2-, and the
C          1/r^2-[1/|p-q|]-potential:
C          if (max(p,q).ge.xcutv) then the three potentials
C          are set to zero in the Lippmann-Schwinger equation

```

```

c   xc0      : 0th order coefficient for the Coulomb potential,
c               see calling example above
c   xc1      : 1st order coefficient for the Coulomb potential
c   xc2      : 2nd order coefficient for the Coulomb potential
c   xcdeltc  : constant of the delta(r)-
c               [= constant in momentum space-] potential
c   xcdeltl  : constant for the additional log(q^2/mu^2)-part of the
c               delta-potential:
c               xcdeltc*1 + xcdeltl*log(q^2/mu^2)
c   xcfullc  : constant of the (p^2+q^2)/(p-q)^2-potential
c   xcfulll  : constant for the additional log(q^2/mu^2)-part of the
c               (p^2+q^2)/(p-q)^2-potential
c   xcrm2    : constant of the 1/r^2-[1/|p-q|]-potential
c   xkincm   : } kinetic corrections in the 0th order Green-function:
c   xkinca   : } G_0(p):=1/[E+iGamma_t-p^2/m_t]*(1+xkincm)+xkinca
c               !!! WATCH THE SIGN IN G_0 !!!
c   jknflg   : flag for these kinetic corrections:
c               0 : no kinetic corrections applied
c               1 : kinetic corrections applied with cutoff xcutv
c                   for xkinca only
c               2 : kinetic corrections applied with cutoff xcutv
c                   for xkinca AND xkincm
c   jgcflg   : flag for G_0(p) in the LS equation:
c               0 (standard choice) : G_0(p) as given above
c               1 (for TIPT)         : G_0(p) = G_c^{0}(p) the 0th
c                                       order Coulomb-Green-function
c                                       in analytical form; not for
c                                       momenta p > 1000*topmass
c   xkincv   : additional kinematic vertexcorrection in G_0, see below:
c   jvflg    : flag for the additional vertexcorrection xkincv in the
c               "zeroth order" G_0(p) in the LS-equation:
c               0 : no correction, means G = G_0 + G_0 int V G
c                   with G_0=1/[E+iGamma_t-p^2/m_t]*(1+xkincm)+xkinca
c               1 : apply the correction in the LS equation as
c                   G = G_0 + xkincv*p^2/m_t^2/[E+iGamma_t-p^2/m_t] +
c                   G_0 int V G
c               and correct the integral over Im[G(p)] to get sigma_tot
c               from the optical theorem by the same factor.
c               The cutoff xcutv is applied for these corrections.
c
c -- Output:
c
c   xim      : R_{ttbar} from the imaginary part of the green
c               function
c   xdi      : R_{ttbar} form the integral over the momentum
c               distribution (no cutoff but the numerical one here!!)
c   np       : number of points used for the grid; fixed in tttoppik
c   xpp      : 1-dim array (max. 900 elements) giving the momenta of
c               the Gauss-Legendre grid (pp(i) in the code)
c   xww      : 1-dim array (max. 900 elements) giving the corresponding
c               Gauss-Legendre weights for the grid
c   xdsdp    : 1-dim array (max. 900 elements) giving the
c               momentum distribution of top: d\sigma/dp,
c               normalized to R,

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```

c          at the momenta of the Gauss-Legendre grid xpp(i)
c  zvfct    : 1-dim array (max. 900 elements) of COMPLEX*16 numbers
c             giving the vertex function K(p), G(p)=K(p)*G_0(p)
c             at the momenta of the grid
c
c *****
c
c
c          implicit none
c          real*8
c
c          u      pi,energy,vzero,eps,
c          u      pp,
c          u      tmass,tgamma,zmass,alphas,alamb5,
c          u      wmass,wgamma,bmass,GFERMI,
c          u      xx,critp,consde,
c          u      w1,w2,sig1,sig2,const,
c          u      gtpcor,etot,
c          u      xenergy,xtm,xtg,xalphas,xscale,xc0,xc1,xc2,xim,xdi,
c          u      xdsdp,xpp,xww,
c          u      cplas,scale,c0,c1,c2,cdeltc,cdeltl,cfullc,cfulll,crm2,
c          u      xcutn,dcut,xcutv,
c          u      xp,xpmax,hmass,
c          u      kincom,kincoa,kincov,xkincm,xkinca,xkincv,
c          u      xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2,chiggs
c          complex*16 bb,gg,a1,a,g0,g0c,zvfct
c          integer i,n,nmax,npot,np,gcflg,kinflg,jknflg,jgcflg,
c          u      jvflg,vflag
c          parameter (nmax=900)
c          dimension pp(nmax), bb(nmax), xx(nmax), gg(nmax),
c          u      w1(nmax), w2(nmax), a1(nmax),
c          u      xdsdp(nmax), xpp(nmax), xww(nmax), zvfct(nmax)
c
c          external a,gtpcor,g0,g0c
c
c          common/ovalco/ pi, energy, vzero, eps, npot
c          COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c          $ WMASS,WGAMMA,BMASS,GFERMI,hmass
c          common/cplcns/cplas,scale,c0,c1,c2,
c          u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c          common/mom/ xp,xpmax,dcut
c          common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
c
c          pi=3.141592653589793238d0
c
c          c Number of points to evaluate on the integral equation
c          c (<=900 and n mod 3 = 0 !!):
c          c          n=66
c          c          n=600
c          c          np=n
c
c          c For second order potential with free parameters:
c          c
c          npot=5
c          c Internal accuracy for TOPPIK, the reachable limit may be smaller,

```

```

c depending on the parameters. But increase in real accuracy only
c in combination with large number of points.
      eps=1.d-3
c Some physical parameters:
      wgamma=2.07d0
      zmass=91.187d0
      wmass=80.33d0
      bmass=4.7d0
c
c Input:
      energy=xenergy
      tmass=xtm
      tgamma=xtg
      cplas=xalphas
      scale=xscale
      c0=xc0
      c1=xc1
      c2=xc2
      cdeltc=xcdeltc
      cdeltl=xcdeltl
      cfullc=xcfullc
      cfulll=xcfulll
      crm2=xcrm2
      kincom=xkincom
      kincoa=xkinca
      kincov=xkincv
      kinflg=jknflg
      gcflg=jgcflg
      vflag=jvflg
c
      alphas=xalphas
c
c Cut for divergent potential-terms for large momenta in the function vhat
c and in the integrals a(p):
      dcut=xcutv
c
c Numerical Cutoff of all momenta (maximal momenta of the grid):
      xpmx=xcutn
      if (dcut.gt.xpmx) then
        write(*,*) ' dcut > xpmx  makes no sense! Stop.'
        stop
      endif
c
c Not needed for the fixed order potentials:
      alamb5=0.2d0
c
      WRITE(*,*) 'INPUT TGAMMA=',TGAMMA
c Needed in subroutine GAMMAT:
      GFERMI=1.16637d-5
c      CALL GAMMAT
c      WRITE(*,*) 'CALCULATED TGAMMA=',TGAMMA
c
      etot=2.d0*tmass+energy
c

```

```

        if ((npot.eq.1).or.(npot.eq.3).or.(npot.eq.4).or.
            (npot.eq.5)) then
    u
c For pure coulomb and fixed order potentials there is no delta-part:
        consde = 0.d0
        else if (npot.eq.2) then
c Initialize QCD-potential common-blocks and calculate constant multiplying
c the delta-part of the 'qcutted' potential in momentum-space:
            call iniphc(1)
            call vqdelt(consde)
        else
            write (*,*) ' Potential not implemented! Stop.'
            stop
        endif
c Delta-part of potential is absorbed by subtracting vzero from the
c original energy (shift from the potential to the free Hamiltonian):
        vzero = consde / (2.d0*pi)**3
c
        write (*,*) 'vzero=', vzero
c
c Find x-values pp(i) and weigths w1(i) for the gaussian quadrature;
c care about large number of points in the important intervals:
c     if (energy-vzero.le.0.d0) then
cc         call gauleg(0.d0, 1.d0, pp, w1, n/3)
cc         call gauleg(1.d0, 5.d0, pp(n/3+1), w1(n/3+1), n/3)
cc         call gauleg(0.d0, 0.2d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c         call gauleg(0.d0, 5.d0, pp, w1, n/3)
c         call gauleg(5.d0, 20.d0, pp(n/3+1), w1(n/3+1), n/3)
c         call gauleg(0.d0, 0.05d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c     else
cc Avoid numerical singular points in the inner of the intervals:
c         critp = dsqrt((energy-vzero)*tmass)
c         if (critp.le.1.d0) then
cc Gauss-Legendre is symmetric => automatically principal-value prescription:
c             call gauleg(0.d0, 2.d0*critp, pp, w1, n/3)
c             call gauleg(2.d0*critp, 20.d0, pp(n/3+1),
c                 u
c                     w1(n/3+1), n/3)
c             call gauleg(0.d0, 0.05d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c         else
cc Better behaviour at the border of the intervals:
c             call gauleg(0.d0, critp, pp, w1, n/3)
c             call gauleg(critp, 2.d0*critp, pp(n/3+1),
c                 u
c                     w1(n/3+1), n/3)
c             call gauleg(0.d0, 1.d0/(2.d0*critp), pp(2*n/3+1),
c                 u
c                     w1(2*n/3+1), n/3)
c             endif
c         endif
c     endif
c
c Or different (simpler) method, good for V_JKT:
        if (energy.le.0.d0) then
            critp=tmass/3.d0
        else
            critp=max(tmass/3.d0,2.d0*dsqrt(energy*tmass))
        endif
        call gauleg(0.d0, critp, pp, w1, 2*n/3)
        call gauleg(1.d0/xpmax, 1.d0/critp, pp(2*n/3+1),

```

```

      u          w1(2*n/3+1), n/3)
c
c Do substitution p => 1/p for the last interval explicitly:
      do 10 i=2*n/3+1,n
          pp(i) = 1.d0/pp(i)
10      continue
c
c Reorder the arrays for the third interval:
      do 20 i=1,n/3
          xx(i) = pp(2*n/3+i)
          w2(i) = w1(2*n/3+i)
20      continue
      do 30 i=1,n/3
          pp(n-i+1) = xx(i)
          w1(n-i+1) = w2(i)
30      continue
c
c Calculate the integrals a(p) for the given momenta pp(i)
c and store weights and momenta for the output arrays:
      do 40 i=1,n
          a1(i) = a(pp(i)) !!! FB: can get stuck in original Toppik!
          !!! FB: abuse 'np' as a flag to communicate unstable runs
          if ( abs(a1(i)) .gt. 1d10 ) then
              np = -1
              return
          endif
          xpp(i)=pp(i)
          xww(i)=w1(i)
40      continue
      do 41 i=n+1,nmax
          xpp(i)=0.d0
          xww(i)=0.d0
41      continue
c
c Solve the integral-equation by solving a system of algebraic equations:
      call sae(pp, w1, bb, a1, n)
c
c (The substitution for the integration to infinity pp => 1/pp
c is done already.)
      do 50 i=1,n
          zvfct(i)=bb(i)
          gg(i) = bb(i)*g0c(pp(i))
cc      gg(i) = (1.d0 + bb(i))*g0c(pp(i))
cc Urspruenglich anderes (Minus) VZ hier, dafuer kein Minus mehr bei der
cc Definition des WQs ueber Im G, 2.6.1998, tt.
cc      gg(i) = - (1.d0 + bb(i))*g0c(pp(i))
50      continue
c
c Normalisation on R:
      const = 8.d0*pi/tmass**2
c
c Proove of the optical theorem for the output values of sae:
c Simply check if sig1 = sig2.
      sig1 = 0.d0

```

```

sig2 = 0.d0
do 60 i=1,n*2/3
c      write(*,*) 'check! p(',i,') = ',pp(i)
cvv
      if (pp(i).lt.dcut.and.vflag.eq.1) then
          sig1 = sig1 + w1(i)*pp(i)**2*aimag(gg(i)
cc      u          *(1.d0+kincov*(pp(i)/tmass)**2)
u      *(1.d0+kincov*g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i)))
u      )
      else
          sig1 = sig1 + w1(i)*pp(i)**2*aimag(gg(i))
      endif
      if (pp(i).lt.dcut.and.kinflg.ne.0) then
          sig2 = sig2 + w1(i)*pp(i)**2*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          *(1.d0-pp(i)**2/2.d0/tmass**2)
cc      u          *tmass/dsqrt(tmass**2+pp(i)**2)
          xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          *(1.d0-pp(i)**2/2.d0/tmass**2)
u          /(2.d0*pi**2)*const
      else
          sig2 = sig2 + w1(i)*pp(i)**2*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
          xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          /(2.d0*pi**2)*const
      endif
c      write(*,*) 'xdsdp = ',xdsdp(i)
c      write(*,*) 'zvfct = ',zvfct(i)
60      continue
c 'p**2' because of substitution p => 1/p in the integration of p**2*G(p)
c to infinity
do 70 i=n*2/3+1,n
c      write(*,*) 'check! p(',i,') = ',pp(i)
cvv
      if (pp(i).lt.dcut.and.vflag.eq.1) then
          sig1 = sig1 + w1(i)*pp(i)**4*aimag(gg(i)
cc      u          *(1.d0+kincov*(pp(i)/tmass)**2)
u      *(1.d0+kincov*g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i)))
u      )
      else
          sig1 = sig1 + w1(i)*pp(i)**4*aimag(gg(i))
      endif
      if (pp(i).lt.dcut.and.kinflg.ne.0) then
          sig2 = sig2 + w1(i)*pp(i)**4*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          *(1.d0-pp(i)**2/2.d0/tmass**2)
cc      u          *tmass/dsqrt(tmass**2+pp(i)**2)
          xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          *(1.d0-pp(i)**2/2.d0/tmass**2)
u          /(2.d0*pi**2)*const
      else

```

```

        sig2 = sig2 + w1(i)*pp(i)**4*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
        xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          /(2.d0*pi**2)*const
        endif
c
c          write(*,*) 'xdsdp = ',xdsdp(i)
c          write(*,*) 'zvfct = ',zvfct(i)
70      continue
        do 71 i=n+1,nmax
            xdsdp(i)=0.d0
            zvfct(i)=(0.d0,0.d0)
71      continue
c
c Normalisation on R:
        sig1 = sig1 / (2.d0*pi**2) * const
        sig2 = sig2 / (2.d0*pi**2) * const
c
c The results from the momentum space approach finally are:
cc Jetzt Minus hier, 2.6.98, tt.
        xim=-sig1
        xdi=sig2
c
        end
c
c
c      complex*16 function g0(p)
c
c      implicit none
c      real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi,energy,vzero,eps,
u      p,gtpcor,hmass
c      integer npot
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      common/ovalco/ pi, energy, vzero, eps, npot
c      external gtpcor
c      save
c      g0=1.d0/cmplx(energy-vzero-p**2/tmass,
u          tgamma*gtpcor(p,2.d0*tmass+energy),
u          kind=kind(0d0))
c      end
c
c      complex*16 function g0c(p)
c
c      implicit none
c      complex*16 hypgeo,green,zk,zi,amd2k,aa,bb,cc,zzp,zzm,
u      hypp,hypm,g0
c      real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,

```



```

u      pi,energy,vzero,eps,
u      p,gtpcor,hmass,
u      kincom,kincoa,kincov,xp,xpmax,dcut
      integer npot,kinflg,gcflg,vflag
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      common/ovalco/ pi, energy, vzero, eps, npot
      common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
      common/mom/ xp,xpmax,dcut
      external hypgeo,gtpcor,g0
      save

c
      if (gcflg.eq.0) then
        if (kinflg.eq.0) then
          g0c=g0(p)
        else if (kinflg.eq.1.and.p.lt.dcut) then
          g0c=g0(p)*(1.d0+kincom)+kincoa
        else if (kinflg.eq.1.and.p.ge.dcut) then
          g0c=g0(p)*(1.d0+kincom)
        else if (kinflg.eq.2.and.p.lt.dcut) then
          g0c=g0(p)*(1.d0+kincom)+kincoa
        else if (kinflg.eq.2.and.p.ge.dcut) then
          g0c=g0(p)
        else
          write(*,*) ' kinflg wrong! Stop.'
          stop
        endif
      else if (gcflg.eq.1) then
        zi=(0.d0,1.d0)
        zk=-tmass*cmplx(energy,tgamma
u                                *gtpcor(p,2.d0*tmass+energy),
u                                kind=kind(0d0))

        zk=sqrt(zk)
        amd2k=4.d0/3.d0*alphas*tmass/2.d0/zk
        aa=(2.d0,0.d0)
        bb=(1.d0,0.d0)
        cc=2.d0-amd2k
        zzp=(1.d0+zi*p/zk)/2.d0
        zzm=(1.d0-zi*p/zk)/2.d0
        if (abs(zzp).gt.20.d0) then
          hypp=(1.d0-zzp)**(-aa)*
u          hypgeo(aa,cc-bb,cc,zzp/(zzp-1.d0))
        else
          hypp=hypgeo(aa,bb,cc,zzp)
        endif
        if (abs(zzm).gt.20.d0) then
          hypm=(1.d0-zzm)**(-aa)*
u          hypgeo(aa,cc-bb,cc,zzm/(zzm-1.d0))
        else
          hypm=hypgeo(aa,bb,cc,zzm)
        endif
        green=-zi*tmass/(4.d0*p*zk)/(1.d0-amd2k)*(hypp-hypm)
c VZ anders herum als in Andres Konvention, da bei ihm G_0=1/[-E-i G*p^2/m]:
        g0c=-green

```

```

        if (p.gt.1.d3*tmass) then
            write(*,*) ' g0cana = ',g0c,' not reliable. Stop.'
            stop
        endif
    else
        write(*,*) ' gcflg wrong! Stop.'
        stop
    endif
end

c
c
c
c      complex*16 function a(p)
c
c      implicit none
c      real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy,ETOT,vzero, eps,
$      QCUT,QMAT1,ALR,PCUT,
u      p,
u      xp,xpmax, xb1,xb2,dcut,ddcut,
u      a1, a2, a3, a4,a5,a6,
u      adglg1, fretil1, fretil2, fimtil1, fimtil2,
u      ALEFVQ, gtpcor, ad8gle, buf,adglg2,
c  u      xerg,
u      kincom,kincoa,kincov,hmass
!      complex*16 zapvq1,ZAPVGP
!      complex*16 ZAPVGP !!! FB
c  u      ,acomp
c      integer npot,ILFLAG,kinflg,gcflg,vflag
c
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$  WMASS,WGAMMA,BMASS,GFERMI,hmass
c      COMMON/PARFLG/ QCUT,QMAT1,ALR,ILFLAG
c      common/ovalco/ pi, energy, vzero, eps, npot
c      common/mom/ xp,xpmax,dcut
c      common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
c
c      external adglg1, fretil1, fretil2, fimtil1, fimtil2,
!      u      zapvq1, ALEFVQ, gtpcor,ZAPVGP,ad8gle,adglg2
u      ALEFVQ, gtpcor,ZAPVGP,ad8gle,adglg2 !!! FB
c
c      if ((npot.eq.1).or.(npot.eq.3).or.(npot.eq.4).or.
u      (npot.eq.5)) then
c
c      xp=p
c      buf=0.d0
c
c      a1=0.d0
c      a2=0.d0
c      a3=0.d0
c      a4=0.d0
c      a5=0.d0

```

```

a6=0.d0
if (gcflg.eq.0) then
  ddcut=xpmax
else if (gcflg.eq.1) then
  ddcut=dcut
else
  write(*,*) ' gcflg wrong! Stop.'
  stop
endif
c
  if (2.d0*xp.lt.ddcut) then
    xb1=xp
    xb2=2.d0*xp
c
c More stable for logarithmically divergent fixed order potentials:
c
    a1=adglg1(fretil1, buf, xb1, eps) !!! FB: can get stuck!
    a2=adglg1(fimtil1, buf, xb1, eps)
c Slightly unstable:
    a3=adglg2(fretil1,xb1,xb2,eps) !!! FB: can get stuck!
c No good:
c    a3=adglg1(fretil1,xb1,xb2,eps)
c Not better:
c    call adqua(xb1,xb2,fretil1,xerg,eps)
c    a3=xerg
c Also not better:
c    a1=adglg1(fretil1, buf, xb2, eps)
c
    a4=adglg2(fimtil1,xb1,xb2,eps)
c    a5 = adglg2(fretil1, xb2, ddcut, eps)
c    a6 = adglg2(fimtil1, xb2, ddcut, eps)
    a5 = adglg2(fretil2, 1.d0/ddcut, 1.d0/xb2, eps)
    a6 = adglg2(fimtil2, 1.d0/ddcut, 1.d0/xb2, eps)
  else if (xp.lt.ddcut) then
    xb1=xp
    xb2=ddcut
    a1=adglg1(fretil1, buf, xb1, eps)
    a2=adglg1(fimtil1, buf, xb1, eps)
    a3=adglg2(fretil1,xb1,xb2,eps)
    a4=adglg2(fimtil1,xb1,xb2,eps)
  else if (ddcut.le.xp) then
  else
    write(*,*) ' Constellation not possible! Stop.'
    stop
  endif
c
  a = 1.d0/(4.d0*pi**2)*cmplx(a1+a3+a5,a2+a4+a6,
u                                kind=kind(0d0))
c
  else if (npot.eq.2) then
    PCUT=QCUT
    ETOT=ENERGY+2*TMASS
    a = ZAPVGP(P,ETOT,VZERO-ENERGY,PCUT,EPS)
c    acomp = zapvq1(ALEFVQ, p, vzero-energy, gtpcor, eps)

```

```

c      a = zapvq1(ALEFVQ, p, vzero-energy, gtpcor, eps)
c      acomp = acomp/a
c      if (abs(acomp-1.d0).gt.1.d-3) then
c          write (*,*) 'p=', p
c          write (*,*) 'acomp/a=', acomp
c      endif
c      else
c          write (*,*) ' Potential not implemented! Stop.'
c          stop
c      endif
c
c  end
c
c  real*8 function fretil1(xk)
c      implicit none
c      real*8 xk, freal
c      external freal
c      fretil1 = freal(xk)
c  end
c
c  real*8 function fretil2(xk)
c      implicit none
c      real*8 xk, freal
c      external freal
c      fretil2 = freal(1.d0/xk) * xk**(-2)
c  end
c
c  real*8 function fimtil1(xk)
c      implicit none
c      real*8 xk, fim
c      external fim
c      fimtil1 = fim(xk)
c  end
c
c  real*8 function fimtil2(xk)
c      implicit none
c      real*8 xk, fim
c      external fim
c      fimtil2 = fim(1.d0/xk) * xk**(-2)
c  end
c
c  real*8 function freal(xk)
c      implicit none
c      complex*16 vhat
c      real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p,pmax, xk, gtpcor,dcut,hmass
c      complex*16 g0,g0c
c      integer npot
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c      $ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      common/ovalco/ pi, energy, vzero, eps, npot

```

```

common/mom/ p,pmax,dcut
external vhat, g0, g0c, gtpcor
c
    freal = real(g0c(xk)*vhat(p, xk)) !!! FB: NaN?
end
c
real*8 function fim(xk)
    implicit none
    complex*16 vhat
    real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p,pmax, xk, gtpcor,dcut,hmass
    complex*16 g0,g0c
    integer npot
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
    common/ovalco/ pi, energy, vzero, eps, npot
    common/mom/ p,pmax,dcut
    external vhat, g0, g0c, gtpcor
    fim = aimag(g0c(xk)*vhat(p, xk))
end
c
c
complex*16 function vhat(p, xk)
c
    implicit none
    complex*16 zi
    real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p, xk,
u      cnspot, phiint, phfqcd, AD8GLE,
u      pm, xkm, ALPHEF,
u      zeta3,cf,ca,tf,xnf,a1,a2,b0,b1,
u      cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,cfulll,crm2,
u      xkpln1st,xkpln2nd,xkpln3rd,
u      pp,pmax,dcut,hmass,chiggs
    integer npot
    parameter(zi=(0.d0,1.d0))
    parameter(zeta3=1.20205690316d0,
u      cf=4.d0/3.d0,ca=3.d0,tf=1.d0/2.d0,
u      xnf=5.d0)
c
    external AD8GLE, phfqcd, ALPHEF
c
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
    common/ovalco/ pi, energy, vzero, eps, npot
    common/pmaxkm/ pm, xkm
    common/mom/ pp,pmax,dcut

```

```

common/cplcns/cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,fullll,crm2,chiggs
c
b0=11.d0-2.d0/3.d0*xnf
b1=102.d0-38.d0/3.d0*xnf
c
a1=31.d0/9.d0*ca-20.d0/9.d0*tf*xnf
a2=(4343.d0/162.d0+4.d0*pi**2-pi**4/4.d0+
u      22.d0/3.d0*zeta3)*ca**2-
u      (1798.d0/81.d0+56.d0/3.d0*zeta3)*ca*tf*xnf-
u      (55.d0/3.d0-16.d0*zeta3)*cf*tf*xnf+
u      (20.d0/9.d0*tf*xnf)**2
c
pm=p
xkm=xk
cnspt=-4.d0/3.d0*4.d0*pi
c
if (p/xk.le.1.d-5.and.p.le.1.d-5) then
  xkpln1st=2.d0
  xkpln2nd=-4.d0*dlog(scale/xk)
  xkpln3rd=-6.d0*dlog(scale/xk)**2
else if (xk/p.le.1.d-5.and.xk.le.1.d-5) then
  xkpln1st=2.d0*(xk/p)**2
  xkpln2nd=-4.d0*(xk/p)**2*dlog(scale/p)
  xkpln3rd=-6.d0*(xk/p)**2*dlog(scale/p)**2
else
c      xkpln1st=xk/p*dlog(dabs((p+xk)/(p-xk)))
      xkpln1st=xk/p*(dlog(p+xk)-dlog(dabs(p-xk)))
      xkpln2nd=xk/p*(-1.d0)*(dlog(scale/(p+xk))**2-
u          dlog(scale/dabs(p-xk))**2)
      xkpln3rd=xk/p*(-4.d0/3.d0)*(dlog(scale/(p+xk))**3-
u          dlog(scale/dabs(p-xk))**3)
endif
c
if (npot.eq.2) then
  if (p/xk.le.1.d-5.and.p.le.1.d-5) then
    vhat = 2.d0 * cnspt * ALPHEF(xk)
  else if (xk/p.le.1.d-5.and.xk.le.1.d-5) then
    vhat = 2.d0 * cnspt * xk**2 / p**2 * ALPHEF(p)
  else
u      phiint = cnspt * (AD8GLE(phfqcd, 0.d0, 0.3d0, 1.d-5)
          +AD8GLE(phfqcd, 0.3d0, 1.d0, 1.d-5))
      vhat = xk / p * dlog(dabs((p+xk)/(p-xk))) * phiint
  endif
else
  if (npot.eq.1) then
    c0=1.d0
    c1=0.d0
    c2=0.d0
  else if (npot.eq.3) then
    c0=1.d0+alphas/(4.d0*pi)*a1
    c1=alphas/(4.d0*pi)*b0
    c2=0
  else if (npot.eq.4) then

```

```

c0=1.d0+alphas/(4.d0*pi)*a1+(alphas/(4.d0*pi))**2*a2
c1=alphas/(4.d0*pi)*b0+
u      (alphas/(4.d0*pi))**2*(b1+2.d0*b0*a1)
c2=(alphas/(4.d0*pi))**2*b0**2
else if (npot.eq.5) then
else
  write(*,*) ' Potential not implemented! Stop.'
  stop
endif
phiint=cnspt*alphas
c
c      if ((xk+p).le.dcut) then
c        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c          -1.d0/2.d0*(1.d0+2.d0*ca/cf)
c          *(pi*cf*alphas)**2/tmass
c          *xk/p*(p+xk-dabs(xk-p))
c      else if (dabs(xk-p).lt.dcut) then
c        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c          -1.d0/2.d0*(1.d0+2.d0*ca/cf)
c          *(pi*cf*alphas)**2/tmass
c          *xk/p*(dcut-dabs(xk-p))
c      else if (dcut.le.dabs(xk-p)) then
c        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      else
c        write(*,*) ' Not possible! Stop.'
c        stop
c      endif
c
c      if (max(xk,p).lt.dcut) then
c Coulomb + first + second order corrections:
c        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c All other potentials:
u          +cdeltc*2.d0*xk**2
u          +cdeltl*xk/p/2.d0*(
u            (p+xk)**2*(dlog(((p+xk)/scale)**2)-1.d0)-
u            (p-xk)**2*(dlog(((p-xk)/scale)**2)-1.d0))
u          +cfullc*(p**2+xk**2)*xkpln1st
u          +cfulll*(p**2+xk**2)*xk/p/4.d0*
u            (dlog(((p+xk)/scale)**2)**2-
u            dlog(((p-xk)/scale)**2)**2)
u          +crm2*xk/p*(p+xk-dabs(xk-p))
c      else
c        vhat=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      endif
c    endif
c
c  end
c
c
c
c --- Routines needed for use of phenomenological potentials ---
c
SUBROUTINE INIPHC(INIFLG)
implicit real*8(a-h,o-z)

```

```

save
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
common/ovalco/ pi, energy, vzero, eps, npot
COMMON/PARFLG/ QCUT,QMAT1,ALR,ILFLAG
CHARACTER QCTCHR,QMTCHR,ALFCHR
DATA QCUTO/.100d0/,QMT1S/5.0d0/

c
zmass= 91.187d0
if(INIFLG.eq.0) then
c
standard set of parameters
ilflag= 1
alphas=.12d0
qcut= qcut0
qmat1= qmt1s
else
c
Parameters of QCD potential specified by USER
5 write(*,*) 'QCD coupling at M_z:  ALPHAS  or  LAMBDA  ?'
write(*,*) 'A/L  :'
read(*,895) ALFCHR
if(ALFCHR.eq.'A'.or.ALFCHR.eq.'a') then
ilflag= 1
write(*,*) 'alpha_s(M_z)= ?'
read(*,*) alphas
elseif(ALFCHR.eq.'L'.or.ALFCHR.eq.'l') then
write(*,*) 'Lambda(nf=5) =?'
read(*,*) alamb5
ilflag= 0
else
write(*,*) '!!! PLEASE TYPE: A OR L  !!!'
goto 5
endif
10 write(*,896) qcut0
read(*,895) QCTCHR
if(QCTCHR.eq.'Y'.or.QCTCHR.eq.'y') then
qcut=qcut0
elseif(QCTCHR.eq.'N'.or.QCTCHR.eq.'n') then
write(*,*) 'QCUT (GeV) = ?'
read(*,*) qcut
else
write(*,*) '!!! PLEASE TYPE: Y OR N  !!!'
goto 10
endif
15 write(*,902) qmt1s
read(*,895) QMTCHR
if(QMTCHR.eq.'Y'.or.QMTCHR.eq.'y') then
qmat1=qmt1s
elseif(QMTCHR.eq.'N'.or.QMTCHR.eq.'n') then
write(*,*) 'QMAT1 (GeV) = ?'
read(*,*) qmat1
else
write(*,*) '!!! PLEASE TYPE: Y OR N  !!!'
goto 15
endif

```



```

endif
895 format(1A)
896 format(1x,'Long distance cut off for QCD potential'/
$ 1x,'QCD = ',f5.4,' GeV. OK ? Y/N')
902 format(1x,
$ 'Matching QCD for NF=5 and Richardson for NF=3 at QMAT1 =',
$ f5.2,' GeV.'/1x,' OK ? Y/N')
end

C
C
      real*8 function phfqcd(x)
C integrand over k ?
      real*8 pm, xkm, x, ALPHEF
      external ALPHEF
      common/pmaxkm/ pm, xkm
      phfqcd = ALPHEF((pm+xkm)*(dabs(pm-xkm)/(pm+xkm))**x)
      end

C
C
FUNCTION ALEFVQ(x)
implicit real*8(a-h,o-z)
external ALPHEF
common/xtr101/ p0
data pi/3.1415926535897930d0/
q= p0*x
ALEFVQ= - 4d0/3* 4*pi*ALPHEF(q)
return
end

C
C
C
C
      COMPLEX*16 FUNCTION ZAPVGP(P,ETOT,VME,PCUT,ACC)

C
C A(p,E)= ZAPVGP(P,ETOT,VME,PCUT,ACC)
C for QCD potential VQGBAR(q) and GAMTPE(P,E) - momentum
C dependent width of top quark in t-tbar system.
C 2-dimensional integration
C P - intrinsic momentum of t quark, ETOT - total energy of t-tbar,
C VME=V0-E, where V0-potential at spatial infinity, E=ETOT-2*TMASS,
C PCUT - cut off in momentum space; e.g. for QCD potential
C given by ALPHEF PCUT=QCUT in COMMON/parflg/,
C ACC - accuracy
C external functions: VQGBAR,GAMTPE,ADQUA,AD8GLE,ADGLG1,ADGLG2
C
      IMPLICIT REAL*8(A-Z)
      EXTERNAL FINO1P,FINO2P,FINO3P,FINO4P,AD8GLE,ADGLG1,ADGLG2
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      COMMON/XTR102/ P0,E0,VMEM,TM,ACCO
      DATA PI/3.14159265/,BUF/1D-10/,SMALL/1D-2/
C For Testing only
      small = 1.d-1
C

```

```

CONST= -TMASS/(8*PI**2*P)
TM= TMASS
ACCO=ACC*SMALL
P0=P
EO=ETOT
VMEM=VME*TMASS
IF(PCUT.LE.P) THEN
    XXRE=AD8GLE(FIN01P,BUF,PCUT,ACC)+ADGLG1(FIN01P,PCUT,P,ACC)+
$    ADGLG1(FIN02P,BUF,1/P,ACC)
    XXIM=AD8GLE(FIN03P,BUF,PCUT,ACC)+ADGLG1(FIN03P,PCUT,P,ACC)+
$    ADGLG1(FIN04P,BUF,1/P,ACC)
ELSE
    XXRE=ADGLG1(FIN01P,BUF,P,ACC)+ADGLG2(FIN01P,P,PCUT,ACC)+
$    AD8GLE(FIN02P,BUF,1/PCUT,ACC)
    XXIM=ADGLG1(FIN03P,BUF,P,ACC)+ADGLG2(FIN03P,P,PCUT,ACC)+
$    AD8GLE(FIN04P,BUF,1/PCUT,ACC)
ENDIF
ZAPVGP=CONST*CMPLX(XXRE,XXIM,KIND=KIND(0d0))
END
C
REAL*8 FUNCTION FIN01P(Q)
C this segment contains FIN01P,FIN02P,FIN03P,FIN04P
IMPLICIT REAL*8(A-C,D-H,O-Z)
EXTERNAL VQGBAR,FIN11P, FIN12P
COMMON/XTR102/ P0,EO,VMEM,TM,ACCO
DATA PI/3.14159265/,BUF/1d-10/
Q0=Q
XL=(P0-Q0)**2
XU=(P0+Q0)**2
CALL ADQUA(XL,XU,FIN11P,Y,ACCO)
FIN01P= VQGBAR(Q0)*Q0*Y
RETURN
ENTRY FIN02P(Q)
Q0=1/Q
XL=(P0-Q0)**2
XU=(P0+Q0)**2
CALL ADQUA(XL,XU,FIN11P,Y,ACCO)
FIN02P= VQGBAR(Q0)*Q0**3*Y
RETURN
ENTRY FIN03P(Q)
Q0=Q
XL=(P0-Q0)**2
XU=(P0+Q0)**2
CALL ADQUA(XL,XU,FIN12P,Y,ACCO)
FIN03P= VQGBAR(Q0)*Q0*Y
RETURN
ENTRY FIN04P(Q)
Q0=1/Q
XL=(P0-Q0)**2
XU=(P0+Q0)**2
CALL ADQUA(XL,XU,FIN12P,Y,ACCO)
FIN04P= VQGBAR(Q0)*Q0**3*Y
END
REAL*8 FUNCTION FIN11P(T)

```

```

C      this segment contains FIN11P,FIN12P
      IMPLICIT REAL*8(A-C,D-H,O-Z)
      EXTERNAL GAMTPE
      COMMON/XTR102/ P0,E0,VMEM,TM,ACCO
      T1= T+VMEM
      TSQRT= SQRT(T)
      GAMMA= TM*GAMTPE(TSQRT,E0)
      FIN11P= T1/(T1**2+GAMMA**2)
      RETURN
      ENTRY FIN12P(T)
      T1= T+VMEM
      TSQRT= SQRT(T)
      GAMMA= TM*GAMTPE(TSQRT,E0)
      FIN12P= GAMMA/(T1**2+GAMMA**2)
      END

C
c
      SUBROUTINE VQDELT(VQ)

c
c      evaluates constants multiplying Dirac delta in potentials VQCUT
c      calls: ADQUA
c
      implicit real*8(a-h,o-z)
      external alphef,fncqct
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      COMMON/PARFLG/ QCUT,QMAT1,ALR,ILFLAG
      data pi/3.141592653589793238D0/

c
      call adqua(1d-8,1d4,fncqct,y,1d-4)
      v=-4d0/3*2/pi*y
      VQ=(-.25-v)*(2*pi)**3
      end

c
      function fncqct(q)
      implicit real*8(a-h,o-z)
      fncqct=sin(q)/q*alphef(q)
      end

c
C
      REAL*8 FUNCTION VQQBAR(P)

C
C      interquark potential for q- qbar singlet state
C
      IMPLICIT REAL*8(A-C,D-H,O-Z)
      EXTERNAL ALPHEF
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      DATA PI/3.14159265/
      VQQBAR = -4D0/3*4*PI*ALPHEF(P)/P**2
      END

C
      FUNCTION ALPHEF(q)
c

```

```

c      V(q) = -4/3 * 4*pi*ALPHEF(q)/q**2
c      input: alphas or alamb5 in COMMON/PHCONS/. If:
c      ILFLAG.EQ.0   alamb5= \Lambda_{\bar{MS}}^{\{5\}} at M_z
c      ILFLAG.EQ.1   alphas = alpha_{strong} at M_z (91.161)
c
c      effective coupling ALPHEF is defined as follows:
c      for q > qmat1=m_b:
c          alphas*( 1 +(31/3-10*nf/9)*alphas/(4*pi) )
c          where alphas=\alpha_{\bar{MS}} for nf=5, i.e.
c          alpha=4*pi/( b0(nf=5)*x + b1(5)/b0(5)*ln(x) )
c          and x = ln(q**2/alamb5**2)
c      for qmat1 > q > qcut:
c          4*pi/b0(nf=3)*(alfmt+1/log(1+q**2/alr**2))
c          where alr=.4 GeV, nefr=3, and continuity --> alfmt
c      below qcut:  alphrc*2*q**2/(q**2+qcut**2) (cont.-->alphrc)
c
c      implicit real*8(a-h,o-z)
c      SAVE
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c      $ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      COMMON/PARFLG/ QCAT,QMAT1,ALR,ILFLAG
c      common/parpot/ a5,b5,c5,alfmt,d,alphrc
c      data pi/3.141592653589793238D0/,
c      $ zold/-1d0/,qctold/-1d0/,alfold/-1d0/,
c      $ olmbd/-1d0/
c
c      if(zmass.le.0d0 .or. qcut.le.0d0) STOP 10001
c      if(zold.ne.zmass .or. qcut.ne.qctold) num=0
c      if(ilflag.eq.0 .and. olmbd.ne.alamb5) num=0
c      if(ilflag.eq.1 .and. alfold.ne.alphas) num=0
c      if(num.eq.0)then
c          num=num+1
c          zold=zmass
c          qctold=qcut
c          call potpar
c          alfold= alphas
c          olmbd= alamb5
c      endif
c      if(q.le.qcut) then
c          alphef=alphrc*(2*q**2)/(qcut**2+q**2)
c      elseif(q.le.qmat1) then
c          alphef=alfmt+d/log(1+q**2/alr**2)
c      else
c          x=2*log(q/alamb5)
c          alfas5=1/(a5*x+b5*log(x))
c          alphef=alfas5*(1+c5*alfas5)
c      endif
c      end
c
c      Only called by ALPHEF:
c      SUBROUTINE POTPAR
c      implicit real*8(a-h,o-z)
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c      $ WMASS,WGAMMA,BMASS,GFERMI,hmass

```

```

COMMON/PARFLG/ QCUT,QMAT1,ALR,ILFLAG
common/parpot/ a5,b5,c5,alfmt,d,alphrc
data pi/3.141592653589793238D0/,nefr/3/
b0(nf)=11-2./3*nf
b1(nf)=102-38./3*nf
cn(nf)=31./3-10./9*nf
alr=400d-3
a5=b0(5)/(4*pi)
b5=b1(5)/b0(5)/(4*pi)
c5=cn(5)/(4*pi)
d=4*pi/b0(nefr)
if(ilflag.eq.0) then
  if(alamb5.le.0d0) STOP 10002
  xa=2*log(zmass/alamb5)
  alphas= 1/(a5*xa + b5*log(xa))
else
  if(alphas.le.0d0) STOP 10003
  t0=0
  t1=max(1d0,alphas*a5)
10  tm=(t0+t1)/2
  fm=tm/alphas+b5*tm*log(tm)-a5
  if(fm.lt.-1d-10) then
    t0=tm
    goto 10
  elseif(fm.gt.1d-10) then
    t1=tm
    goto 10
  endif
  alamb5=zmass*exp(-5d-1/tm)
endif
x=2*log(qmat1/alamb5)
alfas=1/(a5*x+b5*log(x))
alfmt=alfas*(1+c5*alfas)-d/log(1+qmat1**2/alr**2)
alphrc=alfmt+ d/log(1+qcut**2/alr**2)
return
end

C
c --- End of routines for phenomenological potentials ---
C
C
c --- Routines for Gamma_top ---
C
SUBROUTINE GAMMAT
C
C on shell width of top quark including QCD corrections, c.f.
C M.Jezabek and J.H. Kuhn, Nucl. Phys. B314(1989)1
C
IMPLICIT REAL*8(A-C,D-H,O-Z)
EXTERNAL DILOG
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
DATA PI/3.14159265/
F(X)= PI**2+2*DILOG(X)-2*DILOG(1-X)+( 4*X*(1-X-2*X**2)*LOG(X)+
$2*(1-X)**2*(5+4*X)*LOG(1-X) - (1-X)*(5+9*X-6*X**2) ) /

```

```

      $(2*(1-X)**2*(1+2*X))
      Y= (WMASS/TMASS)**2
cc alpha_s(M_t) corresponding to alpha_s(M_Z)=0.118:
cc      alphas=0.107443d0
cc      write(*,*) 'alphas=',alphas
c Usage of alpha_s as given as input for the potential.. better use
c alpha_s at a scale close to m_t..
      TGAMMA= GFERMI*TMASS**3/(8*SQRT(2D0)*PI)*(1-Y)**2*(1+2*Y)*
      $(1- 2D0/3*ALPHAS/PI*F(Y))
      END
C
C
      REAL*8 FUNCTION GAMTPE(P,ETOT)
C
C      momentum dependent width of top quark in t-tbar system
C      GAMTPE = TGAMMA*GTPCOR(P,E), where TGAMMA includes
C      QCD corrections, see JKT, eq.(8), and
C      GTPCOR - correction factor for bound t quark
C
      IMPLICIT REAL*8(A-C,D-H,O-Z)
      EXTERNAL GTPCOR
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      GAMTPE= TGAMMA*GTPCOR(P,ETOT)
      END
C
C
C      GTPCOR and GTPCOR1 should be merged (M.J.) !!!!
C
      real*8 function gtpcor(topp,etot)
      real*8 topp,etot,
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,hmass
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      if (topp.ge.tmass/2.d0) then
c          gtpcor1=0.001d0
c      else
c          gtpcor=1.d0
c      endif
c      end
C
C
c Correction function for non-constant (energy and momentum dependent) width:
      FUNCTION GTPCOR1(TOPP,ETOT)
C
C      TOPP - momentum of t quark = - momentum of tbar
C      ETOT - total energy of t-tbar system
C      calls: GENWDS, RAN2
C
C      Evaluates a correction factor to the width of t-tbar system.
C      in future has to be replaced by a function evaluating
C      width including radiative corrections and GTPCOR.
C      I include two factors reducing the width:

```

```

c      a - time dilatation: for decay in flight lifetime
c      increased accordingly to relativistic kinematics
c      b - overall energy-momentum conservation: I assume that
c      t and tbar decay in flight and in this decays energies
c      of Ws follow from 2-body kinematics. Then I calculate
c      effective mass squared of b-bar system (it may be
c      negative!) from en-momentum conservation.
c      If effective mass is < 2*Mb + 2 GeV configuration
c      is rejected. The weight is acceptance.
c
      IMPLICIT REAL*8(A-H,O-Z)
      real ran2
      external ran2
      PARAMETER(NG=20,NC=4)
      dimension gamma(0:NG),pw1(0:3),pw2(0:3),AIJ(NC,NC),BJ(NC),
$AI(NC),SIG2IN(0:NG),XIK(0:NG,NC),INDX(NC)
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
      SAVE NUM,EOLD,TOLD,AI
      data nevent/10000/, num/0/, eold/-1d5/, told/-1d0/

c
C      for test runs!!
C      nevent=1000
C
      if(etot.ne.eold) num=0
      if(tmass.ne.told) num=0
5      if(num.eq.0) then
c          xdumm= ran2(-2)
          do 10 itp=0,NG
              tp=itp*tmass/NG*2
              gamma(itp)=0
              do 10 ix=1,nevent
                  call GENWDS(tp,etot,pw1,pw2,efmsq)
                  if(efmsq.gt.0d0) then
                      efms=sqrt(efmsq)
                      if(efms.ge. 2*bmass+2) gamma(itp)=gamma(itp)+1
                  endif
10              continue
              do 15 ix=0,NG
15              SIG2IN(IX)= MAX(1D0,GAMMA(IX))
              DO 17 JX=1,NC
                  IF(JX.EQ.1)THEN
                      XIK(0,JX)= .5D0
                  ELSE
                      XIK(0,JX)= 0D0
                  ENDIF
              DO 17 IX=1,NG
                  tp= 2D0*ix/NG
17              XIK(IX,JX)= tp**(JX-1)/(1+EXP(tp*3))
              DO 20 I=1,NC
                  BJ(I)=0
20              DO 20 J=1,NC
                  AIJ(I,J)=0
              DO 30 I=1,NC

```

```

DO 25 IX=0,NG
25  BJ(I)= BJ(I)+GAMMA(IX)*XIK(IX,I)*SIG2IN(IX)
DO 30 J=1,I
DO 30 IX=0,NG
30  AIJ(I,J)= AIJ(I,J)+XIK(IX,I)*XIK(IX,J)*SIG2IN(IX)
DO 35 I=1,NC
DO 35 J=I,NC
35  AIJ(I,J)= AIJ(J,I)
CALL LUDCMP(AIJ,NC,NC,INDX,D)
CALL LUBKSB(AIJ,NC,NC,INDX,BJ)
DO 40 I=1,NC
40  AI(I)= BJ(I)/NEVENT
do 42 i=1,nc
42  write(*,*)'a(' ,i,')=' ,ai(i)
do 100 ix=0,NG
100  gamma(ix)= gamma(ix)/nevent
eold=etot
told=tmass
num= 1
endif
SUM=AI(1)
DO 110 I=2,NC
110 SUM= SUM+AI(I)*(TOPP/TMASS)**(I-1)
C  CORR2= SUM/(1+ EXP(TOPP/TMASS*3))
C  CORR2= SUM/(1+ EXP(MIN(1d1,TOPP/TMASS*3)))
C  if(topp.gt. 2d0*tmass) then
C  corr1= 0.001d0
C  else
C  ip= NG*topp/tmass/2
C  corr1= gamma(ip)
C  endif
C  write(*,*)'ratio=' ,corr1/corr2
C  GTPCOR1 = CORR2
GTPCOR1 = CORR2*SQRT(1-TOPP**2/(TOPP**2+TMASS**2))
END
c
c Generator: only called by GTPCOR1
SUBROUTINE GENWDS(tp,etot,pw1,pw2,efm2)
c
c generates 4-momenta of W's and effective mass of b-bbar
c from t and tbar quarks decays at flight (tp = momentum of t
c = - momentum of tbar (in GeV) ) in Oz direction
c
implicit real*8(a-h,o-z)
c  real ran2
real ranf
c  external ran2
external ranf
dimension pw1(0:3),pw2(0:3)
save
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
data PI/3.141592653589793238D0/
real idum

```



```

c 3  s1= wmass**2+wmass*wgamma*TAN((2*ran2(idum)-1)*pi/2)
3  s1= wmass**2+wmass*wgamma*TAN((2*ranf(idum)-1)*pi/2)
    if(s1.le.0d0) goto 3
    wmass1= sqrt(s1)
    if(abs(wmass1-wmass).ge.3*wgamma) goto 3
c 4  s2= wmass**2+wmass*wgamma*TAN((2*ran2(idum)-1)*pi/2)
4  s2= wmass**2+wmass*wgamma*TAN((2*ranf(idum)-1)*pi/2)
    if(s2.le.0d0) goto 4
    wmass2= sqrt(s2)
    if(abs(wmass2-wmass).ge.3*wgamma) goto 4
    ew1= (tmass**2+wmass1**2-bmass**2)/(2*tmass)
    pwt1= sqrt(ew1**2-wmass1**2)
    ew2= (tmass**2+wmass2**2-bmass**2)/(2*tmass)
    pwt2= sqrt(ew2**2-wmass2**2)
5  p=tp
c    u1= 2*ran2(idum)-1
    u1= 2*ranf(idum)-1
    pw1z= pwt1*u1
c    u2= 2*ran2(idum)-1
    u2= 2*ranf(idum)-1
    pw2z= pwt2*u2
    et= sqrt(tmass**2+p**2)
    bet= p/et
    gam= et/tmass
    pw1(0)= gam*(ew1+bet*pw1z)
    pw1(3)= gam*(pw1z+bet*ew1)
    pw2(0)= gam*(ew2-bet*pw2z)
    pw2(3)= gam*(pw2z-bet*ew2)
    pw1tr= sqrt(pw1(0)**2-pw1(3)**2-wmass1**2)
    pw2tr= sqrt(pw2(0)**2-pw2(3)**2-wmass2**2)
c    phi1= 2*pi*ran2(idum)
    phi1= 2*pi*ranf(idum)
c    phi2= 2*pi*ran2(idum)
    phi2= 2*pi*ranf(idum)
    pw1(1)= pw1tr*cos(phi1)
    pw1(2)= pw1tr*sin(phi1)
    pw2(1)= pw2tr*cos(phi2)
    pw2(2)= pw2tr*sin(phi2)
    prec2= (pw1(1)+pw2(1))**2+(pw1(2)+pw2(2))**2+(pw1(3)+pw2(3))**2
    erest=etot-pw1(0)-pw2(0)
c
    efm2= erest*abs(erest)-prec2
    END
c
c --- End of routines for Gamma_top ---
c
c --- Routines for solving linear equations and matrix inversion (complex) ---
c
    subroutine sae(pp, w1, bb, a1, n)
c
        implicit none
        complex*16 vhat
        real*8
u        tmass,tgamma,zmass,alphas,alamb5,

```

```

u      wmass, wgamma, bmass, GFERMI,
u      pi, energy, vzero, eps,
u      d, pp, w1, gtpcor, hmass,
u      xp, xpm, dcut, kincom, kincoa, kincov
      complex*16 a, a1, bb, ff, cw, svw, g0, g0c
      integer i, j, npot, n, nmax, indx, kinflg, gcflg, vflag
      parameter (nmax=900)
      dimension bb(nmax), ff(nmax,nmax), pp(nmax), w1(nmax),
u      indx(nmax), cw(nmax), a1(nmax)

c
      COMMON/PHCONS/TMASS, TGAMMA, ZMASS, ALPHAS, ALAMB5,
$ WMASS, WGAMMA, BMASS, GFERMI, hmass
      common/ovalco/ pi, energy, vzero, eps, npot
      common/mom/ xp, xpm, dcut
      common/g0inf/kincom, kincoa, kincov, kinflg, gcflg, vflag

c
      external a, vhat, gtpcor, g0, g0c

c
      do 10 i=1, n*2/3
          cw(i) = w1(i) / (4.d0*pi**2) * g0c(pp(i))
c      cw(i) = w1(i) / (4.d0*pi**2 *
c      u      (cmplx(energy-vzero, tgamma*
c      u      gtpcor(pp(i), 2.d0*tmass+energy),
c      u      kind=kind(0d0))-pp(i)**2/tmass))
10      continue
      do 20 i=n*2/3+1, n
          cw(i) = w1(i) / (4.d0*pi**2) * g0c(pp(i)) * pp(i)**2
c      cw(i) = w1(i) / (4.d0*pi**2 *
c      u      (cmplx(energy-vzero, tgamma*
c      u      gtpcor(pp(i), 2.d0*tmass+energy),
c      u      kind=kind(0d0)) /
c      u      pp(i)**2 - 1.d0/tmass))
20      continue
c
      do 30 i=1, n
cc      bb(i) = a1(i)
cvv
          if (pp(i).lt.dcut.and.vflag.eq.1) then
c      bb(i) = cmplx(1.d0+kincov*(pp(i)/tmass)**2, 0.d0,
c      u      kind=kind(0d0))
          bb(i)=1.d0+kincov*
u      g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i))
          else
              bb(i) = (1.d0, 0.d0)
          endif
          svw = (0.d0, 0.d0)
          do 40 j=1, n
              if (i.ne.j) then
                  ff(i,j) = - vhat(pp(i), pp(j)) * cw(j)
                  svw = svw + ff(i,j)
              endif
40          continue
          ff(i,i) = 1.d0 - a1(i) - svw
30      continue

```

```

c
      call zldcmp(ff, n, nmax, indx, d)
      call zlbksb(ff, n, nmax, indx, bb)
c
      end
c
c
      SUBROUTINE ZLBKSB(A,N,NP,INDX,B)
C complex version of lubksb
      IMPLICIT NONE
      INTEGER I, II, INDX, J, LL, N, NP
      COMPLEX*16 A, B, SUM
      DIMENSION A(NP,NP),INDX(N),B(N)
      II=0
      DO 12 I=1,N
        LL=INDX(I)
        SUM=B(LL)
        B(LL)=B(I)
        IF (II.NE.0)THEN
          DO 11 J=II,I-1
            SUM=SUM-A(I,J)*B(J)
11          CONTINUE
          ELSE IF (SUM.NE.(0.DO,0.DO)) THEN
            II=I
          ENDIF
          B(I)=SUM
12        CONTINUE
      DO 14 I=N,1,-1
        SUM=B(I)
        IF(I.LT.N)THEN
          DO 13 J=I+1,N
            SUM=SUM-A(I,J)*B(J)
13          CONTINUE
          ENDIF
          B(I)=SUM/A(I,I)
14        CONTINUE
      RETURN
      END
c
      SUBROUTINE ZLDCMP(A,N,NP,INDX,D)
C complex version of ludcmp
      IMPLICIT NONE
      INTEGER I, IMAX, INDX, J, K, N, NP, NMAX
      REAL*8 AAMAX, D, TINY, VV
      COMPLEX*16 A, DUM, SUM
      PARAMETER (NMAX=900)
      DIMENSION A(NP,NP), INDX(N), VV(NMAX)
c
      tiny=1.d-5
c
      D=1.DO
      DO 12 I=1,N
        AAMAX=0.DO
        DO 11 J=1,N

```

```

      IF (ABS(A(I,J)).GT.AAMAX) AAMAX=ABS(A(I,J))
11  CONTINUE
c    IF (AAMAX.EQ.0.DO) PAUSE 'Singular matrix.'
      IF (AAMAX.EQ.0.DO) print *, "Singular matrix."
      VV(I)=1.DO/AAMAX
12  CONTINUE
      DO 19 J=1,N
        IF (J.GT.1) THEN
          DO 14 I=1,J-1
            SUM=A(I,J)
            IF (I.GT.1) THEN
              DO 13 K=1,I-1
                SUM=SUM-A(I,K)*A(K,J)
13          CONTINUE
                A(I,J)=SUM
            ENDIF
          CONTINUE
14        ENDIF
        AAMAX=0.DO
        DO 16 I=J,N
          SUM=A(I,J)
          IF (J.GT.1) THEN
            DO 15 K=1,J-1
              SUM=SUM-A(I,K)*A(K,J)
15          CONTINUE
              A(I,J)=SUM
            ENDIF
            DUM=VV(I)*ABS(SUM)
            IF (ABS(DUM).GE.AAMAX) THEN
              IMAX=I
              AAMAX=DUM
            ENDIF
16          CONTINUE
          IF (J.NE.IMAX) THEN
            DO 17 K=1,N
              DUM=A(IMAX,K)
              A(IMAX,K)=A(J,K)
              A(J,K)=DUM
17          CONTINUE
            D=-D
            VV(IMAX)=VV(J)
          ENDIF
          INDX(J)=IMAX
          IF (J.NE.N) THEN
            IF (A(J,J).EQ.(0.DO,0.DO)) A(J,J)=cmplx(TINY, 0.d0,
u              kind=kind(0d0))
            DUM=1.DO/A(J,J)
            DO 18 I=J+1,N
              A(I,J)=A(I,J)*DUM
18          CONTINUE
          ENDIF
19        CONTINUE
        IF (A(N,N).EQ.(0.DO,0.DO)) A(N,N)=cmplx(TINY, 0.d0,
u              kind=kind(0d0))

```

```

        RETURN
        END
C
C
C *** TOOLS ***
C
C
C ***** ROUTINES FOR GAUSSIAN INTEGRATIONS
C
C
C SUBROUTINE GAULEG(X1,X2,X,W,N)
C
C Given the lower and upper limits of integration X1 and X2
C and given N, this routine returns arrays X(N) and W(N)
C containing the abscissas and weights of the Gauss-Legendre
C N-point quadrature formula
C
C IMPLICIT REAL*8 (A-H,O-Z)
C REAL*8 X1,X2,X(N),W(N)
C PARAMETER (EPS=3.D-14)
C save
C M=(N+1)/2
C XM=0.5D0*(X2+X1)
C XL=0.5D0*(X2-X1)
C DO 12 I=1,M
C   Z=DCOS(3.141592653589793238D0*(I-.25D0)/(N+.5D0))
1  CONTINUE
C   P1=1.D0
C   P2=0.D0
C   DO 11 J=1,N
C     P3=P2
C     P2=P1
C     P1=((2.D0*J-1.D0)*Z*P2-(J-1.D0)*P3)/J
11  CONTINUE
C   PP=N*(Z*P1-P2)/(Z*Z-1.D0)
C   Z1=Z
C   Z=Z1-P1/PP
C   IF(DABS(Z-Z1).GT.EPS)GO TO 1
C   X(I)=XM-XL*Z
C   X(N+1-I)=XM+XL*Z
C   W(I)=2.D0*XL/((1.D0-Z*Z)*PP*PP)
C   W(N+1-I)=W(I)
12  CONTINUE
C RETURN
C END
C
C
C DOUBLE PRECISION FUNCTION AD8GLE(F,A,B,EPS)
C implicit double precision (a-h,o-z)
C EXTERNAL F
C DIMENSION W(12),X(12)
C   SAVE W, X
C   SAVE
C

```

```

C *****
C
C ADAPTIVE GAUSSIAN QUADRATURE.
C
C AD8GLE IS SET EQUAL TO THE APPROXIMATE VALUE OF THE INTEGRAL OF
C THE FUNCTION F OVER THE INTERVAL (A,B), WITH ACCURACY PARAMETER
C EPS.
C *****
C
C DATA W / 0.10122 85362 90376 25915 25313 543D0,
$ 0.22238 10344 53374 47054 43559 944D0,
$ 0.31370 66458 77887 28733 79622 020D0,
$ 0.36268 37833 78361 98296 51504 493D0,
$ 0.27152 45941 17540 94851 78057 246D-1,
$ 0.62253 52393 86478 92862 84383 699D-1,
$ 0.95158 51168 24927 84809 92510 760D-1,
$ 0.12462 89712 55533 87205 24762 822D0,
$ 0.14959 59888 16576 73208 15017 305D0,
$ 0.16915 65193 95002 53818 93120 790D0,
$ 0.18260 34150 44923 58886 67636 680D0,
$ 0.18945 06104 55068 49628 53967 232D0/
C
C DATA X / 0.96028 98564 97536 23168 35608 686D0,
$ 0.79666 64774 13626 73959 15539 365D0,
$ 0.52553 24099 16328 98581 77390 492D0,
$ 0.18343 46424 95649 80493 94761 424D0,
$ 0.98940 09349 91649 93259 61541 735D0,
$ 0.94457 50230 73232 57607 79884 155D0,
$ 0.86563 12023 87831 74388 04678 977D0,
$ 0.75540 44083 55003 03389 51011 948D0,
$ 0.61787 62444 02643 74844 66717 640D0,
$ 0.45801 67776 57227 38634 24194 430D0,
$ 0.28160 35507 79258 91323 04605 015D0,
$ 0.95012 50983 76374 40185 31933 543D-1/
C
C *****
C
C GAUSS=0.0D0
C AD8GLE=GAUSS
C IF(B.EQ.A) RETURN
C CONST=EPS/(B-A)
C BB=A
C
C COMPUTATIONAL LOOP.
1 AA=BB
  BB=B
2 C1=0.5D0*(BB+AA)
  C2=0.5D0*(BB-AA)
  S8=0.0D0
  DO 3 I=1,4
    U=C2*X(I)
    S8=S8+W(I)*(F(C1+U)+F(C1-U))
3 CONTINUE

```

```

      S8=C2*S8
      S16=0.0D0
      DO 4 I=5,12
        U=C2*X(I)
        S16=S16+W(I)*(F(C1+U)+F(C1-U))
4     CONTINUE
      S16=C2*S16
      IF( ABS(S16-S8) .LE. EPS*(abs(s8)+ABS(S16))*0.5D0 ) GO TO 5
      BB=C1
      IF( 1.D0+ABS(CONST*C2) .NE. 1.D0) GO TO 2
      AD8GLE=0.0D0
      write(*,*)'too high accuracy required in function ad8gle!'
      RETURN
5     GAUSS=GAUSS+S16
      IF(BB.NE.B) GO TO 1
      AD8GLE=GAUSS
      RETURN
      END
C
C
      DOUBLE PRECISION FUNCTION ADGLG1(F,A,B,EPS)
      IMPLICIT REAL*8 (A-H,O-Z)
      EXTERNAL F,AD8GLE,adqua
      DIMENSION W(6),X(6),xx(6)
c     SAVE W, XX, NUM
      SAVE
C
C
      *****
C
C     ADAPTIVE GAUSSIAN QUADRATURE.
C     For x->b   f(x) = 0 (ln^k (b-x) )
C     A - lower limit, B - upper limit (integrable singularity)
C     AD8GLE IS SET EQUAL TO THE APPROXIMATE VALUE OF THE INTEGRAL OF
C     THE FUNCTION F OVER THE INTERVAL (A,B), WITH ACCURACY PARAMETER
C     EPS.
C
C
      *****
C
      DATA W / 4.58964 673950d-1,
$           4.17000 830772d-1,
$           1.13373 382074d-1,
$           1.03991 974531d-2,
$           2.61017 202815d-4,
$           8.98547 906430d-7/
C
      DATA X / 0.22284 66041 79d0,
$           1.18893 21016 73d0,
$           2.99273 63260 59d0,
$           5.77514 35691 05d0,
$           9.83746 74183 83d0,
$           15.98287 39806 02d0/
      DATA NUM/0/
      IF(NUM.eq.0d0) then
        do 1 ix=1,6
1     xx(ix)= EXP(-x(ix))

```

```

        ENDIF
        num=num+1
        sum=0d0
        c=b-a
        sum6=0d0
        do 10 in=1,6
10      sum6= sum6+ w(in)*f(b-c*xx(in))
        sum6=sum6*c
        a1=a
15      a2= (a1+b)/2
        c=b-a2
        sumn=0d0
        do 20 in=1,6
            !!! FB: catch NaN
            if ( c/b .lt. 1d-9 ) then
                adglg1 = 1d15
                return
            endif
20      sumn= sumn+ w(in)*f(b-c*xx(in)) !!! FB: f(b) = NaN !
        sumn=sumn*c
ctt
c      call adqua(a1,a2,f,sum1,eps)
c      sum1=sum1+sum
        sum1=AD8GLE(F,A1,A2,eps)+sum
        IF(ABS( (sum+sum6)/(sum1+sumn)-1d0 ).lt.EPS) THEN
ctt
c      call adqua(a,a2,f,sum2,eps)
        sum2=AD8GLE(F,A,A2,eps)
        IF(ABS( (sum2+sumn)/(sum1+sumn)-1d0 ).gt.EPS) THEN
            sum=sum2
            a1=a2
            sum6=sumn
            goto 15
        ENDIF
        ADGLG1= SUM1+SUMN
        RETURN
    ELSE
        sum=sum1
        a1=a2
        sum6=sumn
        goto 15
    ENDIF
END
END

C
DOUBLE PRECISION FUNCTION ADGLG2(F,A,B,EPS)
IMPLICIT REAL*8 (A-H,O-Z)
EXTERNAL F,AD8GLE
DIMENSION W(6),X(6),xx(6)
c      SAVE W,XX,NUM
SAVE
C
C      *****
C
C      ADAPTIVE GAUSSIAN QUADRATURE.

```



```

C      For x->A   f(x) = 0 (ln^k (x-a) )
C      A - lower limit (integrable singularity), B - upper limit
C      AD8GLE IS SET EQUAL TO THE APPROXIMATE VALUE OF THE INTEGRAL OF
C      THE FUNCTION F OVER THE INTERVAL (A,B), WITH ACCURACY PARAMETER
C      EPS.
C
C      *****
DATA W / 4.58964 673950d-1,
$      4.17000 830772d-1,
$      1.13373 382074d-1,
$      1.03991 974531d-2,
$      2.61017 202815d-4,
$      8.98547 906430d-7/
C
DATA X / 0.22284 66041 79d0,
$      1.18893 21016 73d0,
$      2.99273 63260 59d0,
$      5.77514 35691 05d0,
$      9.83746 74183 83d0,
$      15.98287 39806 02d0/
DATA NUM/0/
IF(NUM.eq.0d0) then
do 1 ix=1,6
1  xx(ix)= EXP(-x(ix))
ENDIF
num=num+1
sum=0d0
c=b-a
sum6=0d0
do 10 in=1,6
10  sum6= sum6+ w(in)*f(A+c*xx(in))
sum6=sum6*c
b1=b
15  b2= (a+b1)/2
c=b2-a
sumn=0d0
do 20 in=1,6
!!! FB: catch NaN
if ( c/a .lt. 1d-9 ) then
adglg2 = 1d15
return
endif
20  sumn= sumn+ w(in)*f(a+c*xx(in)) !!! FB: f(a) = NaN !
sumn=sumn*c
sum1=AD8GLE(F,b2,b1,eps)+sum
IF(ABS( (sum+sum6)/(sum1+sumn)-1d0 ).lt.EPS) THEN
sum2=AD8GLE(F,b2,b,eps)
IF(ABS( (sum2+sumn)/(sum1+sumn)-1d0 ).gt.EPS) THEN
sum=sum2
b1=b2
sum6=sumn
goto 15
ENDIF
ADGLG2= SUM1+SUMN

```

```

        RETURN
    ELSE
        sum=sum1
        b1=b2
        sum6=sumn
        goto 15
    ENDIF
END
C
C
C-----
C INTEGRATION ROUTINE ADQUA written by M. Jezabek      -----
C-----
C
    SUBROUTINE ADQUA(XL,XU,F,Y,ACC)
C
C    ADAPTIVE GAUSS-LEGENDRE + SIMPSON'S RULE QUADRATURE
C    XL - LOWER LIMIT, XU - UPPER LIMIT, F - FUNCTION TO INTEGRATE
C    Y - INTEGRAL
C    ACC - ACCURACY (IF .LE. 0. ACC=1.D-6)
C    ***** new constants, 1 error removed, Oct '92
C
C    CALLS: SIMPSA
C
C    PARAMETERS: NSUB > NO OF SUBDIVISION LEVELS IN GAUSS INTEGRATION
C                 100*2**IMAX > NO OF POINTS IN SIMPSON INTEGRATION
C
    IMPLICIT REAL*8 (A-H,O-Z)
    EXTERNAL F
    DIMENSION VAL(25,2), BOUND(25,2,2), LEV(25),SING(25,3)
    DIMENSION W8(4),X8(4)
    DATA W8
    $/0.101228536290376D0, 0.222381034453374D0, 0.313706645877887D0,
    $ 0.362683783378362D0/
    DATA X8
    $/0.960289856497536D0, 0.796666477413627D0, 0.525532409916329D0,
    $ 0.183434642495650D0/
    save
C
    IF(ACC.LE.0.D0) ACC=1.D-6
    NSUB=24
    NSG=25
    NSC=0
    A=XL
    B=XU
    C1=0.5d0*(A+B)
    C2=C1-A
    S8=0d0
    DO 1 I=1,4
    U=X8(I)*C2
1 S8=S8+W8(I)*(F(C1+U)+F(C1-U))
    S8=S8*C2
    XM=(XL+XU)/2.d0
    BOUND(1,1,1)=XL

```

```

        BOUND(1,1,2)=XM
        BOUND(1,2,1)=XM
        BOUND(1,2,2)=XU
        NC=1
        DO 3 IX=1,2
            A=BOUND(NC,IX,1)
            B=BOUND(NC,IX,2)
            C1=0.5d0*(A+B)
            C2=C1-A
            VAL(NC,IX)=0.d0
        DO 2 I=1,4
            U=X8(I)*C2
2 VAL(NC,IX)=VAL(NC,IX)+W8(I)*(F(C1+U)+F(C1-U))
3 VAL(NC,IX)=VAL(NC,IX)*C2
        S16=VAL(NC,1)+VAL(NC,2)
        IF(DABS(S8-S16).GT.ACC*DABS(S16)) GOTO 4
        Y=S16
        RETURN
4 DO 5 I=1,NSUB
5 LEV(I)=0
        NC1= NC+1
11 XM=(BOUND(NC,1,1)+BOUND(NC,1,2))/2.d0
        BOUND(NC1,1,1)=BOUND(NC,1,1)
        BOUND(NC1,1,2)=XM
        BOUND(NC1,2,1)=XM
        BOUND(NC1,2,2)=BOUND(NC,1,2)
        DO 13 IX=1,2
            A=BOUND(NC1,IX,1)
            B=BOUND(NC1,IX,2)
            C1=0.5d0*(A+B)
            C2=C1-A
            VAL(NC1,IX)=0.d0
        DO 12 I=1,4
            U=X8(I)*C2
12 VAL(NC1,IX)=VAL(NC1,IX)+W8(I)*(F(C1+U)+F(C1-U))
13 VAL(NC1,IX)=VAL(NC1,IX)*C2
        S16=VAL(NC1,1)+VAL(NC1,2)
        S8=VAL(NC,1)
        IF(DABS(S8-S16).LE.ACC*DABS(S16)) GOTO 20
        NC=NC1
        NC1= NC+1
        IF(NC1.LE.NSUB) GOTO 11
C   NC=NSUB   USE SIMPSON'S RULE
        NSC=NSC+1
        IF(NSC.LE.NSG) GOTO 15
        WRITE(*,911)
911 FORMAT(1X,'ADQUA: TOO MANY SINGULARITIES')
        STOP
15 SING(NSC,1)=BOUND(NC,1,1)
        SING(NSC,2)=BOUND(NC,2,2)
        SING(NSC,3)=S16
        S16=0.d0
        NC=NC-1
20 VAL(NC,1)= S16

```

```

121 LEV(NC)=1
21 XM=(BOUND(NC,2,1)+BOUND(NC,2,2))/2.d0
   BOUND(NC1,1,1)=BOUND(NC,2,1)
   BOUND(NC1,1,2)=XM
   BOUND(NC1,2,1)=XM
   BOUND(NC1,2,2)=BOUND(NC,2,2)
   DO 23 IX=1,2
     A=BOUND(NC1,IX,1)
     B=BOUND(NC1,IX,2)
     C1=0.5d0*(A+B)
     C2=C1-A
     VAL(NC1,IX)=0.d0
   DO 22 I=1,4
     U=X8(I)*C2
22 VAL(NC1,IX)=VAL(NC1,IX)+W8(I)*(F(C1+U)+F(C1-U))
23 VAL(NC1,IX)=VAL(NC1,IX)*C2
   S16=VAL(NC1,1)+VAL(NC1,2)
   S8=VAL(NC,2)
   IF(DABS(S8-S16).LE.ACC*DABS(S16)) GOTO 40
   NC=NC+1
   NC1=NC+1
   IF(NC1.LE.NSUB) GOTO 11
C   NC=NSUB   USE SIMPSON'S RULE
   NSC=NSC+1
   IF(NSC.LE.NSG) GOTO 35
   WRITE(*,911)
   STOP
35 SING(NSC,1)=BOUND(NC,1,1)
   SING(NSC,2)=BOUND(NC,2,2)
   SING(NSC,3)=S16
   S16=0.d0
   NC=NC-1
40 VAL(NC,2)= S16
45 IF(NC.GT.1) GOTO 50
   Y1=VAL(1,1)+VAL(1,2)
   GOTO 100
50 NCO=NC-1
   IF(LEV(NCO).EQ.0) IX=1
   IF(LEV(NCO).EQ.1) IX=2
   LEV(NC)=0
   NC1=NC
   VAL(NCO,IX)=VAL(NC,1)+VAL(NC,2)
   NC=NCO
   IF(IX.EQ.1) GOTO 121
   GOTO 45
100 CONTINUE
   IF(NSC.GT.0) GOTO 101
   Y=Y1
   RETURN
101 FSUM=0.d0
   DO 102 IK=1,NSC
102 FSUM=FSUM+DABS(SING(IK,3))
   ACCR=ACC*DMAX1(FSUM,DABS(Y1))/FSUM/10.d0
   DO 104 IK=1,NSC

```

```

104 CALL SIMPSA(SING(IK,1),SING(IK,2),F,SING(IK,3),ACCR)
    DO 106 IK=1,NSC
106 Y1=Y1+SING(IK,3)
    Y=Y1
    RETURN
    END
C
    SUBROUTINE SIMPSA(A,B,F,F0,ACC)
C    SIMPSON'S ADAPTIVE QUADRATURE
    IMPLICIT REAL*8 (A-H,O-Z)
    save
    EXTERNAL F
    IMAX=5
    NO=100
    H=(B-A)/NO
    NO2=NO/2
    S2=0.d0
    IC=1
    S0=F(A)+F(B)
    DO 5 K=1,NO2
5    S2=S2+F(A+2.d0*K*H)
7    S1=0.d0
    DO 10 K=1,NO2
10   S1=S1+F(A+(2.d0*K-1.d0)*H)
    Y=H/3.d0*(S0+4.d0*S1+2.d0*S2)
    IF(DABS(F0/Y-1.d0).GT.ACC) GOTO 20
    RETURN
20   NO2=NO
    NO=2*NO
    S2=S1+S2
    H=H/2.d0
    IF(IC.GT.IMAX) GOTO 30
    F0=Y
    IC=IC+1
    GOTO 7
30   ACCO=DABS(Y/F0-1.d0)
    WRITE(*,900) A,B,ACCO
    STOP
900  FORMAT(1H , 'SIMPSA: TOO HIGH ACCURACY REQUIRED' /
/1X, 29HSINGULARITY IN THE INTERVAL ,D20.12,1X,D20.12/
/1X, 29HACCURACY ACHIEVED ,D20.12)
    END
C
C
C ***** matrix-inversion-routines
C
    SUBROUTINE LUDCMP(A,N,NP,INDX,D)
    IMPLICIT REAL*8(A-H,O-Z)
    PARAMETER (NMAX=100,TINY=1.OE-20)
    DIMENSION A(NP,NP),INDX(N),VV(NMAX)
    D=1.
    DO 12 I=1,N
        AAMAX=0.
        DO 11 J=1,N

```

```

      IF (ABS(A(I,J)).GT.AAMAX) AAMAX=ABS(A(I,J))
11  CONTINUE
!    IF (AAMAX.EQ.0.) PAUSE 'Singular matrix.'
      IF (AAMAX.EQ.0.) print *, 'Singular matrix.'
      VV(I)=1./AAMAX
12  CONTINUE
DO 19 J=1,N
  IF (J.GT.1) THEN
    DO 14 I=1,J-1
      SUM=A(I,J)
      IF (I.GT.1) THEN
        DO 13 K=1,I-1
          SUM=SUM-A(I,K)*A(K,J)
13      CONTINUE
          A(I,J)=SUM
        ENDIF
      CONTINUE
    ENDIF
14    CONTINUE
  ENDIF
  AAMAX=0.
DO 16 I=J,N
  SUM=A(I,J)
  IF (J.GT.1) THEN
    DO 15 K=1,J-1
      SUM=SUM-A(I,K)*A(K,J)
15    CONTINUE
      A(I,J)=SUM
    ENDIF
    DUM=VV(I)*ABS(SUM)
    IF (DUM.GE.AAMAX) THEN
      IMAX=I
      AAMAX=DUM
    ENDIF
16  CONTINUE
  IF (J.NE.IMAX) THEN
    DO 17 K=1,N
      DUM=A(IMAX,K)
      A(IMAX,K)=A(J,K)
      A(J,K)=DUM
17    CONTINUE
    D=-D
    VV(IMAX)=VV(J)
  ENDIF
  INDX(J)=IMAX
  IF (J.NE.N) THEN
    IF (A(J,J).EQ.0.) A(J,J)=TINY
    DUM=1./A(J,J)
    DO 18 I=J+1,N
      A(I,J)=A(I,J)*DUM
18    CONTINUE
  ENDIF
19  CONTINUE
  IF (A(N,N).EQ.0.) A(N,N)=TINY
  RETURN
END

```

```

C      SUBROUTINE LUBKSB(A,N,NP,INDX,B)
C      IMPLICIT REAL*8(A-H,O-Z)
C      DIMENSION A(NP,NP),INDX(N),B(N)
C      II=0
C      DO 12 I=1,N
C          LL=INDX(I)
C          SUM=B(LL)
C          B(LL)=B(I)
C          IF (II.NE.0)THEN
C              DO 11 J=II,I-1
C                  SUM=SUM-A(I,J)*B(J)
11          CONTINUE
C              ELSE IF (SUM.NE.0.) THEN
C                  II=I
C              ENDIF
C              B(I)=SUM
12      CONTINUE
C      DO 14 I=N,1,-1
C          SUM=B(I)
C          IF(I.LT.N)THEN
C              DO 13 J=I+1,N
C                  SUM=SUM-A(I,J)*B(J)
13          CONTINUE
C              ENDIF
C              B(I)=SUM/A(I,I)
14      CONTINUE
C      RETURN
C      END

C
C
C      *****  RANDOM NUMBER GENERATORS
C
C
C      FUNCTION RANF(DUMMY)
C
C      RANDOM NUMBER FUNCTION TAKEN FROM KNUTH
C      (SEMINUMERICAL ALGORITHMS).
C      METHOD IS  $X(N)=MOD(X(N-55)-X(N-24),1/FMODUL)$ 
C      NO PROVISION YET FOR CONTROL OVER THE SEED NUMBER.
C
C      RANF GIVES ONE RANDOM NUMBER BETWEEN 0 AND 1.
C      IRN55 GENERATES 55 RANDOM NUMBERS BETWEEN 0 AND 1/FMODUL.
C      IN55  INITIALIZES THE 55 NUMBERS AND WARMS UP THE SEQUENCE.
C
C      PARAMETER (FMODUL=1.E-09)
C      SAVE /CIRN55/
C      COMMON /CIRN55/NCALL,MCALL,IA(55)
C      INTEGER IA
C      CALL RANDAT
C      IF( NCALL.EQ.0 ) THEN
C          CALL IN55 ( IA,234612947 )
C          MCALL = 55
C          NCALL = 1

```

```

ENDIF
IF ( MCALL.EQ.0 ) THEN
    CALL IRN55(IA)
    MCALL=55
ENDIF
RANF=IA(MCALL)*FMODUL
MCALL=MCALL-1
RETURN
END

C
    SUBROUTINE RANDAT
C
C INITIALISES THE NUMBER NCALL TO 0 TO FLAG THE FIRST CALL
C OF THE RANDOM NUMBER GENERATOR
C
C     SAVE /CIRN55/
C     SAVE FIRST
    SAVE
    COMMON /CIRN55/NCALL,MCALL,IA(55)
    INTEGER IA
    LOGICAL FIRST
    DATA FIRST /.TRUE./
    IF(FIRST)THEN
        FIRST=.FALSE.
        NCALL=0
    ENDIF
    RETURN
    END

C
    SUBROUTINE IN55(IA,IX)
    PARAMETER (MODULO=1000000000)
    INTEGER IA(55)
C
    IA(55)=IX
    J=IX
    K=1
    DO 10 I=1,54
        II=MOD(21*I,55)
        IA(II)=K
        K=J-K
        IF(K.LT.0)K=K+MODULO
        J=IA(II)
10    CONTINUE
    DO 20 I=1,10
        CALL IRN55(IA)
20    CONTINUE
    RETURN
    END

C
    SUBROUTINE IRN55(IA)
    PARAMETER (MODULO=1000000000)
    INTEGER IA(55)
    DO 10 I=1,24
        J=IA(I)-IA(I+31)

```



```

        IF(J.LT.0)J=J+MODULO
        IA(I)=J
10    CONTINUE
        DO 20 I=25,55
            J=IA(I)-IA(I-24)
            IF(J.LT.0)J=J+MODULO
            IA(I)=J
20    CONTINUE
        RETURN
    END

C
C
    FUNCTION RAN2(IDUM)
C    *****
    REAL RDM(31)
    DATA IWARM/0/
C
        IF (IDUM.LT.0.OR.IWARM.EQ.0) THEN
C    INITIALIZATION OR REINITIALISATION
            IWARM=1
            IA1=          1279
            IC1=          351762
            M1=          1664557
            IA2=           2011
            IC2=          221592
            M2=          1048583
            IA3=          15091
            IC3=           6171
            M3=          29201
            IX1=MOD(-IDUM,M1)
            IX1=MOD(IA1*IX1+IC1,M1)
            IX2=MOD(IX1,M2)
            IX1=MOD(IA1*IX1+IC1,M1)
            IX3=MOD(IX1,M3)
            RM1=1./FLOAT(M1)
            RM2=1./FLOAT(M2)
            DO 10 J=1,31
                IX1=MOD(IA1*IX1+IC1,M1)
                IX2=MOD(IA2*IX2+IC2,M2)
10        RDM(J)=(FLOAT(IX1)+FLOAT(IX2)*RM2)*RM1
            ENDIF
C
C    GENERATE NEXT NUMBER IN SEQUENCE
            IF(IWARM.EQ.0) GOTO 901
            IX1=MOD(IA1*IX1+IC1,M1)
            IX2=MOD(IA2*IX2+IC2,M2)
            IX3=MOD(IA3*IX3+IC3,M3)
            J=1+(31*IX3)/M3
            RAN2=RDM(J)
            RDM(J)=(FLOAT(IX1)+FLOAT(IX2)*RM2)*RM1
            RETURN
901    PRINT 9010
9010   FORMAT('    RAN2: LACK OF ITINIALISATION')
        STOP

```

```

      END
C
C
C      *****      SPECIAL FUNCTIONS
C
C      DOUBLE PRECISION FUNCTION DILOG(X)
C
C      SPENCE'S DILOGARITHM IN DOUBLE PRECISION
C
      IMPLICIT REAL*8 (A-H,O-Z)
      Z=-1.644934066848226
      IF(X .LT.-1.0) GO TO 1
      IF(X .LE. 0.5) GO TO 2
      IF(X .EQ. 1.0) GO TO 3
      IF(X .LE. 2.0) GO TO 4
      Z=3.289868133696453
1  T=1.0/X
   S=-0.5
   Z=Z-0.5*DLOG(DABS(X))**2
   GO TO 5
2  T=X
   S=0.5
   Z=0.
   GO TO 5
3  DILOG=1.644934066848226
   RETURN
4  T=1.0-X
   S=-0.5
   Z=1.644934066848226-DLOG(X)*DLOG(DABS(T))
5  Y=2.666666666666667*T+0.666666666666667
   B=      0.00000 00000 00001
   A=Y*B +0.00000 00000 00004
   B=Y*A-B+0.00000 00000 00011
   A=Y*B-A+0.00000 00000 00037
   B=Y*A-B+0.00000 00000 00121
   A=Y*B-A+0.00000 00000 00398
   B=Y*A-B+0.00000 00000 01312
   A=Y*B-A+0.00000 00000 04342
   B=Y*A-B+0.00000 00000 14437
   A=Y*B-A+0.00000 00000 48274
   B=Y*A-B+0.00000 00001 62421
   A=Y*B-A+0.00000 00005 50291
   B=Y*A-B+0.00000 00018 79117
   A=Y*B-A+0.00000 00064 74338
   B=Y*A-B+0.00000 00225 36705
   A=Y*B-A+0.00000 00793 87055
   B=Y*A-B+0.00000 02835 75385
   A=Y*B-A+0.00000 10299 04264
   B=Y*A-B+0.00000 38163 29463
   A=Y*B-A+0.00001 44963 00557
   B=Y*A-B+0.00005 68178 22718
   A=Y*B-A+0.00023 20021 96094
   B=Y*A-B+0.00100 16274 96164

```

```

A=Y*B-A+0.00468 63619 59447
B=Y*A-B+0.02487 93229 24228
A=Y*B-A+0.16607 30329 27855
A=Y*A-B+1.93506 43008 69969
DILOG=S*T*(A-B)+Z
RETURN
END

```

c

```

SUBROUTINE pzext0(iest,xest,yest,yz,dy,nv)
implicit none
INTEGER iest,nv,IMAX,NMAX
REAL*8 xest,dy(nv),yest(nv),yz(nv)
PARAMETER (IMAX=13,NMAX=50)
INTEGER j,k1
REAL*8 delta,f1,f2,q,d(NMAX),qcol(NMAX,IMAX),x(IMAX)
SAVE qcol,x
x(iest)=xest
do 11 j=1,nv
    dy(j)=yest(j)
    yz(j)=yest(j)
11 continue
if(iest.eq.1) then
    do 12 j=1,nv
        qcol(j,1)=yest(j)
12 continue
else
    do 13 j=1,nv
        d(j)=yest(j)
13 continue
    do 15 k1=1,iest-1
        delta=1.d0/(x(iest-k1)-xest)
        f1=xest*delta
        f2=x(iest-k1)*delta
        do 14 j=1,nv
            q=qcol(j,k1)
            qcol(j,k1)=dy(j)
            delta=d(j)-q
            dy(j)=f1*delta
            d(j)=f2*delta
            yz(j)=yz(j)+dy(j)
14 continue
15 continue
    do 16 j=1,nv
        qcol(j,iest)=dy(j)
16 continue
endif
return
END

```

c

c

```

complex*16 function zdigamma(z)
implicit none
complex*16 z,psi,psipr1,psipr2
call mkpsi(z,psi,psipr1,psipr2)

```

```

        zdigamma=psi
    end
c
    subroutine mkpsi(z,psi,psipr1,psipr2)
    implicit none
    complex*16 tmp,tmps2,tmps3,tmp0,tmp1,tmp2,ser0,ser1,ser2,ser3,
    .          zz,z,psi,psipr1,psipr2,off0,off1,off2,zcf,ser02,ser12,
    .          z1,z2
    real*8 cof(6),re1
    integer i
    data cof/76.18009173d0,-86.50532033d0,24.01409822d0,
    .      -1.231739516d0,.120858003d-2,-.536382d-5/
    save
    zz=z
    off0=cmplx(0.d0,0.d0,kind=kind(0d0))
    off1=cmplx(0.d0,0.d0,kind=kind(0d0))
    off2=cmplx(0.d0,0.d0,kind=kind(0d0))
5  re1=real(zz)
    if (re1.le.0.d0) then
        off0=off0+1.d0/zz
        z1=zz*zz
        off1=off1-1.d0/z1
        z2=z1*zz
        off2=off2+2.d0/z2
        zz=zz+(1.d0,0.d0)
        goto 5
    endif
    tmp=zz+cmplx(4.5d0,0.d0,kind=kind(0d0))
    tmps2=tmp*tmp
    tmps3=tmp*tmps2
    tmp0=(zz-cmplx(0.5d0,0.d0,kind=kind(0d0)))/tmp+log(tmp)
u    -cmplx(1.d0,0.d0,kind=kind(0d0))
    tmp1=(5.d0,0.d0)/tmps2+1.d0/tmp
    tmp2=(-10.0d0,0.d0)/tmps3-1.d0/tmps2
    ser0=cmplx(1.d0,0.d0,kind=kind(0d0))
    ser1=cmplx(0.d0,0.d0,kind=kind(0d0))
    ser2=cmplx(0.d0,0.d0,kind=kind(0d0))
    ser3=cmplx(0.d0,0.d0,kind=kind(0d0))
    do 10 i=1,6
        zcf=cof(i)/zz
        ser0=ser0+zcf
        zcf=zcf/zz
        ser1=ser1+zcf
        zcf=zcf/zz
        ser2=ser2+zcf
        zcf=zcf/zz
        ser3=ser3+zcf
        zz=zz+(1.d0,0.d0)
10  continue
    ser1=-ser1
    ser2=2.d0*ser2
    ser3=-6.d0*ser3
    ser02=ser0*ser0
    ser12=ser1*ser1

```

```

        psi=tmp0+ser1/ser0-off0
        psipr1=tmp1+(ser2*ser0-ser12)/ser02-off1
        psipr2=tmp2+(ser3*ser02-3.d0*ser2*ser1*ser0+2.d0*ser12*ser1)
        .          /ser02/ser0-off2
        return
    end
<toppik_axial.f>≡
! WHIZARD <Version> <Date>

! TOPPIK code by M. Jezabek, T. Teubner (v1.1, 1992), T. Teubner (1998)
!
! NOTE: axial part (p-wave) only
!
! FB: -commented out numerical recipes code for hypergeometric 2F1
!      included in hypgeo.f90;
!      -replaced function 'cdabs' by 'abs';
!      -replaced function 'dabs' by 'abs';
!      -replaced function 'dimag' by 'aimag';
!      -replaced function 'dcmplx(,)' by 'cmplx(,kind=kind(0d0))';
!      -replaced function 'dreal' by 'real';
!      -replaced function 'dlog' by 'log';
!      -replaced function 'dsqrt' by 'sqrt';
!      -renamed function 'a' to 'aax'
!      -renamed function 'fretil1' to 'fretil1ax'
!      -renamed function 'fretil2' to 'fretil2ax'
!      -renamed function 'fimtil1' to 'fimtil1ax'
!      -renamed function 'fimtil2' to 'fimtil2ax'
!      -renamed function 'freal' to 'frealax'
!      -renamed function 'fim' to 'fimax'
!      -renamed subroutine 'vhat' to 'vhatax'
!      -renamed subroutine 'sae' to 'saeax'
!      -commented out many routines identically defined in 'toppik.f'
!      -modified 'tttoppikaxial' to catch unstable runs.
!
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!

C *****
C      Version tuned to provide 0(1%) relative accuracy for Coulomb axial
C      vertex function at first and second order (search for 'cctt'):
C      - integrals A(p), Vhat, Vhhat provided analytically w/out cut-off
C      - grid range fixed to 0.1 ... 10**6 absolut
C      - and grid size enhanced to 600 points (900 foreseen in arrays).
C
C      This provides a compromise between stability and accuracy:
C      We need a relatively high momentum resolution and large maximal
C      momenta to achieve a ~1 percent accuracy, but the method of
C      direct inversion of the discretised integral equation for objects
C      whose integral is divergent induces instabilities at small
C      momenta. As the behaviour there is known, they can be cut off and
C      the vertex function fixed by hand; but limiting the grid
C      further would impact on the accuracy.
C      22.3.2017, tt
C *****
C

```

```

c Working version with all the different original potentials
c like  $(p^2+q^2)/|p-q|^2$ , not transformed in terms of delta and  $1/r^2$ ;
c accuracy  $\text{eps}=1.d-3$  possible (only), but should be save, 13.8.'98, tt.
c cleaned up a bit, 24.2.1999, tt.
c
c *****
c
c
c      subroutine tttoppikaxial(xenergy,xtm,xtg,xalphas,xscale,xcutn,
u      xcutv,
u      xc0,xc1,xc2,xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2,
u      xkincm,xkinca,jknflg,jgcflg,xkincv,jvflg,
u      xim,xdi,np,xpp,xww,xsdsp,zftild)
c
c *****
c
c !! THIS IS NOT A PUBLIC VERSION !!
c
c !!! Only P wave result given as output!!! 9.4.1999, tt.
c
c -- Calculation of the Green function in momentum space by solving the
c    Lippmann-Schwinger equation
c     $F(p) = G_0(p) + G_0(p) \int_0^{\text{xcutn}} V(p,q) q.p/p^2 F(q) dq$ 
c
c -- Written by Thomas Teubner, Hamburg, November 1998
c    * Based on TOPPIK Version 1.1
c      from M. Jezabek and TT, Karlsruhe, June 1992
c    * Version originally for non-constant top-width
c    * Constant width supplied here
c    * No generator included
c
c -- Use of double precision everywhere
c
c -- All masses, momenta, energies, widths in GeV
c
c -- Input parameters:
c
c    xenergy  :  $E=\text{Sqrt}[s]-2*\text{topmass}$ 
c    xtm      : topmass (in the Pole scheme)
c    xtg      : top-width
c    xalphas  :  $\alpha_s^{\{\text{MSbar},n_f=5\}}(\text{xscale})$ 
c    xscale   : soft scale  $\mu_{\{\text{soft}\}}$ 
c    xcutn    : numerical UV cutoff on all momenta
c              (UV cutoff of the Gauss-Legendre grid)
c    xcutv    : renormalization cutoff on the
c              delta-, the  $(p^2+q^2)/(p-q)^2$ -, and the
c               $1/r^2-[1/|p-q|]$ -potential:
c              if  $(\max(p,q).\text{ge.xcutv})$  then the three potentials
c              are set to zero in the Lippmann-Schwinger equation
c    xc0      : 0th order coefficient for the Coulomb potential,
c              see calling example above
c    xc1      : 1st order coefficient for the Coulomb potential
c    xc2      : 2nd order coefficient for the Coulomb potential
c    xcdeltc  : constant of the delta(r)-

```

```

c          [= constant in momentum space-] potential
c  xcdeltl : constant for the additional  $\log(q^2/\mu^2)$ -part of the
c            delta-potential:
c             $xcdeltc*1 + xcdeltl*\log(q^2/\mu^2)$ 
c  xcfullc : constant of the  $(p^2+q^2)/(p-q)^2$ -potential
c  xcfulll : constant for the additional  $\log(q^2/\mu^2)$ -part of the
c             $(p^2+q^2)/(p-q)^2$ -potential
c  xcrm2   : constant of the  $1/r^2-[1/|p-q|]$ -potential
c  xkincm  : } kinetic corrections in the 0th order Green function:
c  xkinca  : }  $G_0(p) := 1/[E+i\Gamma_t-p^2/m_t]*(1+xkincm)+xkinca$ 
c            !!! WATCH THE SIGN IN  $G_0$  !!!
c  jknflg  : flag for these kinetic corrections:
c            0 : no kinetic corrections applied
c            1 : kinetic corrections applied with cutoff xcutv
c              for xkinca only
c            2 : kinetic corrections applied with cutoff xcutv
c              for xkinca AND xkincm
c  jgcflg  : flag for  $G_0(p)$  in the LS equation:
c            0 (standard choice) :  $G_0(p)$  as given above
c            1 (for TIPT)         :  $G_0(p) = G_c^{\{0\}}(p)$  the 0th
c                                  order Coulomb Green function
c                                  in analytical form; not for
c                                  momenta  $p > 1000*topmass$ 
c  xkincv  : additional kinematic vertexcorrection in  $G_0$ , see below:
c  jvflg   : flag for the additional vertexcorrection xkincv in the
c            'zeroth order'  $G_0(p)$  in the LS-equation:
c            0 : no correction, means  $G = G_0 + G_0 \int V G$ 
c              with  $G_0 = 1/[E+i\Gamma_t-p^2/m_t]*(1+xkincm)+xkinca$ 
c            1 : apply the correction in the LS equation as
c               $G = G_0 + xkincv*p^2/m_t^2/[E+i\Gamma_t-p^2/m_t] +$ 
c               $G_0 \int V G$ 
c              and correct the integral over  $\text{Im}[G(p)]$  to get  $\sigma_{tot}$ 
c              from the optical theorem by the same factor.
c              The cutoff xcutv is applied for these corrections.
c
c -- Output:
c
c  xim      :  $R^{\{P \text{ wave}\}}_{\{ttbar\}}$  from the imaginary part of the Green
c            function
c  xdi      :  $R^{\{P \text{ wave}\}}_{\{ttbar\}}$  from the integral over the momentum
c            distribution:  $\int_0^{xcutv} dp p^3/m_t * |F(p,E)|^2$ 
c  np       : number of points used for the grid; fixed in tttoppik
c  xpp      : 1-dim array (max. 900 elements) giving the momenta of
c            the Gauss-Legendre grid (pp(i) in the code)
c  xww      : 1-dim array (max. 900 elements) giving the corresponding
c            Gauss-Legendre weights for the grid
c  xdsdp    : 1-dim array (max. 900 elements) giving the
c            momentum distribution of top:  $d\sigma^{\{P \text{ wave}\}}/dp$ ,
c            normalized to R,
c            at the momenta of the Gauss-Legendre grid xpp(i)
c  zftild   : 1-dim array (max. 900 elements) of COMPLEX*16 numbers
c            giving the vertex function  $K_A$  for the P-wave
c            at the momenta of the grid.
c            Then  $F(p) = K_A(p) * G_0(p)$  corresponding to  $G = K_V * G_0$ .

```

```

C
C *****
C
C
C      implicit none
C      real*8
C
C      u      pi,energy,vzero,eps,
C      u      pp,
C      u      tmass,tgamma,zmass,alphas,alamb5,
C      u      wmass,wgamma,bmass,GFERMI,hmass,
C      u      xx,critp,consde,
C      u      w1,w2,sig1,sig2,const,
C      u      gtpcor,etot,
C      u      xenergy,xtm,xtg,xalphas,xscale,xc0,xc1,xc2,xim,xdi,
C      u      xaai,xaad,xsdp,xpp,xww,
C      u      cplas,scale,c0,c1,c2,cdeltc,cdeltl,cfullc,cfulll,crm2,
C      u      chiggs,xcutn,dcut,xcutv,
C      u      xp,xpmax,
C      u      kincom,kincoa,kincov,xkincm,xkinca,xkincv,
C      u      xcdeltc,xcdeltl,xcfullc,xcfulll,xcrm2
C      complex*16 bb,vec,gg,a1,aax,g0,g0c,zvfct,zftild
C      integer i,n,nmax,npot,np,gcflg,kinflg,jknflg,jgcflg,
C      u      jvflg,vflag
C      parameter (nmax=900)
C      dimension pp(nmax),bb(nmax),vec(nmax),xx(nmax),gg(nmax),
C      u      w1(nmax),w2(nmax),a1(nmax),
C      u      xsdp(nmax),xpp(nmax),xww(nmax),
C      u      zvfct(nmax),zftild(nmax)
C
C      external aax,gtpcor,g0,g0c
C
C      common/ovalco/ pi, energy, vzero, eps, npot
C      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
C      $ WMASS,WGAMMA,BMASS,GFERMI,hmass
C      common/cplcns/cplas,scale,c0,c1,c2,
C      u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
C      common/mom/ xp,xpmax,dcut
C      common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
C
C      pi=3.141592653589793238d0
C
C      c Number of points to evaluate on the integral equation
C      c (<=900 and n mod 3 = 0 !!):
C      n=600
C      np=n
C
C      c For second order potential with free parameters:
C
C      npot=5
C      c Internal accuracy for TOPPIK, the reachable limit may be smaller,
C      c depending on the parameters. But increase in real accuracy only
C      c in combination with large number of points.
C      eps=1.d-3
C      c Some physical parameters:

```



```

        wgamma=2.07d0
        zmass=91.187d0
        wmass=80.33d0
        bmass=4.7d0
c
c Input:
        tmass=xm
        energy=xenergy
        tgamma=xtg
        cplas=xalphas
        scale=xscale
        c0=xc0
        c1=xc1
        c2=xc2
        cdeltc=xcdeltc
        cdeltl=xcdeltl
        cfullc=xcfullc
        cfulll=xcfulll
        crm2=xcrm2
        kincom=xkincom
        kincoa=xkincoa
        kincov=xkincov
        kinflg=jknflg
        gcflg=jgcflg
        vflag=jvflg
c
        alphas=xalphas
c
c Cut for divergent potential-terms for large momenta in the function vhatx
c and in the integrals aax(p):
        dcut=xcutv
c
c Numerical Cutoff of all momenta (maximal momenta of the grid):
        xpmx=xcutn
        if (dcut.gt.xpmx) then
            write(*,*) ' dcut > xpmx  makes no sense! Stop.'
            stop
        endif
c
c Not needed for the fixed order potentials:
        alamb5=0.2d0
c
c      WRITE(*,*) 'INPUT TGAMMA=',TGAMMA
c Needed in subroutine GAMMAT:
        GFERMI=1.16637d-5
c      CALL GAMMAT
c      WRITE(*,*) 'CALCULATED TGAMMA=',TGAMMA
c
        etot=2.d0*tmass+energy
c
        if ((npot.eq.1).or.(npot.eq.3).or.(npot.eq.4).or.
            u      (npot.eq.5)) then
c For pure coulomb and fixed order potentials there is no delta-part:
            consde = 0.d0

```

```

        else if (npot.eq.2) then
c Initialize QCD-potential common-blocks and calculate constant multiplying
c the delta-part of the 'qcutted' potential in momentum-space:
c     call iniphc(1)
c     call vqdelc(consde)
c     write(*,*) ' Not supplied with this version. Stop.'
c     stop
        else
c     write (*,*) ' Potential not implemented! Stop. 1'
c     stop
        endif
c Delta-part of potential is absorbed by subtracting vzero from the
c original energy (shift from the potential to the free Hamiltonian):
vzero = consde / (2.d0*pi)**3
c     write (*,*) 'vzero=', vzero
c
c Find x-values pp(i) and weights w1(i) for the gaussian quadrature;
c care about large number of points in the important intervals:
c     if (energy-vzero.le.0.d0) then
cc     call gauleg(0.d0, 1.d0, pp, w1, n/3)
cc     call gauleg(1.d0, 5.d0, pp(n/3+1), w1(n/3+1), n/3)
cc     call gauleg(0.d0, 0.2d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c     call gauleg(0.d0, 5.d0, pp, w1, n/3)
c     call gauleg(5.d0, 20.d0, pp(n/3+1), w1(n/3+1), n/3)
c     call gauleg(0.d0, 0.05d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c     else
cc Avoid numerical singular points in the inner of the intervals:
c     critp = sqrt((energy-vzero)*tmass)
c     if (critp.le.1.d0) then
cc Gauss-Legendre is symmetric => automatically principal-value prescription:
c     call gauleg(0.d0, 2.d0*critp, pp, w1, n/3)
c     call gauleg(2.d0*critp, 20.d0, pp(n/3+1),
c     u     w1(n/3+1), n/3)
c     call gauleg(0.d0, 0.05d0, pp(2*n/3+1), w1(2*n/3+1), n/3)
c     else
cc Better behaviour at the border of the intervals:
c     call gauleg(0.d0, critp, pp, w1, n/3)
c     call gauleg(critp, 2.d0*critp, pp(n/3+1),
c     u     w1(n/3+1), n/3)
c     call gauleg(0.d0, 1.d0/(2.d0*critp), pp(2*n/3+1),
c     u     w1(2*n/3+1), n/3)
c     endif
c     endif
c
c Or different (simpler) method, good for V_JKT:
c     if (energy.le.0.d0) then
c     critp=tmass/3.d0
c     else
c     critp=max(tmass/3.d0,2.d0*sqrt(energy*tmass))
c     endif
c     call gauleg(0.d0, critp, pp, w1, 2*n/3)
c     call gauleg(1.d0/xpmax, 1.d0/critp, pp(2*n/3+1),
c     u     w1(2*n/3+1), n/3)
cctt Tuned March 2017 for best possible numerical behaviour of P-wave

```

```

        call gauleg(0.1d0, 2.d0, pp, w1, 10)
        call gauleg(2.d0, critp, pp(11), w1(11), 2*n/3-10)
        call gauleg(1.d-6, 1.d0/critp, pp(2*n/3+1),
u           w1(2*n/3+1), n/3)
c
c Do substitution  $p \Rightarrow 1/p$  for the last interval explicitly:
        do 10 i=2*n/3+1,n
            pp(i) = 1.d0/pp(i)
10         continue
c
c Reorder the arrays for the third interval:
        do 20 i=1,n/3
            xx(i) = pp(2*n/3+i)
            w2(i) = w1(2*n/3+i)
20         continue
        do 30 i=1,n/3
            pp(n-i+1) = xx(i)
            w1(n-i+1) = w2(i)
30         continue
c
c Calculate the integrals aax(p) for the given momenta pp(i)
c and store weights and momenta for the output arrays:
        do 40 i=1,n
            a1(i) = aax(pp(i)) !!! FB: can get stuck in original Toppik!
            !!! FB: abuse 'np' as a flag to communicate unstable runs
            if ( abs(a1(i)) .gt. 1d10 ) then
                np = -1
                return
            endif
            xpp(i)=pp(i)
            xww(i)=w1(i)
40         continue
        do 41 i=n+1,nmax
            xpp(i)=0.d0
            xww(i)=0.d0
41         continue
c
c Solve the integral-equation by solving a system of algebraic equations:
        call saeax(pp, w1, bb, vec, a1, n)
c
c (The substitution for the integration to infinity  $pp \Rightarrow 1/pp$ 
c is done already.)
        do 50 i=1,n
            zvfct(i)=bb(i)
            zftild(i)=vec(i)
            gg(i) = bb(i)*g0c(pp(i))
cc         gg(i) = (1.d0 + bb(i))*g0c(pp(i))
cc Urspruenglich anderes (Minus) VZ hier, dafuer kein Minus mehr bei der
cc Definition des WQs ueber Im G, 2.6.1998, tt.
cc         gg(i) = - (1.d0 + bb(i))*g0c(pp(i))
50         continue
c
c Normalisation on R:
        const = 8.d0*pi/tmass**2

```

```

c
c Proove of the optical theorem for the output values of saeax:
c Simply check if sig1 = sig2.
      sig1 = 0.d0
      sig2 = 0.d0
      xaai = 0.d0
      xaad = 0.d0
      do 60 i=1,n*2/3
c          write(*,*) 'check! p(',i,') = ',pp(i)
cvv
          if (pp(i).lt.dcut.and.vflag.eq.1) then
              sig1 = sig1 + w1(i)*pp(i)**2*aimag(gg(i)
cc          u          *(1.d0+kincov*(pp(i)/tmass)**2)
u          *(1.d0+kincov*g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i)))
u          )
          else
              sig1 = sig1 + w1(i)*pp(i)**2*aimag(gg(i))
          endif
          if (pp(i).lt.dcut.and.kinflg.ne.0) then
              sig2 = sig2 + w1(i)*pp(i)**2*abs(gg(i))**2 *
u              tgamma*gtpcor(pp(i),etot)
u              *(1.d0-pp(i)**2/2.d0/tmass**2)
cc          u              *tmass/sqrt(tmass**2+pp(i)**2)
c              xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
c          u              tgamma*gtpcor(pp(i),etot)
c          u              *(1.d0-pp(i)**2/2.d0/tmass**2)
c          u              /(2.d0*pi**2)*const
          else
              sig2 = sig2 + w1(i)*pp(i)**2*abs(gg(i))**2 *
u              tgamma*gtpcor(pp(i),etot)
c              xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
c          u              tgamma*gtpcor(pp(i),etot)
c          u              /(2.d0*pi**2)*const
          endif
          xdsdp(i)=pp(i)**4/tmass**2*abs(zftild(i)*g0c(pp(i)))**2
u              *tgamma*gtpcor(pp(i),etot)
u              /(2.d0*pi**2)*const
          xaai=xaai+w1(i)*pp(i)**4/tmass**2*
u              aimag(zftild(i)*g0c(pp(i)))
          xaad=xaad+w1(i)*pp(i)**4/tmass**2*
u              abs(zftild(i)*g0c(pp(i)))**2 *
u              tgamma*gtpcor(pp(i),etot)
c          write(*,*) 'xdsdp = ',xdsdp(i)
c          write(*,*) 'zvfct = ',zvfct(i)
c          write(*,*) 'zftild = ',zftild(i)
60      continue
c '*p**2' because of substitution p => 1/p in the integration of p**2*G(p)
c to infinity
      do 70 i=n*2/3+1,n
c          write(*,*) 'check! p(',i,') = ',pp(i)
cvv
          if (pp(i).lt.dcut.and.vflag.eq.1) then
              sig1 = sig1 + w1(i)*pp(i)**4*aimag(gg(i)
cc          u              *(1.d0+kincov*(pp(i)/tmass)**2)

```

```

u      *(1.d0+kincov*g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i)))
u      )
      else
        sig1 = sig1 + w1(i)*pp(i)**4*aimag(gg(i))
      endif
      if (pp(i).lt.dcut.and.kinflg.ne.0) then
        sig2 = sig2 + w1(i)*pp(i)**4*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
u          *(1.d0-pp(i)**2/2.d0/tmass**2)
cc      u          *tmass/sqrt(tmass**2+pp(i)**2)
c          xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
c      u          tgamma*gtpcor(pp(i),etot)
c      u          *(1.d0-pp(i)**2/2.d0/tmass**2)
c      u          /(2.d0*pi**2)*const
      else
        sig2 = sig2 + w1(i)*pp(i)**4*abs(gg(i))**2 *
u          tgamma*gtpcor(pp(i),etot)
c          xdsdp(i)=pp(i)**2*abs(gg(i))**2 *
c      u          tgamma*gtpcor(pp(i),etot)
c      u          /(2.d0*pi**2)*const
      endif
      xdsdp(i)=pp(i)**4/tmass**2*abs(zftild(i)*g0c(pp(i)))**2
u          *tgamma*gtpcor(pp(i),etot)
u          /(2.d0*pi**2)*const
      xaai=xaai+w1(i)*pp(i)**6/tmass**2*
u          aimag(zftild(i)*g0c(pp(i)))
      xaad=xaad+w1(i)*pp(i)**6/tmass**2*
u          abs(zftild(i)*g0c(pp(i)))**2 *
u          tgamma*gtpcor(pp(i),etot)
c      write(*,*) 'xdsdp = ',xdsdp(i)
c      write(*,*) 'zvfct = ',zvfct(i)
c      write(*,*) 'zftild = ',zftild(i)
70      continue
      do 71 i=n+1,nmax
        xdsdp(i)=0.d0
        zvfct(i)=(0.d0,0.d0)
        zftild(i)=(0.d0,0.d0)
71      continue
c
c Normalisation on R:
      sig1 = sig1 / (2.d0*pi**2) * const
      sig2 = sig2 / (2.d0*pi**2) * const
c
c The results from the momentum space approach finally are:
cc Jetzt Minus hier, 2.6.98, tt.
c      xim=-sig1
c      xdi=sig2
      xaai=-xaai / (2.d0*pi**2) * const
      xaad=xaad / (2.d0*pi**2) * const
c Output of P wave part only:
      xim=xaai
      xdi=xaad
c      write(*,*) 'vvi = ',-sig1,' . vvd = ',sig2
c      write(*,*) 'aai = ',xim,' . aad = ',xdi

```

```

c
c      end
c
c
c
c
c      complex*16 function aax(p)
c
c Neue Funktion fuer die Integrale aax(p), die hier im Falle Cutoff -> infinity
c fuer reine Coulombpotentiale vollstaendig analytisch loesbar sind.
c 22.3.2001, tt.
c
c      implicit none
c      complex*16 zi,zb,zlp,zlm,zalo,zanlo,zannlo,zahig,za
c      real*8
c
c      u      tmass,tgamma,zmass,alphas,alamb5,
c      u      wmass,wgamma,bmass,GFERMI,hmass,
c      u      pi,energy,vzero,eps,
c      u      p,zeta3,cf,ca,tf,xnf,b0,b1,a1,a2,cnspot,phiint,
c      u      cplas,scale,c0,c1,c2,
c      u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c      integer npot
c      parameter(zi=(0.d0,1.d0),zeta3=1.20205690316d0,
c      u      cf=4.d0/3.d0,ca=3.d0,tf=1.d0/2.d0,xnf=5.d0)
c
c      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
c $ WMASS,WGAMMA,BMASS,GFERMI,hmass
c      common/ovalco/ pi, energy, vzero, eps, npot
c      common/cplcns/cplas,scale,c0,c1,c2,
c      u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c
c      b0=11.d0-2.d0/3.d0*xnf
c      b1=102.d0-38.d0/3.d0*xnf
c
c      a1=31.d0/9.d0*ca-20.d0/9.d0*tf*xnf
c      a2=(4343.d0/162.d0+4.d0*pi**2-pi**4/4.d0+
c      u      22.d0/3.d0*zeta3)*ca**2-
c      u      (1798.d0/81.d0+56.d0/3.d0*zeta3)*ca*tf*xnf-
c      u      (55.d0/3.d0-16.d0*zeta3)*cf*tf*xnf+
c      u      (20.d0/9.d0*tf*xnf)**2
c
c      cnspot=-4.d0/3.d0*4.d0*pi
c      phiint=cnspot*alphas
c
c      zb=sqrt(tmass*cmlpx(energy,tgamma,kind=kind(0d0)))
c      zlp=log(zb+p)
c      zlm=log(zb-p)
c L0: no log in z-integral
c      zalo=zi*pi/2.d0/p*(zlp-zlm)
c from NL0: log in the z-integral
c      zanlo=pi/2.d0/p*(zlp-zlm)*(pi+zi*(zlp+zlm))
c from NNLO: log**2 in the z-integral
c      zannlo=pi/3.d0/p*(zlp-zlm)
c      u      *(3.d0*pi*(zlp+zlm)+2.d0*zi*(zlm**2+zlm*zlp+zlp**2))

```

```

c Sum of the Coulomb contributions:
      za=c0*zalo-c1*(zanlo-2.d0*dlog(scale)*zalo)
      u      +c2*(zannlo-4.d0*dlog(scale)*zanlo
      u      +4.d0*dlog(scale)**2*zalo)
c (Higgs) Yukawa contribution
cctt      zahig=zi*pi/2.d0/p*log((zb+p+zi*hmass)/(zb-p+zi*hmass))
c Alltogether:
cctt      aax=-tmass/(4.d0*pi**2)*(phiint*za+chiggs*zahig)
      aax=-tmass/(4.d0*pi**2)*phiint*za

c
c      write(*,*) 'aax(',p,')= ',aax
      end

c
      real*8 function fretillax(xk)
      implicit none
      real*8 xk, frealax
      external frealax
      fretillax = frealax(xk)
      end

c
      real*8 function fretil2ax(xk)
      implicit none
      real*8 xk, frealax
      external frealax
      fretil2ax = frealax(1.d0/xk) * xk**(-2)
      end

c
      real*8 function fimtil1ax(xk)
      implicit none
      real*8 xk, fimax
      external fimax
      fimtil1ax = fimax(xk)
      end

c
      real*8 function fimtil2ax(xk)
      implicit none
      real*8 xk, fimax
      external fimax
      fimtil2ax = fimax(1.d0/xk) * xk**(-2)
      end

c
      real*8 function frealax(xk)
      implicit none
      complex*16 vhatax
      real*8
      u      tmass,tgamma,zmass,alphas,alamb5,
      u      wmass,wgamma,bmass,GFERMI,
      u      pi, energy, vzero, eps,
      u      p,pmax, xk, gtpcor,dcut,hmass
      complex*16 g0,g0c
      integer npot
      COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
      $ WMASS,WGAMMA,BMASS,GFERMI,hmass
      common/ovalco/ pi, energy, vzero, eps, npot

```

```

        common/mom/ p,pmax,dcut
        external vhatax, g0, g0c, gtpcor
c
        frealax = real(g0c(xk)*vhatax(p, xk))
end
c
        real*8 function fimax(xk)
        implicit none
        complex*16 vhatax
        real*8
u          tmass,tgamma,zmass,alphas,alamb5,
u          wmass,wgamma,bmass,GFERMI,
u          pi, energy, vzero, eps,
u          p,pmax, xk, gtpcor,dcut,hmass
        complex*16 g0,g0c
        integer npot
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
        common/ovalco/ pi, energy, vzero, eps, npot
        common/mom/ p,pmax,dcut
        external vhatax, g0, g0c, gtpcor
        fimax = aimag(g0c(xk)*vhatax(p, xk))
end
c
c
        complex*16 function vhatax(p, xk)
c
        implicit none
        complex*16 zi
        real*8
u          tmass,tgamma,zmass,alphas,alamb5,
u          wmass,wgamma,bmass,GFERMI,
u          pi, energy, vzero, eps,
u          p, xk,
u          cnspot, phiint, AD8GLE,
u          pm, xkm,
c u          phfqcd, ALPHEF,
u          zeta3,cf,ca,tf,xnf,a1,a2,b0,b1,
u          cplas,scale,c0,c1,c2,
u          cdeltc,cdeltl,cfullc,cfulll,crm2,
u          xkpln1st,xkpln2nd,xkpln3rd,
u          pp,pmax,dcut,hmass,chiggs
        integer npot
        parameter(zi=(0.d0,1.d0))
        parameter(zeta3=1.20205690316d0,
u          cf=4.d0/3.d0,ca=3.d0,tf=1.d0/2.d0,
u          xnf=5.d0)
c
        external AD8GLE
c u          , phfqcd, ALPHEF
c
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
        common/ovalco/ pi, energy, vzero, eps, npot

```



```

common/pmaxkm/ pm, xkm
common/mom/ pp,pmax,dcut
common/cplcns/cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c
b0=11.d0-2.d0/3.d0*xnf
b1=102.d0-38.d0/3.d0*xnf
c
a1=31.d0/9.d0*ca-20.d0/9.d0*tf*xnf
a2=(4343.d0/162.d0+4.d0*pi**2-pi**4/4.d0+
u      22.d0/3.d0*zeta3)*ca**2-
u      (1798.d0/81.d0+56.d0/3.d0*zeta3)*ca*tf*xnf-
u      (55.d0/3.d0-16.d0*zeta3)*cf*tf*xnf+
u      (20.d0/9.d0*tf*xnf)**2
c
pm=p
xkm=xk
cnspot=-4.d0/3.d0*4.d0*pi
c
if (p/xk.le.1.d-5.and.p.le.1.d-5) then
  xkpln1st=2.d0
  xkpln2nd=-4.d0*log(scale/xk)
  xkpln3rd=-6.d0*log(scale/xk)**2
else if (xk/p.le.1.d-5.and.xk.le.1.d-5) then
  xkpln1st=2.d0*(xk/p)**2
  xkpln2nd=-4.d0*(xk/p)**2*log(scale/p)
  xkpln3rd=-6.d0*(xk/p)**2*log(scale/p)**2
else
c      xkpln1st=xk/p*log(abs((p+xk)/(p-xk)))
      xkpln1st=xk/p*(log(p+xk)-log(abs(p-xk)))
cctt sign checked again, 2.2.2017, tt.
      xkpln2nd=xk/p*(-1.d0)*(log(scale/(p+xk))**2-
u      log(scale/abs(p-xk))**2)
      xkpln3rd=xk/p*(-4.d0/3.d0)*(log(scale/(p+xk))**3-
u      log(scale/abs(p-xk))**3)
endif
c
c      if (npot.eq.2) then
c      if (p/xk.le.1.d-5.and.p.le.1.d-5) then
c      vhatax = 2.d0 * cnspot * ALPHEF(xk)
c      else if (xk/p.le.1.d-5.and.xk.le.1.d-5) then
c      vhatax = 2.d0 * cnspot * xk**2 / p**2 * ALPHEF(p)
c      else
c      phiint = cnspot * (AD8GLE(phfqcd, 0.d0, 0.3d0, 1.d-5)
c      u      +AD8GLE(phfqcd, 0.3d0, 1.d0, 1.d-5))
c      vhatax = xk / p * log(abs((p+xk)/(p-xk))) * phiint
c      endif
c      else
c      if (npot.eq.1) then
c      c0=1.d0
c      c1=0.d0
c      c2=0.d0
c      else if (npot.eq.3) then
c      c0=1.d0+alphas/(4.d0*pi)*a1

```

```

c1=alphas/(4.d0*pi)*b0
c2=0
else if (npot.eq.4) then
c0=1.d0+alphas/(4.d0*pi)*a1+(alphas/(4.d0*pi))**2*a2
c1=alphas/(4.d0*pi)*b0+
u      (alphas/(4.d0*pi))**2*(b1+2.d0*b0*a1)
c2=(alphas/(4.d0*pi))**2*b0**2
else if (npot.eq.5) then
else
write (*,*) ' Potential not implemented! Stop. 3'
stop
endif
phiint=cnspt*alphas
c
c      if ((xk+p).le.dcut) then
c          vhatax=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      u          -1.d0/2.d0*(1.d0+2.d0*ca/cf)
c      u          *(pi*cf*alphas)**2/tmass
c      u          *xk/p*(p+xk-abs(xk-p))
c      else if (abs(xk-p).lt.dcut) then
c          vhatax=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      u          -1.d0/2.d0*(1.d0+2.d0*ca/cf)
c      u          *(pi*cf*alphas)**2/tmass
c      u          *xk/p*(dcut-abs(xk-p))
c      else if (dcut.le.abs(xk-p)) then
c          vhatax=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      else
c          write(*,*) ' Not possible! Stop.'
c          stop
c      endif
c
c      ctt
c      Cut not applied here, should be left hard-wired in gauleg for stability of axial part. March 201
c      if (max(xk,p).lt.dcut) then
c      Coulomb + first + second order corrections:
c          vhatax=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      All other potentials:
c      u          +cdeltc*2.d0*xk**2
c      u          +cdeltl*xk/p/2.d0*(
c      u          (p+xk)**2*(log(((p+xk)/scale)**2)-1.d0)-
c      u          (p-xk)**2*(log(((p-xk)/scale)**2)-1.d0))
c      u          +cfullc*(p**2+xk**2)*xkpln1st
c      u          +cfulll*(p**2+xk**2)*xk/p/4.d0*
c      u          (log(((p+xk)/scale)**2)**2-
c      u          log(((p-xk)/scale)**2)**2)
c      u          +crm2*xk/p*(p+xk-abs(xk-p))
c      else
c          vhatax=phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd)
c      endif
c      endif
c      endif
c
c      end
c
c

```

```

complex*16 function vhat(p, xk)
c
    implicit none
    complex*16 zi
    real*8
u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      p, xk,
u      cnspot, phiint, AD8GLE,
u      pm, xkm,
u      zeta3,cf,ca,tf,xnf,a1,a2,b0,b1,
u      cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,cfulll,crm2,
u      xkpln1st,xkpln2nd,
u      pp,pmax,dcut,hmass,chiggs
    integer npot
    parameter(zi=(0.d0,1.d0))
    parameter(zeta3=1.20205690316d0,
u          cf=4.d0/3.d0,ca=3.d0,tf=1.d0/2.d0,
u          xnf=5.d0)
c
    external AD8GLE
c
    COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
    common/ovalco/ pi, energy, vzero, eps, npot
    common/pmaxkm/ pm, xkm
    common/mom/ pp,pmax,dcut
    common/cplcns/cplas,scale,c0,c1,c2,
u      cdeltc,cdeltl,cfullc,cfulll,crm2,chiggs
c
    b0=11.d0-2.d0/3.d0*xnf
    b1=102.d0-38.d0/3.d0*xnf
c
    a1=31.d0/9.d0*ca-20.d0/9.d0*tf*xnf
    a2=(4343.d0/162.d0+4.d0*pi**2-pi**4/4.d0+
u      22.d0/3.d0*zeta3)*ca**2-
u      (1798.d0/81.d0+56.d0/3.d0*zeta3)*ca*tf*xnf-
u      (55.d0/3.d0-16.d0*zeta3)*cf*tf*xnf+
u      (20.d0/9.d0*tf*xnf)**2
c
    pm=p
    xkm=xk
    cnspot=-4.d0/3.d0*4.d0*pi
c
    if (npot.eq.1) then
        c0=1.d0
        c1=0.d0
        c2=0.d0
    else if (npot.eq.3) then
        c0=1.d0+alphas/(4.d0*pi)*a1
        c1=alphas/(4.d0*pi)*b0
        c2=0

```

```

        else if (npot.eq.4) then
            write(*,*) '2nd order Coulomb in Vhhat not implemented yet.'
            stop
            c0=1.d0+alphas/(4.d0*pi)*a1+(alphas/(4.d0*pi))**2*a2
            c1=alphas/(4.d0*pi)*b0+
u            (alphas/(4.d0*pi))**2*(b1+2.d0*b0*a1)
            c2=(alphas/(4.d0*pi))**2*b0**2
            else if (npot.eq.5) then
                else
                    write(*,*) ' Potential not implemented! Stop. 4'
                    stop
                endif
            phiint=cnspot*alphas
c
cctt No cut-off description used here either.
c            if (max(xk,p).lt.dcut) then
cctt Pure Coulomb in first order and second order only:
c
c            xkpln1st=-(xk/p)**2*(1.d0+(xk**2+p**2)/(2.d0*xk*p)*
u            (dlog(dabs(p-xk))-dlog(p+xk)))
c            xkpln1st=-(xk/p)**2*(1.d0+(xk**2+p**2)/(4.d0*xk*p)*
c            u            (dlog((p-xk)**2)-2.d0*dlog(p+xk)))
c
c            xkpln2nd=((xk/p)**2/2.d0+xk*(xk**2+p**2)/8.d0/p**3*
u            (dlog((p-xk)**2)-2.d0*dlog(p+xk)))*
u            (-2.d0+dlog((xk-p)**2/scale**2)
u            +dlog((xk+p)**2/scale**2))
c
cctt 3rd order not yet.            xkpln3rd=
            if (c2.ne.0.d0) then
                write(*,*) ' Vhhat: 2nd order not implemented yet. Stop.'
                stop
            endif
c
cctt            vhhath=dcmplx(phiint*(c0*xkpln1st+c1*xkpln2nd+c2*xkpln3rd),
cctt            u            0.d0)
cctt            vhhath=cmplx(phiint*(c0*xkpln1st+c1*xkpln2nd),
u            0.d0,kind=kind(0d0))
c            else
c            vhhath=(0.d0,0.d0)
c            endif
c
c            end
c
c
c
c
c --- Routines for solving linear equations and matrix inversion (complex) ---
c
c            subroutine saeax(pp, w1, bb, vec, a1, n)
c
c            implicit none
c            complex*16 vhatax,vhhath
c            real*8

```

```

u      tmass,tgamma,zmass,alphas,alamb5,
u      wmass,wgamma,bmass,GFERMI,
u      pi, energy, vzero, eps,
u      d, d1, pp, w1, gtpcor,hmass,
u      xp,xpmax,dcut,kincom,kincoa,kincov
complex*16 aax, a1, bb, vec, ff, kk, cw, svw, g0, g0c
integer i, j, npot, n, nmax, indx,kinflg,gcflg,vflag
parameter (nmax=900)
dimension bb(nmax),vec(nmax),ff(nmax,nmax),kk(nmax,nmax),
u      pp(nmax),w1(nmax),indx(nmax),cw(nmax),a1(nmax)
c
COMMON/PHCONS/TMASS,TGAMMA,ZMASS,ALPHAS,ALAMB5,
$ WMASS,WGAMMA,BMASS,GFERMI,hmass
common/ovalco/ pi, energy, vzero, eps, npot
common/mom/ xp,xpmax,dcut
common/g0inf/kincom,kincoa,kincov,kinflg,gcflg,vflag
c
external aax, vatax, gtpcor, g0, g0c, vhat
c
do 10 i=1,n*2/3
cw(i) = w1(i) / (4.d0*pi**2) * g0c(pp(i))
c      cw(i) = w1(i) / (4.d0*pi**2 *
c      u      (cmplx(energy-vzero, tgamma*
c      u      gtpcor(pp(i),2.d0*tmass+energy),
c      u      kind=kind(0d0))-pp(i)**2/tmass))
10 continue
do 20 i=n*2/3+1,n
cw(i) = w1(i) / (4.d0*pi**2) * g0c(pp(i)) * pp(i)**2
c      cw(i) = w1(i) / (4.d0*pi**2 *
c      u      (cmplx(energy-vzero, tgamma*
c      u      gtpcor(pp(i),2.d0*tmass+energy),kind=kind(0d0)) /
c      u      pp(i)**2 - 1.d0/tmass))
20 continue
c
do 30 i=1,n
cc      bb(i) = a1(i)
cvv
      if (pp(i).lt.dcut.and.vflag.eq.1) then
c          bb(i) = cmplx(1.d0+kincov*(pp(i)/tmass)**2,0.d0,
c      u          kind=kind(0d0))
          bb(i)=1.d0+kincov*
u          g0(pp(i))*(pp(i)/tmass)**2/g0c(pp(i))
      else
          bb(i) = (1.d0,0.d0)
      endif
c
c Without extra kinematic corrections:
      vec(i)=(1.d0,0.d0)
c
      svw = (0.d0,0.d0)
do 40 j=1,n
      if (i.ne.j) then
          ff(i,j) = - vatax(pp(i),pp(j)) * cw(j)
          kk(i,j) = - vhat(pp(i),pp(j)) * cw(j)

```

```

                svw = svw + ff(i,j)
            endif
40          continue
            ff(i,i) = 1.d0 - a1(i) - svw
            kk(i,i) = ff(i,i)
30        continue
c
            call zldcmp(ff, n, nmax, indx, d)
            call zldcmp(kk, n, nmax, indx, d1)
            call zlbksb(ff, n, nmax, indx, bb)
            call zlbksb(kk, n, nmax, indx, vec)
c
            end
c
c
c
<ttv_formfactors.f90>≡
<File header>

module ttv_formfactors

    use kinds
    <Use debug>
    use constants
    use numeric_utils
    use physics_defs, only: CF, CA, TR
    use sm_physics
    use lorentz
    use interpolation
    use nr_tools
    use io_units, only: free_unit, given_output_unit
    use string_utils
    use iso_varying_string, string_t => varying_string
    use system_dependencies
    use, intrinsic :: iso_fortran_env !NODEP!
    use diagnostics
    <Standard module head>
    save

    <ttv_formfactors: public>

    <ttv_formfactors: parameters>

    <ttv_formfactors: types>

    <ttv_formfactors: global variables>

    <ttv_formfactors: interfaces>

contains

    <ttv_formfactors: procedures>

end module ttv_formfactors

```

```

<ttv formfactors: public>≡
    public :: onshell_projection_t

<ttv formfactors: types>≡
    type :: onshell_projection_t
        logical :: production
        logical :: decay
        logical :: width
        logical :: boost_decay
    contains
        <ttv formfactors: onshell projection: TBP>
    end type onshell_projection_t

<ttv formfactors: onshell projection: TBP>≡
    procedure :: debug_write => onshell_projection_debug_write

<ttv formfactors: procedures>≡
    subroutine onshell_projection_debug_write (onshell_projection)
        class(onshell_projection_t), intent(in) :: onshell_projection
        if (debug_on) call msg_debug (D_THRESHOLD, "onshell_projection%production", &
            onshell_projection%production)
        if (debug_on) call msg_debug (D_THRESHOLD, "onshell_projection%decay", &
            onshell_projection%decay)
        if (debug_on) call msg_debug (D_THRESHOLD, "onshell_projection%width", &
            onshell_projection%width)
        if (debug_on) call msg_debug (D_THRESHOLD, "onshell_projection%boost_decay", &
            onshell_projection%boost_decay)
    end subroutine onshell_projection_debug_write

<ttv formfactors: onshell projection: TBP>+≡
    procedure :: set_all => onshell_projection_set_all

<ttv formfactors: procedures>+≡
    pure subroutine onshell_projection_set_all (onshell_projection, flag)
        class(onshell_projection_t), intent(inout) :: onshell_projection
        logical, intent(in) :: flag
        onshell_projection%production = flag
        onshell_projection%decay = flag
    end subroutine onshell_projection_set_all

<ttv formfactors: onshell projection: TBP>+≡
    procedure :: active => onshell_projection_active

<ttv formfactors: procedures>+≡
    pure function onshell_projection_active (onshell_projection) result (active)
        logical :: active
        class(onshell_projection_t), intent(in) :: onshell_projection
        active = onshell_projection%production .or. &
            onshell_projection%decay
    end function onshell_projection_active

```

```

<ttv formfactors: types>+≡
  type :: helicity_approximation_t
    logical :: simple = .false.
    logical :: extra = .false.
    logical :: ultra = .false.
  contains
    <ttv formfactors: helicity approximation: TBP>
  end type helicity_approximation_t

<ttv formfactors: public>+≡
  public :: settings_t

<ttv formfactors: types>+≡
  type :: settings_t
    ! look what is set by initialized_parameters, bundle them in a class and rename to initialize
    logical :: initialized_parameters
    ! this belongs to init_threshold_phase_space_grid in phase_space_grid_t
    logical :: initialized_ps
    ! this belongs to the ff_grid_t, its usefulness is doubtful
    logical :: initialized_ff
    logical :: mpole_dynamic
    integer :: offshell_strategy
    logical :: factorized_computation
    logical :: interference
    logical :: only_interference_term
    logical :: nlo
    logical :: no_nlo_width_in_signal_propagators
    logical :: force_minus_one
    logical :: flip_relative_sign
    integer :: sel_hel_top = 0
    integer :: sel_hel_topbar = 0
    logical :: Z_disabled
    type(onshell_projection_t) :: onshell_projection
    type(helicity_approximation_t) :: helicity_approximation
  contains
    <ttv formfactors: settings: TBP>
  end type settings_t

<ttv formfactors: settings: TBP>≡
  procedure :: setup_flags => settings_setup_flags

<ttv formfactors: procedures>+≡
  ! TODO: (bcn 2016-03-21) break this up into a part regarding the
  ! FF grid and a part regarding the settings
  subroutine settings_setup_flags (settings, ff_in, offshell_strategy_in, &
    top_helicity_selection)
    class(settings_t), intent(inout) :: settings
    integer, intent(in) :: ff_in, offshell_strategy_in, top_helicity_selection
    logical :: bit_top, bit_topbar
    !!! RESUMMED_SWITCHOFF = - 2
    !!! MATCHED = -1, &
    SWITCHOFF_RESUMMED = ff_in < 0
    TOPPIK_RESUMMED = ff_in <= 1
    settings%nlo = btest(offshell_strategy_in, 0)

```



```

settings%factorized_computation = btest(offshell_strategy_in, 1)
settings%interference = btest(offshell_strategy_in, 2)
call settings%onshell_projection%set_all(btest(offshell_strategy_in, 3))
settings%no_nlo_width_in_signal_propagators = btest(offshell_strategy_in, 4)
settings%helicity_approximation%simple = btest(offshell_strategy_in, 5)
if (.not. settings%onshell_projection%active ()) then
    settings%onshell_projection%production = btest(offshell_strategy_in, 6)
    settings%onshell_projection%decay = btest(offshell_strategy_in, 7)
end if
settings%onshell_projection%width = .not. btest(offshell_strategy_in, 8)
settings%onshell_projection%boost_decay = btest(offshell_strategy_in, 9)
settings%helicity_approximation%extra = btest(offshell_strategy_in, 10)
settings%force_minus_one = btest(offshell_strategy_in, 11)
settings%flip_relative_sign = btest(offshell_strategy_in, 12)
if (top_helicity_selection > -1) then
    settings%helicity_approximation%ultra = .true.
    bit_top = btest (top_helicity_selection, 0)
    bit_topbar = btest (top_helicity_selection, 1)
    if (bit_top) then
        settings%sel_hel_top = 1
    else
        settings%sel_hel_top = -1
    end if
    if (bit_topbar) then
        settings%sel_hel_topbar = 1
    else
        settings%sel_hel_topbar = -1
    end if
end if
settings%only_interference_term = btest(offshell_strategy_in, 14)
settings%Z_disabled = btest(offshell_strategy_in, 15)
if (ff_in == MATCHED .or. ff_in == MATCHED_NOTSOHARD) then
    settings%onshell_projection%width = .true.
    settings%onshell_projection%production = .true.
    settings%onshell_projection%decay = .true.
    settings%factorized_computation = .true.
    settings%interference = .true.
    settings%onshell_projection%boost_decay = .true.
end if
if (debug_on) call msg_debug (D_THRESHOLD, "SWITCHOFF_RESUMMED", SWITCHOFF_RESUMMED)
if (debug_on) call msg_debug (D_THRESHOLD, "TOPPIK_RESUMMED", TOPPIK_RESUMMED)
if (debug_active (D_THRESHOLD)) &
    call settings%write ()
end subroutine settings_setup_flags

```

(ttv formfactors: settings: TBP)+≡
 procedure :: write => settings_write

(ttv formfactors: procedures)+≡
 subroutine settings_write (settings, unit)
 class(settings_t), intent(in) :: settings
 integer, intent(in), optional :: unit
 integer :: u
 u = given_output_unit (unit)

```

write (u, '(A,L1)') "settings%helicity_approximation%simple = ", &
    settings%helicity_approximation%simple
write (u, '(A,L1)') "settings%helicity_approximation%extra = ", &
    settings%helicity_approximation%extra
write (u, '(A,L1)') "settings%helicity_approximation%ultra = ", &
    settings%helicity_approximation%ultra
write (u, '(A,L1)') "settings%initialized_parameters = ", &
    settings%initialized_parameters
write (u, '(A,L1)') "settings%initialized_ps = ", &
    settings%initialized_ps
write (u, '(A,L1)') "settings%initialized_ff = ", &
    settings%initialized_ff
write (u, '(A,L1)') "settings%mpole_dynamic = ", &
    settings%mpole_dynamic
write (u, '(A,I5)') "settings%offshell_strategy = ", &
    settings%offshell_strategy
write (u, '(A,L1)') "settings%factorized_computation = ", &
    settings%factorized_computation
write (u, '(A,L1)') "settings%interference = ", settings%interference
write (u, '(A,L1)') "settings%only_interference_term = ", &
    settings%only_interference_term
write (u, '(A,L1)') "settings%Z_disabled = ", &
    settings%Z_disabled
write (u, '(A,L1)') "settings%nlo = ", settings%nlo
write (u, '(A,L1)') "settings%no_nlo_width_in_signal_propagators = ", &
    settings%no_nlo_width_in_signal_propagators
write (u, '(A,L1)') "settings%force_minus_one = ", settings%force_minus_one
write (u, '(A,L1)') "settings%flip_relative_sign = ", settings%flip_relative_sign
call settings%onshell_projection%debug_write ()
end subroutine settings_write

```

<ttv formfactors: settings: TBP>+≡

```

procedure :: use_nlo_width => settings_use_nlo_width

```

<ttv formfactors: procedures>+≡

```

pure function settings_use_nlo_width (settings, ff) result (nlo)
    logical :: nlo
    class(settings_t), intent(in) :: settings
    integer, intent(in) :: ff
    nlo = settings%nlo
end function settings_use_nlo_width

```

<ttv formfactors: public>+≡

```

public :: formfactor_t

```

<ttv formfactors: types>+≡

```

type :: formfactor_t
    logical :: active
contains
    <ttv formfactors: formfactor: TBP>
end type formfactor_t

```

<ttv formfactors: formfactor: TBP>≡

```

procedure :: activate => formfactor_activate

```

```

<ttv formfactors: procedures>+≡
  pure subroutine formfactor_activate (formfactor)
    class(formfactor_t), intent(inout) :: formfactor
    formfactor%active = .true.
  end subroutine formfactor_activate

```

```

<ttv formfactors: formfactor: TBP>+≡
  procedure :: disable => formfactor_disable

```

```

<ttv formfactors: procedures>+≡
  pure subroutine formfactor_disable (formfactor)
    class(formfactor_t), intent(inout) :: formfactor
    formfactor%active = .false.
  end subroutine formfactor_disable

```

This function actually returns \tilde{F} , i.e. $F - 1$.

```

<ttv formfactors: formfactor: TBP>+≡
  procedure :: compute => formfactor_compute

<ttv formfactors: procedures>+≡
  function formfactor_compute (formfactor, ps, vec_type, FF_mode) result (FF)
    complex(default) :: FF
    class(formfactor_t), intent(in) :: formfactor
    type(phase_space_point_t), intent(in) :: ps
    integer, intent(in) :: vec_type, FF_mode
    real(default) :: f
    if (threshold%settings%initialized_parameters .and. formfactor%active) then
      select case (FF_mode)
        case (MATCHED, MATCHED_NOTSOHARD, RESUMMED, RESUMMED_SWITCHOFF)
          FF = resummed_formfactor (ps, vec_type) - one
        case (MATCHED_EXPANDED)
          f = f_switch_off (v_matching (ps%sqrts, GAM_M1S))
          FF = - expanded_formfactor (f * AS_HARD, f * AS_HARD, ps, vec_type) &
            + resummed_formfactor (ps, vec_type)
        case (MATCHED_EXPANDED_NOTSOHARD)
          f = f_switch_off (v_matching (ps%sqrts, GAM_M1S))
          FF = - expanded_formfactor (f * alphas_notsohard (ps%sqrts), f * &
            alphas_notsohard (ps%sqrts), ps, vec_type) &
            + resummed_formfactor (ps, vec_type)
        case (EXPANDED_HARD)
          FF = expanded_formfactor (AS_HARD, AS_HARD, ps, vec_type) - one
        case (EXPANDED_NOTSOHARD)
          FF = expanded_formfactor (alphas_notsohard (ps%sqrts), &
            alphas_notsohard (ps%sqrts), ps, vec_type) - one
        case (EXPANDED_SOFT)
          FF = expanded_formfactor (AS_HARD, alphas_soft (ps%sqrts), ps, &
            vec_type) - one
        case (EXPANDED_SOFT_SWITCHOFF)
          f = f_switch_off (v_matching (ps%sqrts, GAM_M1S))
          FF = expanded_formfactor (f * AS_HARD, &
            f * alphas_soft (ps%sqrts), ps, vec_type) - one
        case (RESUMMED_ANALYTIC_LL)
          FF = formfactor_LL_analytic (alphas_soft (ps%sqrts), ps%sqrts, &
            ps%p, vec_type) - one
      end select
    end if
  end function formfactor_compute

```

```

        case (TREE)
            FF = zero
        case default
            FF = zero
        end select
    else
        FF = zero
    end if
    if (debug2_active (D_THRESHOLD)) then
        call update_global_sqrts_dependent_variables (ps%sqrts)
        call msg_debug2 (D_THRESHOLD, "threshold%settings%initialized_parameters", threshold%setting)
        call msg_debug2 (D_THRESHOLD, "formfactor%active", formfactor%active)
        call msg_debug2 (D_THRESHOLD, "FF_mode", FF_mode)
        call msg_debug2 (D_THRESHOLD, "FF", FF)
        call msg_debug2 (D_THRESHOLD, "v", sqrts_to_v (ps%sqrts, GAM))
        call msg_debug2 (D_THRESHOLD, "vec_type", vec_type)
        call ps%write ()
    end if
end function formfactor_compute

<ttv formfactors: public>+≡
    public :: width_t

<ttv formfactors: types>+≡
    type :: width_t
        real(default) :: aem
        real(default) :: sw
        real(default) :: mw
        real(default) :: mb
        real(default) :: vtb
        real(default) :: gam_inv
    contains
        <ttv formfactors: width: TBP>
    end type width_t

<ttv formfactors: width: TBP>≡
    procedure :: init => width_init

<ttv formfactors: procedures>+≡
    pure subroutine width_init (width, aemi, sw, mw, mb, vtb, gam_inv)
        class(width_t), intent(inout) :: width
        real(default), intent(in) :: aemi, sw, mw, mb, vtb, gam_inv
        width%aem = one / aemi
        width%sw = sw
        width%mw = mw
        width%mb = mb
        width%vtb = vtb
        width%gam_inv = gam_inv
    end subroutine width_init

<ttv formfactors: width: TBP>+≡
    procedure :: compute => width_compute

```

```

<ttv formfactors: procedures>+≡
pure function width_compute (width, top_mass, sqrts, initial) result (gamma)
  real(default) :: gamma
  class(width_t), intent(in) :: width
  real(default), intent(in) :: top_mass, sqrts
  logical, intent(in), optional :: initial
  real(default) :: alphas
  logical :: ini
  ini = .false.; if (present (initial)) ini = initial
  if (ini) then
    alphas = AS_HARD
  else
    alphas = alphas_notsohard (sqrts)
  end if
  if (threshold%settings%nlo) then
    gamma = top_width_sm_qcd_nlo_jk (width%aem, width%sw, width%vtb, &
      top_mass, width%mw, width%mb, alphas) + width%gam_inv
  else
    gamma = top_width_sm_lo (width%aem, width%sw, width%vtb, top_mass, &
      width%mw, width%mb) + width%gam_inv
  end if
end function width_compute

```

Use singleton pattern instead of global variables. At least shows where the variables are from.

```

<ttv formfactors: public>+≡
  public :: threshold

<ttv formfactors: global variables>≡
  type(threshold_t) :: threshold

<ttv formfactors: public>+≡
  public :: threshold_t

<ttv formfactors: types>+≡
  type :: threshold_t
    type(settings_t) :: settings
    type(formfactor_t) :: formfactor
    type(width_t) :: width
  contains
    <ttv formfactors: threshold: TBP>
  end type threshold_t

```

```

<ttv formfactors: parameters>≡
integer, parameter :: VECTOR = 1
integer, parameter :: AXIAL = 2
integer, parameter, public :: MATCHED_EXPANDED_NOTSOHARD = -5, &
  MATCHED_NOTSOHARD = -4, &
  MATCHED_EXPANDED = - 3, &
  RESUMMED_SWITCHOFF = - 2, &
  MATCHED = -1, &
  RESUMMED = 1, &
  EXPANDED_HARD = 4, &
  EXPANDED_SOFT = 5, &

```

```

EXPANDED_SOFT_SWITCHOFF = 6, &
RESUMMED_ANALYTIC_LL = 7, &
EXPANDED_NOTSOHARD = 8, &
TREE = 9
real(default), parameter :: NF = 5.0_default

real(default), parameter :: z3 = 1.20205690315959428539973816151_default
real(default), parameter :: A1 = 31./9.*CA - 20./9.*TR*NF
real(default), parameter :: A2 = (4343./162. + 4.*pi**2 - pi**4/4. + &
22./3.*z3)*CA**2 - (1798./81. + 56./3.*z3)*CA*TR*NF - &
(55./3. - 16.*z3)*CF*TR*NF + (20./9.*TR*NF)**2
complex(default), parameter :: iep5 = imago*tiny_10

```

gam_m1s is only used for the scale nustar

```

<ttv formfactors: public>+≡
public :: GAM, GAM_M1S

<ttv formfactors: global variables>+≡
real(default) :: M1S, GAM, GAM_M1S
integer :: NRQCD_ORDER
real(default) :: MTPOLE = - one
real(default) :: mtpole_init
real(default) :: RESCALE_H, MU_HARD, AS_HARD
real(default) :: AS_MZ, MASS_Z
real(default) :: MU_USOFT, AS_USOFT

```

NUSTAR_FIXED is normally not used

```

<ttv formfactors: public>+≡
public :: AS_SOFT
public :: AS_LL_SOFT
public :: AS_USOFT
public :: AS_HARD
public :: SWITCHOFF_RESUMMED
public :: TOPPIK_RESUMMED

<ttv formfactors: global variables>+≡
real(default) :: RESCALE_F, MU_SOFT, AS_SOFT, AS_LL_SOFT, NUSTAR_FIXED
logical :: NUSTAR_DYNAMIC, SWITCHOFF_RESUMMED, TOPPIK_RESUMMED
real(default) :: B0
real(default) :: B1

real(default), dimension(2) :: aa2, aa3, aa4, aa5, aa8, aa0
character(len=200) :: parameters_ref
type(nr_spline_t) :: ff_p_spline
real(default) :: v1, v2

integer :: POINTS_SQ, POINTS_P, POINTS_P0, n_q
real(default), dimension(:), allocatable :: sq_grid, p_grid, p0_grid, q_grid
complex(default), dimension(:,:,:), allocatable :: ff_grid
complex(single), dimension(:,:,:), allocatable :: Vmatrix

```

Explicit range and step size of the sqrts-grid relative to 2*M1S:

```

<ttv formfactors: global variables>+≡

```

```

real(default) :: sqrts_min, sqrts_max, sqrts_it

<ttv formfactors: interfaces>≡
  interface char
    module procedure int_to_char, real_to_char, complex_to_char, logical_to_char
  end interface char

<ttv formfactors: public>+≡
  public :: mis_to_mpole

<ttv formfactors: types>+≡
  type, public :: phase_space_point_t
    real(default) :: p2 = 0, k2 = 0, q2 = 0
    real(default) :: sqrts = 0, p = 0, p0 = 0
    real(default) :: mpole = 0, en = 0
    logical :: inside_grid = .false., onshell = .false.
  contains
    <ttv formfactors: phase space point: TBP>
  end type phase_space_point_t

<ttv formfactors: phase space point: TBP>≡
  procedure :: init => phase_space_point_init_rel

<ttv formfactors: procedures>+≡
  pure subroutine phase_space_point_init_rel (ps_point, p2, k2, q2, m)
    class(phase_space_point_t), intent(inout) :: ps_point
    real(default), intent(in) :: p2
    real(default), intent(in) :: k2
    real(default), intent(in) :: q2
    real(default), intent(in), optional :: m
    ps_point%p2 = p2
    ps_point%k2 = k2
    ps_point%q2 = q2
    call rel_to_nonrel (p2, k2, q2, ps_point%sqrts, ps_point%p, ps_point%p0)
    ps_point%mpole = mis_to_mpole (ps_point%sqrts)
    ps_point%en = sqrts_to_en (ps_point%sqrts)
    ps_point%inside_grid = sqrts_within_range (ps_point%sqrts)
    if ( present(m) ) ps_point%onshell = ps_point%is_onshell (m)
  end subroutine phase_space_point_init_rel

<ttv formfactors: phase space point: TBP>+≡
  procedure :: init_nonrel => phase_space_point_init_nonrel

<ttv formfactors: procedures>+≡
  pure subroutine phase_space_point_init_nonrel (ps_point, sqrts, p, p0, m)
    class(phase_space_point_t), intent(inout) :: ps_point
    real(default), intent(in) :: sqrts
    real(default), intent(in) :: p
    real(default), intent(in) :: p0
    real(default), intent(in), optional :: m
    ps_point%sqrts = sqrts
    ps_point%p = p
    ps_point%p0 = p0

```

```

    call nonrel_to_rel (sqrts, p, p0, ps_point%p2, ps_point%k2, ps_point%q2)
    ps_point%mpole = m1s_to_mpole (sqrts)
    ps_point%en = sqrts_to_en (sqrts, ps_point%mpole)
    ps_point%inside_grid = sqrts_within_range (sqrts)
    if ( present(m) ) ps_point%onshell = ps_point%is_onshell (m)
end subroutine phase_space_point_init_nonrel

```

(ttv formfactors: procedures)+≡

```

!!! convert squared 4-momenta into sqrts, p0 = E_top-sqrts/2 and abs. 3-momentum p
pure subroutine rel_to_nonrel (p2, k2, q2, sqrts, p, p0)
    real(default), intent(in) :: p2
    real(default), intent(in) :: k2
    real(default), intent(in) :: q2
    real(default), intent(out) :: sqrts
    real(default), intent(out) :: p
    real(default), intent(out) :: p0
    sqrts = sqrt(q2)
    p0 = abs(p2 - k2) / (2. * sqrts)
    p = sqrt (0.5_default * (- p2 - k2 + sqrts**2/2. + 2.* p0**2))
end subroutine rel_to_nonrel

```

(ttv formfactors: procedures)+≡

```

!!! convert sqrts, p0 = E_top-sqrts/2 and abs. 3-momentum p into squared 4-momenta
pure subroutine nonrel_to_rel (sqrts, p, p0, p2, k2, q2)
    real(default), intent(in) :: sqrts
    real(default), intent(in) :: p
    real(default), intent(in) :: p0
    real(default), intent(out) :: p2
    real(default), intent(out) :: k2
    real(default), intent(out) :: q2
    p2 = (sqrts/2.+p0)**2 - p**2
    k2 = (sqrts/2.-p0)**2 - p**2
    q2 = sqrts**2
end subroutine nonrel_to_rel

```

(ttv formfactors: procedures)+≡

```

pure function complex_m2 (m, w) result (m2c)
    real(default), intent(in) :: m
    real(default), intent(in) :: w
    complex(default) :: m2c
    m2c = m**2 - imago*m*w
end function complex_m2

```

(ttv formfactors: phase space point: TBP)+≡

```

procedure :: is_onshell => phase_space_point_is_onshell

```

(ttv formfactors: procedures)+≡

```

pure function phase_space_point_is_onshell (ps_point, m) result (flag)
    logical :: flag
    class(phase_space_point_t), intent(in) :: ps_point
    real(default), intent(in) :: m
    flag = nearly_equal (ps_point%p2 , m**2, rel_smallness=1E-5_default) .and. &

```



```

        nearly_equal (ps_point%k2 , m**2, rel_smallness=1E-5_default)
end function phase_space_point_is_onshell

```

```

<ttv formfactors: phase space point: TBP>+=
    procedure :: write => phase_space_point_write

```

```

<ttv formfactors: procedures>+=
    subroutine phase_space_point_write (psp, unit)
        class(phase_space_point_t), intent(in) :: psp
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, '(A)') char ("p2 = " // str (psp%p2))
        write (u, '(A)') char ("k2 = " // str (psp%k2))
        write (u, '(A)') char ("q2 = " // str (psp%q2))
        write (u, '(A)') char ("sqrts = " // str (psp%sqrts))
        write (u, '(A)') char ("p = " // str (psp%p))
        write (u, '(A)') char ("p0 = " // str (psp%p0))
        write (u, '(A)') char ("mpole = " // str (psp%mpole))
        write (u, '(A)') char ("en = " // str (psp%en))
        write (u, '(A)') char ("inside_grid = " // str (psp%inside_grid))
        write (u, '(A)') char ("onshell = " // str (psp%onshell))
    end subroutine phase_space_point_write

```

```

<ttv formfactors: procedures>+=
    function set_nrqcd_order (nrqcd_order_in) result (nrqcdorder)
        integer :: nrqcdorder
        real(default), intent(in) :: nrqcd_order_in
        nrqcdorder = 1
        if ( int(nrqcd_order_in) > nrqcdorder ) then
            call msg_warning ("reset to highest available NRQCD_ORDER = " // char(nrqcdorder))
        else
            nrqcdorder = int(nrqcd_order_in)
        end if
    end function set_nrqcd_order

```

```

<ttv formfactors: public>+=
    public :: init_parameters

```

```

<ttv formfactors: procedures>+=
    subroutine init_parameters (mpole_out, gam_out, m1s_in, Vtb, gam_inv, &
        aemi, sw, az, mz, mw, mb, h_in, f_in, nrqcd_order_in, ff_in, &
        offshell_strategy_in, v1_in, v2_in, scan_sqrts_min, &
        scan_sqrts_max, scan_sqrts_stepsize, mpole_fixed, top_helicity_selection)
        real(default), intent(out) :: mpole_out
        real(default), intent(out) :: gam_out
        real(default), intent(in) :: m1s_in
        real(default), intent(in) :: Vtb
        real(default), intent(in) :: gam_inv
        real(default), intent(in) :: aemi
        real(default), intent(in) :: sw
        real(default), intent(in) :: az
        real(default), intent(in) :: mz
    end subroutine init_parameters

```

```

real(default), intent(in) :: mw
real(default), intent(in) :: mb
real(default), intent(in) :: h_in
real(default), intent(in) :: f_in
real(default), intent(in) :: nrqcd_order_in
real(default), intent(in) :: ff_in
real(default), intent(in) :: offshell_strategy_in
real(default), intent(in) :: v1_in
real(default), intent(in) :: v2_in
real(default), intent(in) :: scan_sqrts_min
real(default), intent(in) :: scan_sqrts_max
real(default), intent(in) :: scan_sqrts_stepsize
logical, intent(in) :: mpole_fixed
real(default), intent(in) :: top_helicity_selection
if (debug_active (D_THRESHOLD)) call show_input()
threshold%settings%initialized_parameters = .false.
M1S = m1s_in
threshold%settings%mpole_dynamic = .not. mpole_fixed
threshold%settings%offshell_strategy = int (offshell_strategy_in)
call threshold%settings%setup_flags (int(ff_in), &
    threshold%settings%offshell_strategy, &
    int (top_helicity_selection))
NRQCD_ORDER = set_nrqcd_order (nrqcd_order_in)
v1 = v1_in
v2 = v2_in
sqrts_min = scan_sqrts_min
sqrts_max = scan_sqrts_max
sqrts_it = scan_sqrts_stepsize
!!! global hard parameters incl. hard alphas used in all form factors
RESCALE_H = h_in
MU_HARD   = M1S * RESCALE_H
AS_MZ     = az
MASS_Z    = mz
AS_HARD   = running_as (MU_HARD, az, mz, 2, NF)
call threshold%width%init (aemi, sw, mw, mb, vtb, gam_inv)
GAM_M1S = threshold%width%compute (M1S, zero, initial=.true.)
call compute_global_auxiliary_numbers ()
!!! soft parameters incl. mtpole
!!! (depend on sqrts: initialize with sqrts ~ 2*M1S)
NUSTAR_FIXED = - one
NUSTAR_DYNAMIC = NUSTAR_FIXED < zero
RESCALE_F = f_in
call update_global_sqrts_dependent_variables (2. * M1S)
mtpole_init = MTPOLE
mpole_out = mtpole_init
gam_out = GAM
threshold%settings%initialized_parameters = .true.
contains
    (ttv formfactors: init parameters: subroutines)
end subroutine init_parameters

```

```

(ttv formfactors: init parameters: subroutines)≡
subroutine show_input()
    if (debug_on) call msg_debug (D_THRESHOLD, "init_parameters")

```

```

if (debug_on) call msg_debug (D_THRESHOLD, "m1s_in", m1s_in)
if (debug_on) call msg_debug (D_THRESHOLD, "Vtb", Vtb)
if (debug_on) call msg_debug (D_THRESHOLD, "gam_inv", gam_inv)
if (debug_on) call msg_debug (D_THRESHOLD, "aemi", aemi)
if (debug_on) call msg_debug (D_THRESHOLD, "sw", sw)
if (debug_on) call msg_debug (D_THRESHOLD, "az", az)
if (debug_on) call msg_debug (D_THRESHOLD, "mz", mz)
if (debug_on) call msg_debug (D_THRESHOLD, "mw", mw)
if (debug_on) call msg_debug (D_THRESHOLD, "mb", mb)
if (debug_on) call msg_debug (D_THRESHOLD, "h_in", h_in)
if (debug_on) call msg_debug (D_THRESHOLD, "f_in", f_in)
if (debug_on) call msg_debug (D_THRESHOLD, "nrqcd_order_in", nrqcd_order_in)
if (debug_on) call msg_debug (D_THRESHOLD, "ff_in", ff_in)
if (debug_on) call msg_debug (D_THRESHOLD, "offshell_strategy_in", offshell_strategy_in)
if (debug_on) call msg_debug (D_THRESHOLD, "top_helicity_selection", top_helicity_selection)
if (debug_on) call msg_debug (D_THRESHOLD, "v1_in", v1_in)
if (debug_on) call msg_debug (D_THRESHOLD, "v2_in", v2_in)
if (debug_on) call msg_debug (D_THRESHOLD, "scan_sqrts_min", scan_sqrts_min)
if (debug_on) call msg_debug (D_THRESHOLD, "scan_sqrts_max", scan_sqrts_max)
if (debug_on) call msg_debug (D_THRESHOLD, "scan_sqrts_stepsize", scan_sqrts_stepsize)
if (debug_on) call msg_debug (D_THRESHOLD, "AS_HARD", AS_HARD)
end subroutine show_input

```

(ttv formfactors: procedures)+≡

```

subroutine compute_global_auxiliary_numbers ()
  !!! auxiliary numbers needed later
  !!! current coefficients Ai(S,L,J), cf. arXiv:hep-ph/0609151, Eqs. (63)-(64)
  !!! 3S1 coefficients (s-wave, vector current)
  B0 = coeff_b0(NF) * (4.*pi)
  B1 = coeff_b1(NF) * (4.*pi)**2
  aa2(1) = (CF*(CA*CF*(9.*CA - 100.*CF) - &
    B0*(26.*CA**2 + 19.*CA*CF - 32.*CF**2)))/(26.*B0**2 *CA)
  aa3(1) = CF**2/( B0**2 *(6.*B0 - 13.*CA)*(B0 - 2.*CA)) * &
    (CA**2 *(9.*CA - 100.*CF) + B0*CA*(74.*CF - CA*16.) - &
    6.*B0**2 *(2.*CF - CA))
  aa4(1) = (24.*CF**2 * (11.*CA - 3.*B0)*(5.*CA + 8.*CF)) / &
    (13.*CA*(6.*B0 - 13.*CA)**2)
  aa5(1) = (CF**2 * (CA*(15.-28) + B0*5.))/(6.*(B0-2.*CA)**2)
  aa8(1) = zero
  aa0(1) = -((8.*CF*(CA + CF)*(CA + 2.*CF))/(3.*B0**2))
  !!! 3P1 coefficients (p-wave, axial vector current)
  aa2(2) = -1./3. * (CF*(CA+2.*CF)/B0 - CF**2/(4.*B0) )
  aa3(2) = zero
  aa4(2) = zero
  aa5(2) = 1./3. * CF**2/(4.*(B0-2.*CA))
  aa8(2) = -1./3. * CF**2/(B0-CA)
  aa0(2) = -1./3. * 8.*CA*CF*(CA+4.*CF)/(3.*B0**2)
end subroutine compute_global_auxiliary_numbers

```

(ttv formfactors: public)+≡

```
public :: init_threshold_grids
```

(ttv formfactors: procedures)+≡

```
subroutine init_threshold_grids (test)
```

```

real(default), intent(in) :: test
if (debug_active (D_THRESHOLD)) then
    call msg_debug (D_THRESHOLD, "init_threshold_grids")
    call msg_debug (D_THRESHOLD, "TOPPIK_RESUMMED", TOPPIK_RESUMMED)
end if
if (test > zero) then
    call msg_message ("TESTING ONLY: Skip threshold initialization and use tree-level SM.")
    return
end if
if (.not. threshold%settings%initialized_parameters) call msg_fatal ("init_threshold_grid: par
!!! !!! !!! MAC OS X and BSD don't load the global module with parameter values stored
!!! if (parameters_ref == parameters_string ()) return
call dealloc_grids ()
if (TOPPIK_RESUMMED) call init_formfactor_grid ()
parameters_ref = parameters_string ()
end subroutine init_threshold_grids

```

(ttv formfactors: procedures)+≡

```

!!! LL/NLL resummation of nonrelativistic Coulomb potential
pure function resummed_formfactor (ps, vec_type) result (c)
    type(phase_space_point_t), intent(in) :: ps
    integer, intent(in) :: vec_type
    complex(default) :: c
    c = one
    if (.not. threshold%settings%initialized_ff .or. .not. ps%inside_grid) return
    if (POINTS_SQ > 1) then
        call interpolate_linear (sq_grid, p_grid, ff_grid(:, :, 1, vec_type), ps%sqrts, ps%p, c)
    else
        call interpolate_linear (p_grid, ff_grid(1, :, 1, vec_type), ps%p, c)
    end if
end function resummed_formfactor

```

(ttv formfactors: procedures)+≡

```

!!! leading nonrelativistic  $O(\alpha_s^1)$  contribution (-> expansion of resummation)
function expanded_formfactor (alphas_hard, alphas_soft, ps, vec_type) result (FF)
    complex(default) :: FF
    real(default), intent(in) :: alphas_hard, alphas_soft
    type(phase_space_point_t), intent(in) :: ps
    integer, intent(in) :: vec_type
    real(default) :: shift_from_hard_current
    complex(default) :: v, contrib_from_potential
    FF = one
    if (.not. threshold%settings%initialized_parameters) return
    call update_global_sqrts_dependent_variables (ps%sqrts)
    v = sqrts_to_v (ps%sqrts, GAM)
    if (NRQCD_ORDER == 1) then
        if (vec_type == AXIAL) then
            shift_from_hard_current = - CF / pi
        else
            shift_from_hard_current = - two * CF / pi
        end if
    else
        shift_from_hard_current = zero
    end if
end function expanded_formfactor

```

```

end if
if (ps%onshell) then
    contrib_from_potential = CF * ps%mpole * Pi / (4 * ps%p)
else
    if (vec_type == AXIAL) then
        contrib_from_potential = - CF * ps%mpole / (two * ps%p) * &
            (imago * ps%mpole * v / ps%p + &
            (ps%mpole**2 * v**2 + (ps%p)**2) / (4 * Pi * (ps%p)**2) * ( &
            (log (- ps%mpole * v - ps%p))**2 - &
            (log (- ps%mpole * v + ps%p))**2 + &
            (log (ps%mpole * v - ps%p))**2 - &
            (log (ps%mpole * v + ps%p))**2 ))
    else
        contrib_from_potential = imago * CF * ps%mpole * &
            log ((ps%p + ps%mpole * v) / &
            (-ps%p + ps%mpole * v) + ieps) / (two * ps%p)
    end if
end if
FF = one + alphas_soft * contrib_from_potential + &
    alphas_hard * shift_from_hard_current
end function expanded_formfactor

```

(ttv formfactors: procedures)+≡

```

subroutine init_formfactor_grid ()
    type(string_t) :: ff_file
    if (debug_on) call msg_debug (D_THRESHOLD, "init_formfactor_grid")
    threshold%settings%initialized_ff = .false.
    ff_file = "SM_tt_threshold.grid"
    call msg_message ()
    call msg_message ("%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%")
    call msg_message (" Initialize e+e- => ttbar threshold resummation:")
    call msg_message (" Use analytic (LL) or TOPPIK (NLL) form factors for ttA/ttZ vector")
    call msg_message (" and axial vector couplings (S/P-wave) in the threshold region.")
    call msg_message (" Cf. threshold shapes from A. Hoang et al.: [arXiv:hep-ph/0107144],")
    call msg_message (" [arXiv:1309.6323].")
    if (NRQCD_ORDER > 0) then
        call msg_message (" Numerical NLL solutions calculated with TOPPIK [arXiv:hep-ph/9904468]")
        call msg_message (" by M. Jezabek, T. Teubner.")
    end if
    call msg_message ("%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%")
    call msg_message ()
    call read_formfactor_grid (ff_file)
    if (.not. threshold%settings%initialized_ff) then
        if (.not. threshold%settings%initialized_ps) call init_threshold_phase_space_grid ()
        call scan_formfactor_over_phase_space_grid ()
        call write_formfactor_grid (ff_file)
    end if
end subroutine init_formfactor_grid

```

(ttv formfactors: procedures)+≡

```

subroutine read_formfactor_grid (ff_file)
    type(string_t), intent(in) :: ff_file
    complex(single), dimension(:, :, :, :), allocatable :: ff_grid_sp

```

```

character(len(parameters_ref)) :: parameters
integer :: u, st
logical :: ex
integer, dimension(4) :: ff_shape
if (debug_on) call msg_debug (D_THRESHOLD, "read_formfactor_grid")
inquire (file=char(ff_file), exist=ex)
if (.not. ex) return
u = free_unit ()
call msg_message ("Opening grid file: " // char(ff_file))
open (unit=u, status='old', file=char(ff_file), form='unformatted', iostat=st)
if (st /= 0) call msg_fatal ("iostat = " // char(st))
read (u) parameters
read (u) ff_shape
if (ff_shape(4) /= 2) call msg_fatal ("read_formfactor_grid: i = " // char(ff_shape(4)))
if (parameters /= parameters_string ()) then
    call msg_message ("Threshold setup has changed: recalculate threshold grid.")
    close (unit=u, status='delete')
    return
end if
call msg_message ("Threshold setup unchanged: reusing existing threshold grid.")
POINTS_SQ = ff_shape(1)
POINTS_P = ff_shape(2)
if (debug_active (D_THRESHOLD)) then
    call msg_debug (D_THRESHOLD, "ff_shape(1) (POINTS_SQ)", ff_shape(1))
    call msg_debug (D_THRESHOLD, "ff_shape(2)", ff_shape(2))
    call msg_debug (D_THRESHOLD, "ff_shape(3) (POINTS_P0)", ff_shape(3))
    call msg_debug (D_THRESHOLD, "ff_shape(4) (==2)", ff_shape(4))
end if
allocate (sq_grid(POINTS_SQ))
read (u) sq_grid
allocate (p_grid(POINTS_P))
read (u) p_grid
POINTS_P0 = ff_shape(3)
allocate (ff_grid_sp(POINTS_SQ,POINTS_P,POINTS_P0,2))
read (u) ff_grid_sp
allocate (ff_grid(POINTS_SQ,POINTS_P,POINTS_P0,2))
ff_grid = cmplx (ff_grid_sp, kind=default)
close (u, iostat=st)
if (st > 0) call msg_fatal ("close " // char(ff_file) // ": iostat = " // char(st))
threshold%settings%initialized_ps = .true.
threshold%settings%initialized_ff = .true.
end subroutine read_formfactor_grid

```

(ttv formfactors: procedures)+≡

```

subroutine write_formfactor_grid (ff_file)
type(string_t), intent(in) :: ff_file
integer :: u, st
if (.not. threshold%settings%initialized_ff) then
    call msg_warning ("write_formfactor_grid: no grids initialized!")
    return
end if
u = free_unit ()
open (unit=u, status='replace', file=char(ff_file), form='unformatted', iostat=st)
if (st /= 0) call msg_fatal ("open " // char(ff_file) // ": iostat = " // char(st))

```

```

write (u) parameters_string ()
write (u) shape(ff_grid)
write (u) sq_grid
write (u) p_grid
write (u) cmplx(ff_grid, kind=single)
close (u, iostat=st)
if (st > 0) call msg_fatal ("close " // char(ff_file) // ": iostat = " // char(st))
end subroutine write_formfactor_grid

```

(ttv formfactors: procedures)+≡

```

pure function parameters_string () result (str)
character(len(parameters_ref)) :: str
str = char(M1S) // " " // char(GAM_M1S) // " " // char(NRQCD_ORDER) &
// " " // char(RESCALE_H) &
// " " // char(RESCALE_F) &
// " " // char(sqrts_min) &
// " " // char(sqrts_max) // " " // char(sqrts_it)
end function parameters_string

```

(ttv formfactors: procedures)+≡

```

subroutine update_global_sqrts_dependent_variables (sqrts)
real(default), intent(in) :: sqrts
real(default) :: nu_soft, f
logical :: only_once_for_fixed_nu, already_done
real(default), save :: last_sqrts = - one
if (debug_on) call msg_debug (D_THRESHOLD, "update_global_sqrts_dependent_variables")
if (debug_on) call msg_debug (D_THRESHOLD, "sqrts", sqrts)
if (debug_on) call msg_debug (D_THRESHOLD, "last_sqrts", last_sqrts)
already_done = threshold%settings%initialized_parameters .and. &
nearly_equal (sqrts, last_sqrts, rel_smallness=1E-6_default)
if (debug_on) call msg_debug (D_THRESHOLD, "already_done", already_done)
only_once_for_fixed_nu = .not. NUSTAR_DYNAMIC .and. MTPOLE > zero
if (debug_on) call msg_debug (D_THRESHOLD, "only_once_for_fixed_nu", only_once_for_fixed_nu)
if (only_once_for_fixed_nu .or. already_done) return
last_sqrts = sqrts
nu_soft = RESCALE_F * nustar (sqrts)
MU_SOFT = M1S * RESCALE_H * nu_soft
MU_USOFT = M1S * RESCALE_H * nu_soft**2
AS_SOFT = running_as (MU_SOFT, AS_HARD, MU_HARD, NRQCD_ORDER, NF)
AS_LL_SOFT = running_as (MU_SOFT, AS_HARD, MU_HARD, 0, NF)
AS_USOFT = running_as (MU_USOFT, AS_HARD, MU_HARD, 0, NF) !!! LL here
if (SWITCHOFF_RESUMMED) then
f = f_switch_off (v_matching (sqrts, GAM_M1S))
AS_SOFT = AS_SOFT * f
AS_LL_SOFT = AS_LL_SOFT * f
AS_USOFT = AS_USOFT * f
end if
MTPOLE = m1s_to_mpole (sqrts)
GAM = threshold%width%compute (MTPOLE, sqrts)
if (debug_on) call msg_debug (D_THRESHOLD, "GAM", GAM)
if (debug_on) call msg_debug (D_THRESHOLD, "nu_soft", nu_soft)
if (debug_on) call msg_debug (D_THRESHOLD, "MTPOLE", MTPOLE)
if (debug_on) call msg_debug (D_THRESHOLD, "AS_SOFT", AS_SOFT)

```

```

    if (debug_on) call msg_debug (D_THRESHOLD, "AS_LL_SOFT", AS_LL_SOFT)
    if (debug_on) call msg_debug (D_THRESHOLD, "AS_USOFT", AS_USOFT)
end subroutine update_global_sqrts_dependent_variables

!!! Coulomb potential coefficients needed by TOPPIK
pure function xc (a_soft, i_xc) result (xci)
    real(default), intent(in) :: a_soft
    integer, intent(in) :: i_xc
    real(default) :: xci
    xci = zero
    select case (i_xc)
    case (0)
        xci = one
        if ( NRQCD_ORDER>0 ) xci = xci + a_soft/(4.*pi) * A1
        if ( NRQCD_ORDER>1 ) xci = xci + (a_soft/(4.*pi))**2 * A2
    case (1)
        if ( NRQCD_ORDER>0 ) xci = xci + a_soft/(4.*pi) * B0
        if ( NRQCD_ORDER>1 ) xci = xci + (a_soft/(4.*pi))**2 * (B1 + 2*B0*A1)
    case (2)
        if ( NRQCD_ORDER>1 ) xci = xci + (a_soft/(4.*pi))**2 * B0**2
    case default
        return
    end select
end function xc

```

(ttv formfactors: procedures)+≡

```

function current_coeff (a_hard, a_soft, a_usoft, i) result (coeff)
    real(default), intent(in) :: a_hard, a_soft, a_usoft
    integer, intent(in) :: i
    real(default) :: coeff
    real(default) :: matching_c, c1
    real(default) :: z, w
    if (debug_on) call msg_debug (D_THRESHOLD, "current_coeff")
    coeff = one
    if (NRQCD_ORDER == 0) return
    z = a_soft / a_hard
    w = a_usoft / a_soft
    !!! hard s/p-wave 1-loop matching coefficients, cf. arXiv:hep-ph/0604072
    select case (i)
    case (1)
        matching_c = one - 2.*(CF/pi) * a_hard
    case (2)
        matching_c = one - (CF/pi) * a_hard
    case default
        call msg_fatal ("current_coeff: unknown coeff i = " // char(i))
    end select
    !!! current coefficient c1, cf. arXiv:hep-ph/0609151, Eq. (62)
    c1 = exp( a_hard * pi * ( aa2(i)*(1.-z) + aa3(i)*log(z) + &
        aa4(i)*(1.-z**(1.-13.*CA/(6.*B0))) + aa5(i)*(1.-z**(1.-2.*CA/B0)) + &
        aa8(i)*(1.-z**(1.-CA/B0)) + aa0(i)*(z-1.-log(w)/w) ) )
    coeff = matching_c * c1
end function current_coeff

```



```

<ttv formfactors: public>+≡
  public :: v_matching

<ttv formfactors: procedures>+≡
  pure function v_matching (sqrts, gamma) result (v)
    real(default) :: v
    real(default), intent(in) :: sqrts, gamma
    v = abs (sqrts_to_v_1S (sqrts, gamma))
  end function v_matching

```

Smooth transition from f1 to f2 between v1 and v2 (simplest polynom).

```

<ttv formfactors: public>+≡
  public :: f_switch_off

<ttv formfactors: procedures>+≡
  pure function f_switch_off (v) result (fval)
    real(default), intent(in) :: v
    real(default) :: fval
    real(default) :: vm, f1, f2, x
    f1 = one
    f2 = zero + tiny_10
    vm = (v1+v2) / 2.
    if ( v < v1 ) then
      fval = f1
    else if (v < v2) then
      x = (v - v1) / (v2 - v1)
      fval = 1 - x**2 * (3 - 2 * x)
    else
      fval = f2
    end if
  end function f_switch_off

```

```

<ttv formfactors: procedures>+≡
  function formfactor_LL_analytic (a_soft, sqrts, p, vec_type) result (c)
    real(default), intent(in) :: a_soft
    real(default), intent(in) :: sqrts
    real(default), intent(in) :: p
    integer, intent(in) :: vec_type
    complex(default) :: c
    real(default) :: en
    c = one
    if (.not. threshold%settings%initialized_parameters) return
    call update_global_sqrts_dependent_variables (sqrts)
    en = sqrts_to_en (sqrts, MTPOLE)
    select case (vec_type)
      case (1)
        c = G0p (CF*a_soft, en, p, MTPOLE, GAM) / G0p_tree (en, p, MTPOLE, GAM)
      case (2)
        c = G0p_ax (CF*a_soft, en, p, MTPOLE, GAM) / G0p_tree (en, p, MTPOLE, GAM)
      case default
        call msg_fatal ("unknown ttZ/ttA vertex component, vec_type = " // char(vec_type))
    end select
  end function formfactor_LL_analytic

```

```

<ttv formfactors: procedures>+≡
!!! Max's LL nonrelativistic threshold Green's function
function G0p (a, en, p, m, w) result (c)
  real(default), intent(in) :: a
  real(default), intent(in) :: en
  real(default), intent(in) :: p
  real(default), intent(in) :: m
  real(default), intent(in) :: w
  complex(default) :: c
  complex(default) :: k, ipk, la, z1, z2
  complex(default) :: one, two, cc, dd
  k = sqrt( -m*en -imago*m*w )
  ipk = imago * p / k
  la = a * m / 2. / k
  one = cmplx (1., kind=default)
  two = cmplx (2., kind=default)
  cc = 2. - la
  dd = ( 1. + ipk ) / 2.
  z1 = nr_hypgeo (two, one, cc, dd)
  dd = ( 1. - ipk ) / 2.
  z2 = nr_hypgeo (two, one, cc, dd)
  c = - imago * m / (4.*p*k) / (1.-la) * ( z1 - z2 )
end function G0p

```

```

<ttv formfactors: procedures>+≡
!!! tree level version: a_soft -> 0
pure function G0p_tree (en, p, m, w) result (c)
  real(default), intent(in) :: en
  real(default), intent(in) :: p
  real(default), intent(in) :: m
  real(default), intent(in) :: w
  complex(default) :: c
  c = m / (p**2 - m*(en+imago*w))
end function G0p_tree

```

```

<ttv formfactors: procedures>+≡
!!! Peter Poier's LL nonrelativistic axial threshold Green's function
function G0p_ax (a, en, p, m, w) result (c)
  real(default), intent(in) :: a
  real(default), intent(in) :: en
  real(default), intent(in) :: p
  real(default), intent(in) :: m
  real(default), intent(in) :: w
  complex(default) :: c
  complex(default) :: k, ipk, la, z1, z2, z3, z4
  complex(default) :: zero, two, three, cc, ddp, ddm
  k = sqrt( -m*en -imago*m*w )
  ipk = imago * p / k
  la = a * m / 2. / k
  zero = cmplx (0., kind=default)
  two = cmplx (2., kind=default)
  three = cmplx (3., kind=default)
  cc = 1. - la

```

```

ddp = ( 1. + ipk ) / 2.
ddm = ( 1. - ipk ) / 2.
z1 = nr_hypgeo (zero, two, cc, ddp)
z2 = nr_hypgeo (zero, two, cc, ddm)
cc = 2. - la
z3 = nr_hypgeo (zero, three, cc, ddm)
z4 = nr_hypgeo (zero, three, cc, ddp)
c = m / 2. / p**3 * ( 2.*p + imago*k*(1.-la)*(z1-z2) + imago*k*(z3-z4) )
end function G0p_ax

```

(ttv formfactors: procedures)+≡

```

pure function nustar (sqrts) result (nu)
  real(default), intent(in) :: sqrts
  real(default) :: nu
  real(default), parameter :: nustar_offset = 0.05_default
  complex(default) :: arg
  if (NUSTAR_DYNAMIC) then
    !!! from [arXiv:1309.6323], Eq. (3.2) (other definitions possible)
    arg = ( sqrts - 2.*M1S + imago*GAM_M1S ) / M1S
    nu = nustar_offset + abs(sqrt(arg))
  else
    nu = NUSTAR_FIXED
  end if
end function nustar

```

We recompute `alpha_soft` for form factors that do not call `update_global_parameters` (it is called in the scan for the (N)LL grid).

(ttv formfactors: procedures)+≡

```

pure function alphas_soft (sqrts) result (a_soft)
  real(default) :: a_soft
  real(default), intent(in) :: sqrts
  real(default) :: mu_soft, nusoft
  nusoft = RESCALE_F * nustar (sqrts)
  mu_soft = RESCALE_H * M1S * nusoft
  a_soft = running_as (mu_soft, AS_HARD, MU_HARD, NRQCD_ORDER, NF)
end function alphas_soft

```

(ttv formfactors: public)+≡

```

public :: alphas_notsohard

```

(ttv formfactors: procedures)+≡

```

pure function alphas_notsohard (sqrts) result (a_soft)
  real(default) :: a_soft
  real(default), intent(in) :: sqrts
  real(default) :: mu_notsohard
  ! complex(default) :: v
  ! v = sqrts_to_v_1S (sqrts, GAM_M1S)
  ! mu_notsohard = RESCALE_H * M1S * sqrt(abs(v))
  mu_notsohard = RESCALE_H * M1S * sqrt(nustar (sqrts))
  a_soft = running_as (mu_notsohard, AS_MZ, MASS_Z, 2, NF)
end function alphas_notsohard

```

(ttv formfactors: procedures)+≡

```

pure function m1s_to_mpole (sqrts) result (mpole)
  real(default), intent(in) :: sqrts
  real(default) :: mpole
  mpole = mtpole_init
  if (threshold%settings%mpole_dynamic) then
    mpole = M1S * ( 1. + deltaM(sqrts) )
  else
    mpole = M1S
  end if
end function m1s_to_mpole

```

(ttv formfactors: procedures)+≡

```

!pure
!function mpole_to_M1S (mpole, sqrts, nl) result (m)
  !real(default), intent(in) :: mpole
  !real(default), intent(in) :: sqrts
  !integer, intent(in) :: nl
  !real(default) :: m
  !m = mpole * ( 1. - deltaM(sqrts, nl) )
!end function mpole_to_M1S

```

(ttv formfactors: procedures)+≡

```

pure function deltaM (sqrts) result (del)
  real(default), intent(in) :: sqrts
  real(default) :: del
  real(default) :: ac
  ac = CF * alphas_soft (sqrts)
  del = ac**2 / 8.
  if (NRQCD_ORDER > 0) then
    del = del + ac**3 / (8. * pi * CF) * &
      (B0 * (log (RESCALE_H * RESCALE_F * nustar (sqrts) / ac) + one) + A1 / 2.)
  end if
end function deltaM

```

(ttv formfactors: procedures)+≡

```

pure function sqrts_within_range (sqrts) result (flag)
  real(default), intent(in) :: sqrts
  logical :: flag
  flag = ( sqrts >= sqrts_min - tiny_07 .and. sqrts <= sqrts_max + tiny_07 )
end function

```

(ttv formfactors: procedures)+≡

```

! The mapping is such that even for min=max, we get three points:
! min - it , min, min + it
pure function sqrts_iter (i_sq) result (sqrts)
  integer, intent(in) :: i_sq
  real(default) :: sqrts
  if (POINTS_SQ > 1) then
    sqrts = sqrts_min - sqrts_it + &
      (sqrts_max - sqrts_min + two * sqrts_it) * &
      real(i_sq - 1) / real(POINTS_SQ - 1)
  end if
end function

```

```

else
  sqrts = sqrts_min
end if
end function sqrts_iter

```

(ttv formfactors: procedures)+≡

```

function scan_formfactor_over_p_LL_analytic (a_soft, sqrts, vec_type) result (ff_analytic)
  real(default), intent(in) :: a_soft
  real(default), intent(in) :: sqrts
  integer, intent(in) :: vec_type
  complex(default), dimension(POINTS_P) :: ff_analytic
  integer :: i_p
  ff_analytic = [(formfactor_LL_analytic (a_soft, sqrts, p_grid(i_p), vec_type), i_p=1, POINTS_P)
end function scan_formfactor_over_p_LL_analytic

```

(ttv formfactors: procedures)+≡

```

!!! tttoppik wrapper
subroutine scan_formfactor_over_p_TOPPIK (a_soft, sqrts, vec_type, p_grid_out, mpole_in, ff_toppik)
  real(default), intent(in) :: a_soft
  real(default), intent(in) :: sqrts
  integer, intent(in) :: vec_type
  real(default), dimension(POINTS_P), intent(out), optional :: p_grid_out
  real(default), intent(in), optional :: mpole_in
  complex(default), dimension(POINTS_P), optional :: ff_toppik
  integer :: i_p
  real(default) :: mpole, alphas_hard, f
  real(default), dimension(POINTS_P) :: p_toppik
  type(nr_spline_t) :: toppik_spline
  real*8 :: xenergy, xtm, xtg, xalphas, xscale, xc0, xc1, xc2, xim, xdi, &
    xcutn, xcutv, xkincm, xkinca, xkincv, xcdeltc, &
    xcdeltl, xcflllc, xcfllll, xcrm2
  integer, parameter :: nmax=900
  real*8 :: xdsdp(nmax), xpp(nmax), xww(nmax)
  complex*16 :: zff(nmax)
  integer :: np, jknflg, jgcflg, jvflg
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_formfactor_over_p_TOPPIK")
  if (POINTS_P > nmax-40) call msg_fatal ("TOPPIK: POINTS_P must be <=" // char(nmax-40))
  if (debug_on) call msg_debug (D_THRESHOLD, "POINTS_P", POINTS_P)
  if (present (ff_toppik)) ff_toppik = zero
  mpole = MTPOLE; if (present (mpole_in)) mpole = mpole_in
  xenergy = sqrts_to_en (sqrts, MTPOLE)
  xtm      = mpole
  xtg      = GAM
  xalphas  = a_soft
  xscale   = MU_SOFT
  xcutn    = 175.E6
  xcutv    = 175.E6
  xc0      = xc (a_soft, 0)
  xc1      = xc (a_soft, 1)
  xc2      = xc (a_soft, 2)
  xcdeltc  = 0.
  xcdeltl  = 0.
  xcflllc  = 0.

```

```

xctfulll = 0.
xcrm2 = 0.
xkincm = 0.
xkinca = 0.
jknflg = 0
jgcflg = 0
xkincv = 0.
jvflg = 0
select case (vec_type)
  case (VECTOR)
    if (debug_on) call msg_debug (D_THRESHOLD, "calling tttoppik")
    call tttoppik &
      (xenergy, xtm, xtg, xalphas, xscale, xcutn, xcutv, xc0, xc1, xc2, &
       xdelc, xdelc1, xcfllc, xcflll, xcrm2, xkincm, xkinca, jknflg, &
       jgcflg, xkincv, jvflg, xim, xdi, np, xpp, xww, xdsdp, zff)
  case (AXIAL)
    if (debug_on) call msg_debug (D_THRESHOLD, "calling tttoppikaxial")
    call tttoppikaxial &
      (xenergy, xtm, xtg, xalphas, xscale, xcutn, xcutv, xc0, xc1, xc2, &
       xdelc, xdelc1, xcfllc, xcflll, xcrm2, xkincm, xkinca, jknflg, &
       jgcflg, xkincv, jvflg, xim, xdi, np, xpp, xww, xdsdp, zff)
    !!! 1st ~10 TOPPIK p-wave entries are ff_unstable: discard them
    zff(1:10) = [(zff(11), i_p=1, 10)]
  case default
    call msg_fatal ("unknown ttZ/ttA vertex component, vec_type = " // char(vec_type))
end select
if (present (p_grid_out)) p_grid_out = xpp(1:POINTS_P)
if (.not. present (ff_topplik)) return
!!! keep track of TOPPIK instabilities and try to repair later
if (np < 0) then
  ff_topplik(1) = 2.d30
  if (debug_active (D_THRESHOLD)) then
    call msg_warning ("caught TOPPIK instability at sqrts = " // char(sqrts))
  end if
  return
end if
p_topplik = xpp(1:POINTS_P)
ff_topplik = zff(1:POINTS_P)
!!! TOPPIK output p-grid scales with en above ~ 4 GeV:
!!! interpolate for global sqrts/p grid
if (.not. nearly_equal (p_topplik(42), p_grid(42), rel_smallness=1E-6_default)) then
  call toppik_spline%init (p_topplik, ff_topplik)
  ff_topplik(2:POINTS_P) = [(topplik_spline%interpolate (p_grid(i_p)), i_p=2, POINTS_P)]
  call toppik_spline%dealloc ()
end if
!!! TOPPIK output includes tree level ~ 1, a_soft @ LL in current coefficient!
if (SWITCHOFF_RESUMMED) then
  f = f_switch_off (v_matching (sqrts, GAM_M1S))
  alphas_hard = AS_HARD * f
else
  alphas_hard = AS_HARD
end if
ff_topplik = ff_topplik * current_coeff (alphas_hard, AS_LL_SOFT, AS_USOFT, vec_type)
if (debug_on) call msg_debug (D_THRESHOLD, &

```

```

        "current_coeff (alphas_hard, AS_LL_SOFT, AS_USOFT, vec_type)", &
        current_coeff (alphas_hard, AS_LL_SOFT, AS_USOFT, vec_type))
end subroutine scan_formfactor_over_p_TOPPIK

```

(ttv formfactors: procedures)+≡

```

function scan_formfactor_over_p (sqrts, vec_type) result (ff)
  real(default), intent(in) :: sqrts
  integer, intent(in) :: vec_type
  complex(default), dimension(POINTS_P) :: ff
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_formfactor_over_p")
  select case (NRQCD_ORDER)
    case (0)
      ! ff = scan_formfactor_over_p_LL_analytic (AS_SOFT, sqrts, vec_type)
      call scan_formfactor_over_p_TOPPIK (AS_SOFT, sqrts, vec_type, ff_topplik=ff)
    case (1)
      call scan_formfactor_over_p_TOPPIK (AS_SOFT, sqrts, vec_type, ff_topplik=ff)
    case default
      call msg_fatal ("NRQCD_ORDER = " // char(NRQCD_ORDER))
  end select
end function scan_formfactor_over_p

```

(ttv formfactors: procedures)+≡

```

subroutine scan_formfactor_over_phase_space_grid ()
  integer :: i_sq, vec_type, unstable_loop
  logical, dimension(:,,:), allocatable :: ff_unstable
  real(default) :: t1, t2, t3, t_topplik, t_p0_dep
  if (debug_on) call msg_debug (D_THRESHOLD, "scan_formfactor_over_phase_space_grid")
  allocate (ff_grid(POINTS_SQ,POINTS_P,POINTS_P0,2))
  allocate (ff_unstable(POINTS_SQ,2))
  t_topplik = zero
  t_p0_dep = zero
  write (msg_buffer, "(3(A,F7.3,1X),A)") "Scanning from ", &
    sqrts_min - sqrts_it, "GeV to ", &
    sqrts_max + sqrts_it, "GeV in steps of ", sqrts_it, "GeV"
  call msg_message ()
  ENERGY_SCAN: do i_sq = 1, POINTS_SQ
    if (signal_is_pending ()) return
    call update_global_sqrts_dependent_variables (sq_grid(i_sq))
    !!! vector and axial vector
    do vec_type = VECTOR, AXIAL
      call cpu_time (t1)
      unstable_loop = 0
      UNTIL_STABLE: do
        ff_grid(i_sq,:,1,vec_type) = scan_formfactor_over_p (sq_grid(i_sq), vec_type)
        ff_unstable(i_sq,vec_type) = abs(ff_grid(i_sq,1,1,vec_type)) > 1.d30
        unstable_loop = unstable_loop + 1
        if (ff_unstable(i_sq,vec_type) .and. unstable_loop < 10) then
          cycle
        else
          exit
        end if
      end do UNTIL_STABLE
    end do
    call cpu_time (t2)
  end do

```

```

        !!! include p0 dependence by an integration over the p0-independent FF
        call cpu_time (t3)
        t_toppiik = t_toppiik + t2 - t1
        t_p0_dep = t_p0_dep + t3 - t2
    end do
    call msg_show_progress (i_sq, POINTS_SQ)
end do ENERGY_SCAN
if (debug_active (D_THRESHOLD)) then
    print *, "time for TOPPIK call: ", t2 - t1, " seconds."
    print *, "time for p0 dependence: ", t3 - t2, " seconds."
end if
if (any (ff_unstable)) call handle_TOPPIK_instabilities (ff_grid, ff_unstable)
if (allocated(Vmatrix)) deallocate(Vmatrix)
if (allocated(q_grid)) deallocate(q_grid)
threshold%settings%initialized_ff = .true.
end subroutine scan_formfactor_over_phase_space_grid

```

(ttv formfactors: procedures)+≡

```

subroutine init_threshold_phase_space_grid ()
    integer :: i_sq
    if (debug_on) call msg_debug (D_THRESHOLD, "init_threshold_phase_space_grid")
    if (sqrts_it > tiny_07) then
        POINTS_SQ = int ((sqrts_max - sqrts_min) / sqrts_it + tiny_07) + 3
    else
        POINTS_SQ = 1
    end if
    if (debug_on) call msg_debug (D_THRESHOLD, "Number of sqrts grid points: POINTS_SQ", POINTS_SQ)
    if (debug_on) call msg_debug (D_THRESHOLD, "sqrts_max", sqrts_max)
    if (debug_on) call msg_debug (D_THRESHOLD, "sqrts_min", sqrts_min)
    if (debug_on) call msg_debug (D_THRESHOLD, "sqrts_it", sqrts_it)
    allocate (sq_grid(POINTS_SQ))
    sq_grid = [(sqrts_iter (i_sq), i_sq=1, POINTS_SQ)]
    POINTS_P = 600
    allocate (p_grid(POINTS_P))
    p_grid = p_grid_from_TOPPIK ()
    POINTS_P0 = 1
    threshold%settings%initialized_ps = .true.
end subroutine init_threshold_phase_space_grid

```

(ttv formfactors: procedures)+≡

```

subroutine init_p0_grid (p_in, n)
    real(default), dimension(:), allocatable, intent(in) :: p_in
    integer, intent(in) :: n
    if (debug_on) call msg_debug (D_THRESHOLD, "init_p0_grid")
    if (debug_on) call msg_debug (D_THRESHOLD, "n", n)
    if (debug_on) call msg_debug (D_THRESHOLD, "size(p_in)", size(p_in))
    if (.not. allocated (p_in)) call msg_fatal ("init_p0_grid: p_in not allocated!")
    if (allocated (p0_grid)) deallocate (p0_grid)
    allocate (p0_grid(n))
    p0_grid(1) = zero
    p0_grid(2:n) = p_in(1:n-1)
end subroutine init_p0_grid

```


(ttv formfactors: procedures)+≡

```

!!! Andre's procedure to refine an existing grid
pure subroutine finer_grid (gr, fgr, n_in)
  real(default), dimension(:), intent(in) :: gr
  real(default), dimension(:), allocatable, intent(inout) :: fgr
  integer, intent(in), optional :: n_in
  integer :: n, i, j
  real(default), dimension(:), allocatable :: igr
  n = 4
  if ( present(n_in) ) n = n_in
  allocate( igr(n) )
  if ( allocated(fgr) ) deallocate( fgr )
  allocate( fgr(n*(size(gr)-1)+1) )
  do i=1, size(gr)-1
    do j=0, n-1
      igr(j+1) = gr(i) + real(j)*(gr(i+1)-gr(i))/real(n)
    end do
    fgr((i-1)*n+1:i*n) = igr
  end do
  fgr(size(fgr)) = gr(size(gr))
  deallocate( igr )
end subroutine finer_grid

```

(ttv formfactors: procedures)+≡

```

subroutine dealloc_grids ()
  if ( allocated(sq_grid) ) deallocate( sq_grid )
  if ( allocated( p_grid) ) deallocate( p_grid )
  if ( allocated(p0_grid) ) deallocate( p0_grid )
  if ( allocated(ff_grid) ) deallocate( ff_grid )
  threshold%settings%initialized_ps = .false.
  threshold%settings%initialized_ff = .false.
end subroutine dealloc_grids

```

(ttv formfactors: procedures)+≡

```

subroutine trim_p_grid (n_p_new)
  integer, intent(in) :: n_p_new
  real(default), dimension(n_p_new) :: p_save
  complex(default), dimension(POINTS_SQ,n_p_new,POINTS_P0,2) :: ff_save
  if (n_p_new > POINTS_P) then
    call msg_fatal ("trim_p_grid: new size larger than old size.")
    return
  end if
  p_save = p_grid(1:n_p_new)
  ff_save = ff_grid(:,1:n_p_new,:,:)
  deallocate( p_grid, ff_grid )
  allocate( p_grid(n_p_new), ff_grid(POINTS_SQ,n_p_new,POINTS_P0,2) )
  p_grid = p_save
  ff_grid = ff_save
end subroutine trim_p_grid

```

(ttv formfactors: procedures)+≡

```

!!! try to repair TOPPIK instabilities by interpolation of adjacent sq_grid points
subroutine handle_TOPPIK_instabilities (ff, nan)

```

```

complex(default), dimension(:,:,:), intent(inout) :: ff
logical, dimension(:,:), intent(in) :: nan
integer :: i, i_sq, n_nan
logical :: interrupt
n_nan = sum (merge ([[1, i=1, 2*POINTS_SQ]], &
    [[0, i=1, 2*POINTS_SQ]], reshape (nan, [2*POINTS_SQ])) )
interrupt = n_nan > 3
do i = 1, 2
    if (interrupt ) exit
    if (.not. any (nan(:,i))) cycle
    do i_sq = 2, POINTS_SQ - 1
        if (.not. nan(i_sq,i)) cycle
        if (nan(i_sq+1,i) .or. nan(i_sq-1,i)) then
            interrupt = .true.
            exit
        end if
        ff(i_sq, :, :, i) = (ff(i_sq-1, :, :, i) + ff(i_sq+1, :, :, i)) / two
    end do
end do
if (.not. interrupt) return
call msg_fatal ("Too many TOPPIK instabilities! Check your parameter setup " &
    // "or slightly vary the scales sh and/or sf.")
end subroutine handle_TOPPIK_instabilities

```

```

<ttv formfactors: procedures>+≡
pure function sqrts_to_v (sqrts, gamma) result (v)
complex(default) :: v
real(default), intent(in) :: sqrts, gamma
real(default) :: m
m = m1s_to_mpole (sqrts)
v = sqrt ((sqrts - two * m + imago * gamma) / m)
end function sqrts_to_v

```

```

<ttv formfactors: procedures>+≡
pure function sqrts_to_v_1S (sqrts, gamma) result (v)
complex(default) :: v
real(default), intent(in) :: sqrts, gamma
v = sqrt ((sqrts - two * M1S + imago * gamma) / M1S)
end function sqrts_to_v_1S

```

```

<ttv formfactors: procedures>+≡
pure function v_to_sqrts (v) result (sqrts)
real(default), intent(in) :: v
real(default) :: sqrts
real(default) :: m
m = mpole_init
sqrts = 2.*m + m*v**2
end function v_to_sqrts

```

```

<ttv formfactors: procedures>+≡
!!! -q^2 times the Coulomb potential V at LO resp. NLO
function minus_q2_V (a, q, p, p0r, vec_type) result (v)

```

```

real(default), intent(in) :: a
real(default), intent(in) :: q
real(default), intent(in) :: p
real(default), intent(in) :: p0r
integer, intent(in) :: vec_type
complex(default) :: p0, log_mppp, log_mmpm, log_mu_s, v
p0 = abs(p0r) + ieps
log_mppp = log( (p-p0+q) * (p+p0+q) )
log_mmpm = log( (p-p0-q) * (p+p0-q) )
select case (vec_type)
  case (1)
    select case (NRQCD_ORDER)
      case (0)
        v = CF*a * 2.*pi*(log_mppp-log_mmpm) * q/p
      case (1)
        log_mu_s = 2.*log(MU_SOFT)
        v = CF*a * (2.*(4.*pi+A1*a)*(log_mppp-log_mmpm) &
          + B0*a*((log_mmpm-log_mu_s)**2-(log_mppp-log_mu_s)**2)) * q/(4.*p)
      case default
        call msg_fatal ("NRQCD_ORDER = " // char(NRQCD_ORDER))
    end select
  case (2)
    !!! not implemented yet
    v = zero
  case default
    call msg_fatal ("unknown ttZ/ttA vertex component, vec_type = " // char(vec_type))
end select
end function minus_q2_V

```

(ttv formfactors: procedures)+≡

```

!!! compute support points (~> q-grid) for numerical integration: trim p-grid and
!!! merge with singular points of integrand: q = p, |p-p0|, p+p0, sqrt(mpole*E)
subroutine compute_support_points (en, i_p, i_p0, n_trim)
  real(default), intent(in) :: en
  integer, intent(in) :: i_p
  integer, intent(in) :: i_p0
  integer, intent(in) :: n_trim
  real(default) :: p, p0
  real(default), dimension(4) :: sing_vals
  integer :: n_sing, i_q
  if (mod (POINTS_P, n_trim) /= 0) call msg_fatal ("trim p-grid for q-integration: POINTS_P = "
    // char(POINTS_P) // " and n_trim = " // char(n_trim))
  n_q = POINTS_P / n_trim + merge(0,1,n_trim==1)
  p = p_grid(i_p)
  p0 = p0_grid(i_p0)
  n_sing = 0
  if ( i_p /= 1 .and. mod(i_p,n_trim) /= 0 ) then
    n_sing = n_sing+1
    sing_vals(n_sing) = p
  end if
  if ( i_p0 /= 1 ) then
    n_sing = n_sing+1
    sing_vals(n_sing) = p0 + p
    if ( i_p0 /= i_p+1 ) then

```

```

        n_sing = n_sing+1
        sing_vals(n_sing) = abs( p0 - p )
    end if
end if
if ( en > 0. ) then
    n_sing = n_sing+1
    sing_vals(n_sing) = sqrt( MTPOLE * en )
end if
if ( allocated(q_grid) ) deallocate( q_grid )
allocate( q_grid(n_q+n_sing) )
q_grid(1) = p_grid(1)
q_grid(2:n_q) = [(p_grid(i_q), i_q=max(n_trim,2), POINTS_P, n_trim)]
if (n_sing > 0 ) q_grid(n_q+1:n_q+n_sing) = sing_vals(1:n_sing)
call nr_sort (q_grid)
end subroutine compute_support_points

```

(ttv formfactors: procedures)+≡

```

!!! cf. arXiv:hep-ph/9503238, validated against arXiv:hep-ph/0008171
pure function formfactor_ttv_relativistic_nlo (alphas, ps, J0) result (c)
    real(default), intent(in) :: alphas
    type(phase_space_point_t), intent(in) :: ps
    complex(default), intent(in) :: J0
    complex(default) :: c
    real(default) :: p2, k2, q2, kp, pq, kq
    complex(default) :: D2, chi, ln1, ln2, L1, L2, z, S, m2, m
    complex(default) :: JA, JB, JC, JD, JE, IA, IB, IC, ID, IE
    complex(default) :: CCmsbar
    complex(default) :: dF1, dF2, dM1, dM2
    complex(default), dimension(12) :: P1
    complex(default), parameter :: ximo = zero
    p2 = ps%p2
    k2 = ps%k2
    q2 = ps%q2
    m2 = complex_m2 (ps/mpole, GAM)
    !!! kinematic abbreviations
    kp = 0.5_default * (-q2 + p2 + k2)
    pq = 0.5_default * ( k2 - p2 - q2)
    kq = 0.5_default * (-p2 + k2 + q2)
    D2 = kp**2 - k2*p2
    chi = p2*k2*q2 + 2.*m2*((p2 + k2)*kp - 2.*p2*k2) + m2**2 * q2
    ln1 = log( (1. - p2/m2)*(1,0) + ieps )
    ln2 = log( (1. - k2/m2)*(1,0) + ieps )
    L1 = (1. - m2/p2) * ln1
    L2 = (1. - m2/k2) * ln2
    z = sqrt( (1.-4.*m2/q2)*(1,0) )
    S = 0.5_default * z * log( (z+1.)/(z-1.) + ieps )
    m = sqrt(m2)

    !!! loop integrals in terms of J0
    JA = 1./D2 * (J0/2.*(-m2*pq - p2*kq) + kp*L2 - p2*L1 - 2.*pq*S)
    JB = 1./D2 * (J0/2.*( m2*kq + k2*pq) + kp*L1 - k2*L2 + 2.*kq*S)
    JC = 1/(4.*D2) * (2.*p2 + 2*kp*m2/k2 - 4.*kp*S + 2.*kp*(1. - m2/k2)*L2 + &
        (2.*kp*(p2 - m2) + 3.*p2*(m2 - k2))*JA + p2*(m2 - p2)*JB)
    JD = 1./(4.*D2) * (2.*kp*((k2 - m2)*JA + (p2 - m2)*JB - 1.) - k2*(2.*m2/k2 &

```

```

- 2.*S + (1. - m2/k2)*L2 + (p2 - m2)*JA) - p2*(-2.*S + (1. - &
m2/p2)*L1 + (k2 - m2)*JB))
JE = 1./(4.*D2) * (2.*k2 + 2.*kp*m2/p2 - 4.*kp*S + 2.*kp*(1. - m2/p2)*L1 + &
(2.*kp*(k2 - m2) + 3.*k2*(m2 - p2))*JB + k2*(m2 - k2)*JA)
IA = 1./D2 * (-(kq/2.)*J0 - 2.*q2/chi *((m2 - p2)*k2 - (m2 - k2)*kp)*S + &
1./(m2 - p2)*(p2 - kp + p2*q2/chi *(k2 - m2)*(m2 + kp))*L1 + &
k2*q2/chi *(m2 + kp)*L2)
IB = 1./D2 * ( (pq/2.)*J0 - 2.*q2/chi *((m2 - k2)*p2 - (m2 - p2)*kp)*S + &
1./(m2 - k2)*(k2 - kp + k2*q2/chi *(p2 - m2)*(m2 + kp))*L2 + &
p2*q2/chi *(m2 + kp)*L1)
IC = 1./(4.*D2) * (2.*p2*J0 - 4.*kp/k2*(1. + m2/(k2 - m2)*L2) + (2.*kp - &
3.*p2)*JA - p2*JB + (-2.*kp*(m2 - p2) + 3.*p2*(m2 - k2))*IA + &
p2*(m2 - p2)*IB)
ID = 1./(4.*D2) * (-2.*kp*J0 + 2.*(1. + m2/(k2 - m2)*L2) + 2.*(1. + &
m2/(p2 - m2)*L1) + (2.*kp - k2)*JA + (2.*kp - p2)*JB + (k2*(m2 - &
p2) - 2.*kp*(m2 - k2))*IA + (p2*(m2 - k2) - 2.*kp*(m2 - p2))*IB)
IE = 1./(4.*D2) * (2.*k2*J0 - 4.*kp/p2*(1. + m2/(p2 - m2)*L1) + (2.*kp - &
3.*k2)*JB - k2*JA + (-2.*kp*(m2 - k2) + 3.*k2*(m2 - p2))*IB + &
k2*(m2 - k2)*IA)

!!! divergent part ~ 1/epsilon: depends on subtraction scheme
CCmsbar = -2.0_default * log(RESALE_H)

! real top mass in the loop numerators
m2 = cmplx(real(m2), kind=default)
! m = sqrt(m2)

!!! quark self energies
dF1 = - (ximo+1.) * (CCmsbar + (1.+m2/p2)*(1.-L1))
dF2 = - (ximo+1.) * (CCmsbar + (1.+m2/k2)*(1.-L2))
dM1 = m/p2 * ( (ximo+1.)*(1.+m2/p2*ln1) - 3.*ln1 )
dM2 = m/k2 * ( (ximo+1.)*(1.+m2/k2*ln2) - 3.*ln2 )

!!! coefficient list: vertex function Gamma_mu (k,p) = sum_i( Vi_mu * Pi )
P1(1) = 2.*JA - 2.*JC + ximo*(m2*IC + p2*ID)
P1(2) = 2.*JB - 2.*JE + ximo*(k2*ID + m2*IE)
P1(3) = -2.*J0 + 2.*JA + 2.*JB - 2.*JD + ximo*(-J0/2. - k2/2.*IC - &
kp*ID + m2*ID + p2/2.*IE + JA)
P1(4) = -2.*JD + ximo*(k2*IC + m2*ID - JA)
P1(5) = J0 - JA - JB + ximo*(J0/4. + k2/4.*IC + kp/2.*ID + p2/4.*IE - &
1./2.*JA - 1./2.*JB)
P1(6) = -m2*J0 - k2*JA - p2*JB + k2/2.*JC + kp*JD + p2/2.*JE + &
(1./2. + CCmsbar - 2.*S) &
+ ximo*(-m2*J0/4. - m2/4.*k2*IC - m2/2.*kp*ID - m2/4.*p2*IE &
- k2/2.*JA - p2/2.*JB + (CCmsbar + 2.))
P1(7) = 2.*m*J0 - 4.*m*JA + ximo*m*(J0/2. - 2.*kp*IC + k2/2.*IC - &
p2*ID - kp*ID - p2/2.*IE - JA)
P1(8) = 2.*m*J0 - 4.*m*JB + ximo*m*(J0/2. + k2/2.*IC - kp*ID + k2*ID - &
p2/2.*IE - JB)
P1(9) = ximo*m*(ID + IE)
P1(10) = ximo*m*(ID + IC)
P1(11) = ximo*m*( p2*ID + kp*IC + p2/2.*IE - k2/2.*IC) + dM2
!!! self energy contribution: ~ gamma_mu.k_slash = V11
P1(12) = ximo*m*(-k2*ID - kp*IE + p2/2.*IE - k2/2.*IC) + dM1

```

```

!!! self energy contribution: ~ gamma_mu.p_slash = V12

!!! leading form factor: V6 = gamma_mu, V5 = gamma_mu.k_slash.p_slash ~> -m^2*gamma_mu
c = one + alphas * CF / (4.*pi) * ( P1(6) - m2*P1(5) &
!!! self energy contributions ~ gamma^mu
+ dF1 + dF2 + m*( dM1 + dM2 ) )
!!! on-shell subtraction: UV divergence cancels
+ 0.5_default*( dF1 + dF2 + m*( dM1 + dM2 ) )
!
end function formfactor_ttv_relativistic_nlo

<ttv formfactors: procedures>+=
pure function sqrts_to_en (sqrts, mpole_in) result (en)
real(default), intent(in) :: sqrts
real(default), intent(in), optional :: mpole_in
real(default) :: mpole, en
if (present (mpole_in)) then
mpole = mpole_in
else
mpole = m1s_to_mpole (sqrts)
end if
en = sqrts - two * mpole
end function sqrts_to_en

<ttv formfactors: procedures>+=
function p_grid_from_TOPPIK (mpole_in) result (p_topplik)
real(default), intent(in), optional :: mpole_in
real(default), dimension(POINTS_P) :: p_topplik
real(default) :: mpole
if (debug_on) call msg_debug (D_THRESHOLD, "p_grid_from_TOPPIK")
mpole = MTPOLE; if (present (mpole_in)) mpole = mpole_in
call scan_formfactor_over_p_TOPPIK &
(alphas_soft(2. * M1S), 2. * M1S, 1, p_topplik, mpole)
if (.not. strictly_monotonous (p_topplik)) &
call msg_fatal ("p_grid NOT strictly monotonous!")
end function p_grid_from_TOPPIK

<ttv formfactors: procedures>+=
pure function int_to_char (i) result (c)
integer, intent(in) :: i
character(len=len(trim(int2fixed(i)))) :: c
c = int2char (i)
end function int_to_char

<ttv formfactors: procedures>+=
pure function real_to_char (r) result (c)
real(default), intent(in) :: r
character(len=len(trim(real2fixed(r)))) :: c
c = real2char (r)
end function real_to_char

```

(ttv formfactors: procedures)+≡

```

pure function complex_to_char (z) result (c)
  complex(default), intent(in) :: z
  character(len=len(trim(real2fixed(real(z))))+len(trim(real2fixed(aimag(z))))+5) :: c
  character(len=len(trim(real2fixed(real(z)))) :: re
  character(len=len(trim(real2fixed(aimag(z)))) :: im
  re = real_to_char (real(z))
  im = real_to_char (aimag(z))
  if (nearly_equal (aimag(z), zero)) then
    c = re
  else
    c = re // " + " // im // "*I"
  end if
end function complex_to_char

```

(ttv formfactors: procedures)+≡

```

pure function logical_to_char (l) result (c)
  logical, intent(in) :: l
  character(len=1) :: c
  write (c, '(l1)') l
end function logical_to_char

```

(ttv formfactors: procedures)+≡

```

subroutine get_rest_frame (p1_in, p2_in, p1_out, p2_out)
  type(vector4_t), intent(in) :: p1_in, p2_in
  type(vector4_t), intent(out) :: p1_out, p2_out
  type(lorentz_transformation_t) :: L
  L = inverse (boost (p1_in + p2_in, (p1_in + p2_in)**1))
  p1_out = L * p1_in; p2_out = L * p2_in
end subroutine get_rest_frame

function shift_momentum (p_in, E, p) result (p_out)
  type(vector4_t) :: p_out
  type(vector4_t), intent(in) :: p_in
  real(default), intent(in) :: E, p
  type(vector3_t) :: vec
  vec = p_in%p(1:3) / space_part_norm (p_in)
  p_out = vector4_moving (E, p * vec)
end function shift_momentum

subroutine evaluate_one_to_two_splitting_threshold (p_origin, &
  p1_in, p2_in, p1_out, p2_out, msq_in, jac)
  type(vector4_t), intent(in) :: p_origin
  type(vector4_t), intent(in) :: p1_in, p2_in
  type(vector4_t), intent(inout) :: p1_out, p2_out
  real(default), intent(in), optional :: msq_in
  real(default), intent(inout), optional :: jac
  type(lorentz_transformation_t) :: L
  type(vector4_t) :: p1_rest, p2_rest
  real(default) :: msq, msq1, msq2
  real(default) :: m
  real(default) :: E1, E2, E_max
  real(default) :: p, lda

```

```

real(default), parameter :: E_offset = 0.001_default
!!! (TODO-cw-2016-10-13) Find a better way to get masses
real(default), parameter :: mb = 4.2_default
real(default), parameter :: mw = 80.419_default

call get_rest_frame (p1_in, p2_in, p1_rest, p2_rest)

msq = p_origin**2; m = sqrt(msq)
msq1 = p1_in**2
msq2 = m * (m - two * p1_rest%p(0))
E1 = (msq + msq1 - msq2) / (two * m)
E_max = (msq - (mb + mw)**2) / (two * m)
E_max = E_max - E_offset
if (E1 > E_max) then
    E1 = E_max
    msq2 = m * (m - two * E_max)
end if

lda = lambda (msq, msq1, msq2)
if (lda < zero) call msg_fatal &
    ("Threshold Splitting: lambda < 0 encountered! Use a higher offset.")
p = sqrt(lda) / (two * m)

E1 = sqrt (msq1 + p**2)
E2 = sqrt (msq2 + p**2)

p1_out = shift_momentum (p1_rest, E1, p)
p2_out = shift_momentum (p2_rest, E2, p)

L = boost (p_origin, p_origin**1)
p1_out = L * p1_out
p2_out = L * p2_out
end subroutine evaluate_one_to_two_splitting_threshold

```

```

<ttv formfactors: public>+≡
    public :: generate_on_shell_decay_threshold

<ttv formfactors: procedures>+≡
    subroutine generate_on_shell_decay_threshold (p_decay, p_top, p_decay_onshell)
        !!! Gluon must be on first position in this array
        type(vector4_t), intent(in), dimension(:) :: p_decay
        type(vector4_t), intent(inout) :: p_top
        type(vector4_t), intent(inout), dimension(:) :: p_decay_onshell
        procedure(evaluate_one_to_two_splitting_special), pointer :: ppointer
        ppointer => evaluate_one_to_two_splitting_threshold
        call generate_on_shell_decay (p_top, p_decay, p_decay_onshell, 1, &
            evaluate_special = ppointer)
    end subroutine generate_on_shell_decay_threshold

```

29.0.1 Unit tests

Test module, followed by the corresponding implementation module.

```

<ttv formfactors.ut.f90>≡

```



```

    <File header>

    module ttv_formfactors_ut
        use unit_tests
        use ttv_formfactors_util

    <Standard module head>

    <ttv formfactors: public test>

    contains

    <ttv formfactors: test driver>

    end module ttv_formfactors_ut
<ttv_formfactors_util.f90>≡
    <File header>

    module ttv_formfactors_util

    <Use kinds>
    <Use debug>
        use constants
        use ttv_formfactors
        use diagnostics
        use sm_physics, only: running_as
        use numeric_utils

    <Standard module head>

    <ttv formfactors: test declarations>

    contains

    <ttv formfactors: tests>

    end module ttv_formfactors_util
API: driver for the unit tests below.
<ttv formfactors: public test>≡
    public :: ttv_formfactors_test
<ttv formfactors: test driver>≡
    subroutine ttv_formfactors_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <ttv formfactors: execute tests>
    end subroutine ttv_formfactors_test

```

Basic setup

```

<ttv formfactors: execute tests>≡

```

```

call test(ttv_formfactors_1, "ttv_formfactors_1", &
        "Basic setup", u, results)

<ttv formfactors: test declarations>≡
public :: ttv_formfactors_1

<ttv formfactors: tests>≡
subroutine ttv_formfactors_1 (u)
    integer, intent(in) :: u
    real(default) :: m1s, Vtb, wt_inv, alphaemi, sw, alphas_mz, mz, &
        mw, mb, sh, sf, NRQCD_ORDER, FF, offshell_strategy, v1, v2, &
        scan_sqrts_max, sqrts, scan_sqrts_min, scan_sqrts_stepsize, &
        test, gam_out, mpole
    type(formfactor_t) :: formfactor
    type(phase_space_point_t) :: ps
    logical :: mpole_fixed
    integer :: top_helicity_selection
    write (u, "(A)")  "* Test output: ttv_formfactors_1"
    write (u, "(A)")  "* Purpose: Basic setup"
    write (u, "(A)")

    m1s = 172.0_default
    Vtb = one
    wt_inv = zero
    alphaemi = 125.0_default
    alphas_mz = 0.118_default
    mz = 91.1876_default
    mw = 80.399_default
    sw = sqrt(one - mw**2 / mz**2)
    mb = 4.2_default
    sh = one
    sf = one
    NRQCD_ORDER = one
    FF = MATCHED
    offshell_strategy = 0
    top_helicity_selection = -1
    v1 = 0.3_default
    v2 = 0.5_default
    scan_sqrts_stepsize = 0.0_default
    test = - one
    write (u, "(A)") "Check high energy behavior"
    sqrts = 500.0_default
    scan_sqrts_min = sqrts
    scan_sqrts_max = sqrts
    write (u, "(A)") "Check that the mass is not fixed"
    mpole_fixed = .false.

    <(re)start grid>
    call threshold%formfactor%activate ()
    call formfactor%activate ()
    call assert (u, m1s_to_mpole (350.0_default) > m1s + 0.1_default, &
        "m1s_to_mpole (350.0_default) > m1s")
    write (u, "(A)")

    ! For simplicity we test on-shell back-to-back tops

```

```

call ps%init (m1s**2, m1s**2, sqrts**2, mpole)
call assert_equal (u, f_switch_off (v_matching (ps%sqrts, GAM_M1S)), tiny_10, &
  "f_switch_off (v_matching (ps%sqrts, GAM_M1S))")
call assert (u, &
  abs (formfactor%compute (ps, 1, EXPANDED_HARD)) > &
  abs (formfactor%compute (ps, 1, RESUMMED)), &
  "expansion with hard alphas should be larger " // &
  "than resummed (with switchoff)")
call assert_equal (u, &
  abs (formfactor%compute (ps, 1, RESUMMED)), zero, &
  "resummed (with switchoff) should be zero", abs_smallness=tiny_10)
call assert_equal (u, &
  abs (formfactor%compute (ps, 1, EXPANDED_SOFT_SWITCHOFF)), zero, &
  "expanded (with switchoff) should be zero", abs_smallness=tiny_10)
write (u, "(A)") ""

write (u, "(A)") "Check global variables"
call assert_equal (u, AS_HARD, &
  running_as (m1s, alphas_mz, mz, 2, 5.0_default), "hard alphas")
call assert_equal (u, AS_SOFT, zero, "soft alphas", abs_smallness=tiny_10)
call assert_equal (u, AS_USOFT, zero, "ultrasoft alphas", abs_smallness=tiny_10)
call assert_equal (u, AS_LL_SOFT, zero, "LL soft alphas", abs_smallness=tiny_10)

!!! care: the formfactor contains the tree level that we usually subtract again
write (u, "(A)") "Check low energy behavior"
sqrts = 2 * m1s + 0.01_default
scan_sqrts_min = sqrts
scan_sqrts_max = sqrts
write (u, "(A)") "Check that the mass is fixed"
mpole_fixed = .true.
<(re)start grid>

call ps%init (m1s**2, m1s**2, sqrts**2, mpole)
call assert_equal (u, m1s_to_mpole (350.0_default), m1s, &
  "m1s_to_mpole (350.0_default) == m1s")
call assert_equal (u, m1s_to_mpole (550.0_default), m1s, &
  "m1s_to_mpole (550.0_default) == m1s")
write (u, "(A)") ""
call assert_equal (u, f_switch_off (v_matching (ps%sqrts, GAM_M1S)), one, "f_switch_off (v_mat
call formfactor%disable ()
call assert_equal (u, &
  abs (formfactor%compute (ps, 1, 1)), &
  zero, &
  "disabled formfactor should return zero")
call formfactor%activate ()
call assert_equal (u, &
  formfactor%compute (ps, 1, EXPANDED_SOFT_SWITCHOFF), &
  formfactor%compute (ps, 1, EXPANDED_SOFT), &
  "switchoff function should do nothing here")
write (u, "(A)") ""

write (u, "(A)") "* Test output end: ttv_formfactors_1"
end subroutine ttv_formfactors_1

```

```

<(re)start grid>≡
  call init_parameters &
    (mpole, gam_out, mls, Vtb, wt_inv, &
     alphaemi, sw, alphas_mz, mz, mw, &
     mb, sh, sf, NRQCD_ORDER, FF, offshell_strategy, &
     v1, v2, scan_sqrts_min, scan_sqrts_max, &
     scan_sqrts_stepsize, mpole_fixed, real(top_helicity_selection, default))
  call init_threshold_grids (test)

```

Test flags

```

<ttv formfactors: execute tests>+≡
  call test(ttv_formfactors_2, "ttv_formfactors_2", &
    "Test flags", u, results)

<ttv formfactors: test declarations>+≡
  public :: ttv_formfactors_2

<ttv formfactors: tests>+≡
  subroutine ttv_formfactors_2 (u)
    integer, intent(in) :: u
    write (u, "(A)")  "* Test output: ttv_formfactors_2"
    write (u, "(A)")  "* Purpose: Test flags"
    write (u, "(A)")

    write (u, "(A)") "RESUMMED_SWITCHOFF + NLO"
    call threshold%settings%setup_flags (-2, 1, -1)
    call assert (u, SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
    call assert (u, TOPPIK_RESUMMED, "TOPPIK_RESUMMED")
    call assert (u, threshold%settings%nlo, "threshold%settings%nlo")
    call assert (u, .not. threshold%settings%factorized_computation, &
      ".not. threshold%settings%factorized_computation")
    call assert (u, .not. threshold%settings%interference, &
      ".not. threshold%settings%interference")
    call assert (u, .not. threshold%settings%no_nlo_width_in_signal_propagators, &
      ".not. threshold%settings%no_nlo_width_in_signal_propagators")

    write (u, "(A)") "MATCHED + FACTORIZATION"
    call threshold%settings%setup_flags (-1, 0+2, -1)
    call assert (u, .not. threshold%settings%nlo, ".not. threshold%settings%nlo")
    call assert (u, TOPPIK_RESUMMED, "TOPPIK_RESUMMED")
    call assert (u, threshold%settings%factorized_computation, &
      "threshold%settings%factorized_computation")

    write (u, "(A)") "RESUMMED + INTERFERENCE"
    call threshold%settings%setup_flags (1, 0+0+4, -1)
    call assert (u, .not. SWITCHOFF_RESUMMED, ".not. SWITCHOFF_RESUMMED")
    call assert (u, TOPPIK_RESUMMED, "TOPPIK_RESUMMED")
    call assert (u, .not. threshold%settings%nlo, ".not. threshold%settings%nlo")
    call assert (u, .not. threshold%settings%factorized_computation, &
      ".not. threshold%settings%factorized_computation")
    call assert (u, threshold%settings%interference, "threshold%settings%interference")

    write (u, "(A)") "EXPANDED_HARD"
    call threshold%settings%setup_flags (4, 0+2+4, -1)

```

```

call assert (u, .not. SWITCHOFF_RESUMMED, ".not. SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, ".not. threshold%settings%nlo")
call assert (u, threshold%settings%factorized_computation, &
    "threshold%settings%factorized_computation")
call assert (u, threshold%settings%interference, "threshold%settings%interference")

write (u, "(A)") "EXPANDED_SOFT"
call threshold%settings%setup_flags (5, 1+2+4, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, ".not. SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, threshold%settings%factorized_computation, &
    "threshold%settings%factorized_computation")
call assert (u, threshold%settings%interference, &
    "threshold%settings%interference")

write (u, "(A)") "EXPANDED_SOFT_SWITCHOFF"
call threshold%settings%setup_flags (6, 0+0+0+8, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, .not. threshold%settings%factorized_computation, &
    "threshold%settings%factorized_computation")
call assert (u, .not. threshold%settings%interference, &
    "threshold%settings%interference")

write (u, "(A)") "RESUMMED_ANALYTIC_LL"
call threshold%settings%setup_flags (7, 0+0+4+8, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, .not. threshold%settings%factorized_computation, &
    "threshold%settings%factorized_computation")
call assert (u, threshold%settings%interference, "threshold%settings%interference")
call assert (u, threshold%settings%onshell_projection%production, &
    "threshold%settings%onshell_projection%production")

write (u, "(A)") "EXPANDED_SOFT_HARD"
call threshold%settings%setup_flags (8, 0+2+0+128, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")
call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, .not. threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, threshold%settings%factorized_computation, &
    "threshold%settings%factorized_computation")
call assert (u, .not. threshold%settings%interference, "threshold%settings%interference")
call assert (u, .not. threshold%settings%onshell_projection%production, &
    "threshold%settings%onshell_projection%production")
call assert (u, threshold%settings%onshell_projection%decay, &
    "threshold%settings%onshell_projection%decay")

write (u, "(A)") "EXTRA_TREE"
call threshold%settings%setup_flags (9, 1+0+0+16+64, -1)
call assert (u, .not. SWITCHOFF_RESUMMED, "SWITCHOFF_RESUMMED")

```

```

call assert (u, .not. TOPPIK_RESUMMED, ".not. TOPPIK_RESUMMED")
call assert (u, threshold%settings%nlo, "threshold%settings%nlo")
call assert (u, .not. threshold%settings%factorized_computation, &
"threshold%settings%factorized_computation")
call assert (u, .not. threshold%settings%interference, "threshold%settings%interference")
call assert (u, threshold%settings%onshell_projection%production, &
"threshold%settings%onshell_projection%production")
call assert (u, .not. threshold%settings%onshell_projection%decay, &
"threshold%settings%onshell_projection%decay")
call assert (u, threshold%settings%no_nlo_width_in_signal_propagators, &
"threshold%settings%no_nlo_width_in_signal_propagators")

write (u, "(A)") "test projection of width"
call threshold%settings%setup_flags (9, 0+0+0+256, -1)
call assert (u, .not. threshold%settings%onshell_projection%production, &
"threshold%settings%onshell_projection%production")
call assert (u, .not. threshold%settings%onshell_projection%decay, &
"threshold%settings%onshell_projection%decay")
call assert (u, .not. threshold%settings%onshell_projection%width, &
"threshold%settings%onshell_projection%width")

write (u, "(A)") "test boost of decay momenta"
call threshold%settings%setup_flags (9, 512, -1)
if (debug_on) call msg_debug (D_THRESHOLD, &
"threshold%settings%onshell_projection%boost_decay", &
threshold%settings%onshell_projection%boost_decay)
call threshold%settings%setup_flags (9, 0, -1)
if (debug_on) call msg_debug (D_THRESHOLD, &
".not. threshold%settings%onshell_projection%boost_decay", &
.not. threshold%settings%onshell_projection%boost_decay)

write (u, "(A)") "test helicity approximations"
call threshold%settings%setup_flags (9, 32, -1)
call assert (u, threshold%settings%helicity_approximation%simple, &
"threshold%settings%helicity_approximation%simple")
call assert (u, .not. threshold%settings%helicity_approximation%extra, &
".not. threshold%settings%helicity_approximation%extra")
call assert (u, .not. threshold%settings%helicity_approximation%ultra, &
".not. threshold%settings%helicity_approximation%ultra")
call threshold%settings%setup_flags (9, 1024, -1)
call assert (u, .not. threshold%settings%helicity_approximation%simple, &
".not. threshold%settings%helicity_approximation%simple")
call assert (u, threshold%settings%helicity_approximation%extra, &
"threshold%settings%helicity_approximation%extra")

write (u, "(A)")
write (u, "(A)") "* Test output end: ttv_formfactors_2"
end subroutine ttv_formfactors_2

```

Chapter 30

Integration and Process Objects

This is the central part of the WHIZARD package. It provides the functionality for evaluating structure functions, kinematics and matrix elements, integration and event generation. It combines the various parts that deal with those tasks individually and organizes the data transfer between them.

subevt_expr This enables process observables as (abstract) expressions, to be evaluated for each process call.

parton_states A `parton_state_t` object represents an elementary partonic interaction. There are two versions: one for the isolated elementary process, one for the elementary process convoluted with the structure-function chain. The parton state is an effective state. It needs not coincide with the seed-kinematics state which is used in evaluating phase space.

process Here, all pieces are combined for the purpose of evaluating the elementary processes. The whole algorithm is coded in terms of abstract data types as defined in the appropriate modules: `prc_core` for matrix-element evaluation, `prc_core_def` for the associated configuration and driver, `sf_base` for beams and structure-functions, `phs_base` for phase space, and `mci_base` for integration and event generation.

process_config

process_counter Very simple object for statistics

process_mci

pcm

kinematics

instances While the above modules set up all static information, the instances have the changing event data. There are term and process instances but no component instances.

process_stacks Process stacks collect process objects.

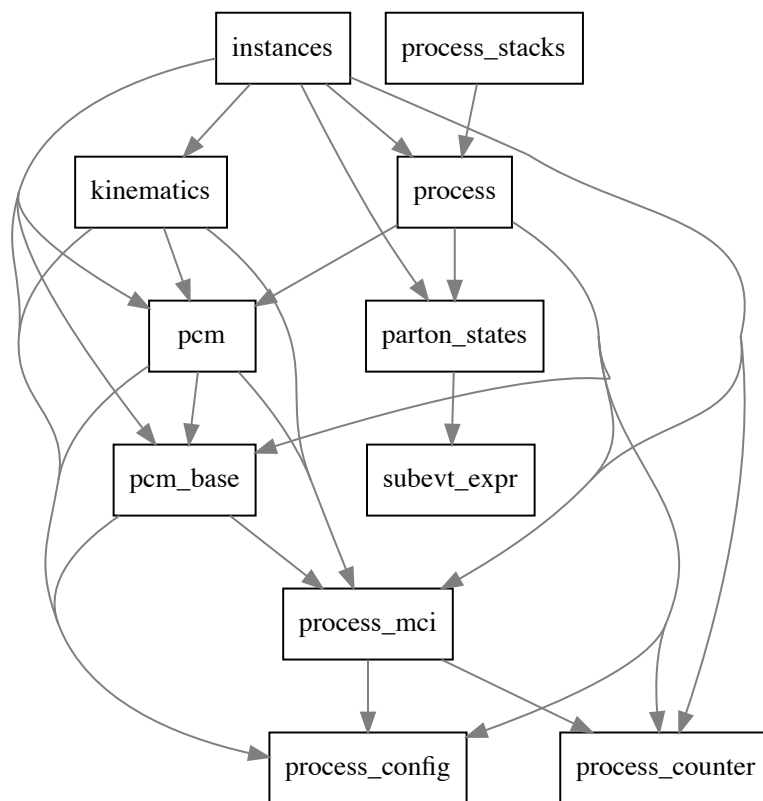


Figure 30.1: Module dependencies in `src/process_integration`.

We combine here hard interactions, phase space, and (for scatterings) structure functions and interfaces them to the integration module.

The process object implements the combination of a fixed beam and structure-function setup with a number of elementary processes. The latter are called process components. The process object represents an entity which is supposedly observable. It should be meaningful to talk about the cross section of a process.

The individual components of a process are, technically, processes themselves, but they may have unphysical cross sections which have to be added for a physical result. Process components may be exclusive tree-level elementary processes, dipole subtraction term, loop corrections, etc.

The beam and structure function setup is common to all process components. Thus, there is only one instance of this part.

The process may be a scattering process or a decay process. In the latter case, there are no structure functions, and the beam setup consists of a single particle. Otherwise, the two classes are treated on the same footing.

Once a sampling point has been chosen, a process determines a set of partons with a correlated density matrix of quantum numbers. In general, each sampling point will generate, for each process component, one or more distinct parton configurations. This is the **computed** state. The computed state is the subject of the multi-channel integration algorithm.

For NLO computations, it is necessary to project the computed states onto another set of parton configurations (e.g., by recombining certain pairs). This is the **observed** state. When computing partonic observables, the information is taken from the observed state.

For the purpose of event generation, we will later select one parton configuration from the observed state and collapse the correlated quantum state. This configuration is then dressed by applying parton shower, decays and hadronization. The decay chain, in particular, combines a scattering process with possible subsequent decay processes on the parton level, which are full-fledged process objects themselves.

30.1 Process observables

We define an abstract **subevt_expr_t** object as an extension of the **subevt_t** type. The object contains a local variable list, variable instances (as targets for pointers in the variable list), and evaluation trees. The evaluation trees reference both the variables and the **subevt**.

There are two instances of the abstract type: one for process instances, one for physical events. Both have a common logical expression **selection** which determines whether the object passes user-defined cuts.

The intention is that we fill the **subevt_t** base object and compute the variables once we have evaluated a kinematical phase space point (or a complete event). We then evaluate the expressions and can use the results in further calculations.

The **process_expr_t** extension contains furthermore scale and weight expressions. The **event_expr_t** extension contains a reweighting-factor expression and a logical expression for event analysis. In practice, we will link the

variable list of the `event_obs` object to the variable list of the currently active `process_obs` object, such that the process variables are available to both objects. Event variables are meaningful only for physical events.

Note that there are unit tests, but they are deferred to the `expr_tests` module.

```

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

    <Use kinds>
    <Use strings>
    use constants, only: zero, one
    use io_units
    use format_utils, only: write_separator
    use diagnostics
    use lorentz
    use subevents
    use variables
    use flavors
    use quantum_numbers
    use interactions
    use particles
    use expr_base

    <Standard module head>

    <Subvt expr: public>

    <Subvt expr: types>

    <Subvt expr: interfaces>

    contains

    <Subvt expr: procedures>

  end module subvt_expr

```

30.1.1 Abstract base type

```

<Subvt expr: types>≡
  type, extends (subvt_t), abstract :: subvt_expr_t
    logical :: subvt_filled = .false.
    type(var_list_t) :: var_list
    real(default) :: sqrts_hat = 0
    integer :: n_in = 0
    integer :: n_out = 0
    integer :: n_tot = 0
    logical :: has_selection = .false.
    class(expr_t), allocatable :: selection
    logical :: colorize_subvt = .false.
  contains
    <Subvt expr: subvt expr: TBP>

```

```
end type subevt_expr_t
```

Output: Base and extended version. We already have a `write` routine for the `subevt_t` parent type.

```
<Subevt expr: subevt expr: TBP>≡
  procedure :: base_write => subevt_expr_write

<Subevt expr: procedures>≡
  subroutine subevt_expr_write (object, unit, pacified)
    class(subevt_expr_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacified
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Local variables:"
    call write_separator (u)
    call var_list_write (object%var_list, u, follow_link=.false., &
      pacified = pacified)
    call write_separator (u)
    if (object%subevt_filled) then
      call object%subevt_t%write (u, pacified = pacified)
      if (object%has_selection) then
        call write_separator (u)
        write (u, "(1x,A)") "Selection expression:"
        call write_separator (u)
        call object%selection%write (u)
      end if
    else
      write (u, "(1x,A)") "subevt: [undefined]"
    end if
  end subroutine subevt_expr_write
```

Finalizer.

```
<Subevt expr: subevt expr: TBP>+≡
  procedure (subevt_expr_final), deferred :: final
  procedure :: base_final => subevt_expr_final

<Subevt expr: procedures>+≡
  subroutine subevt_expr_final (object)
    class(subevt_expr_t), intent(inout) :: object
    call object%var_list%final ()
    if (object%has_selection) then
      call object%selection%final ()
    end if
  end subroutine subevt_expr_final
```

30.1.2 Initialization

Initialization: define local variables and establish pointers.

The common variables are `sqrts` (the nominal beam energy, fixed), `sqrts_hat` (the actual energy), `n.in`, `n.out`, and `n.tot` for the `subevt`. With the exception

of `sqrts`, all are implemented as pointers to subobjects.

```

<Subevt expr: subevt expr: TBP>+≡
  procedure (subevt_expr_setup_vars), deferred :: setup_vars
  procedure :: base_setup_vars => subevt_expr_setup_vars

<Subevt expr: procedures>+≡
  subroutine subevt_expr_setup_vars (expr, sqrts)
    class(subevt_expr_t), intent(inout), target :: expr
    real(default), intent(in) :: sqrts
    call expr%var_list%final ()
    call var_list_append_real (expr%var_list, &
      var_str ("sqrts"), sqrts, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_real_ptr (expr%var_list, &
      var_str ("sqrts_hat"), expr%sqrts_hat, &
      is_known = expr%subevt_filled, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_int_ptr (expr%var_list, &
      var_str ("n_in"), expr%n_in, &
      is_known = expr%subevt_filled, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_int_ptr (expr%var_list, &
      var_str ("n_out"), expr%n_out, &
      is_known = expr%subevt_filled, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_int_ptr (expr%var_list, &
      var_str ("n_tot"), expr%n_tot, &
      is_known = expr%subevt_filled, &
      locked = .true., verbose = .false., intrinsic = .true.)
  end subroutine subevt_expr_setup_vars

```

Append the subevent `expr` (its base-type core) itself to the variable list, if it is not yet present.

```

<Subevt expr: subevt expr: TBP>+≡
  procedure :: setup_var_self => subevt_expr_setup_var_self

<Subevt expr: procedures>+≡
  subroutine subevt_expr_setup_var_self (expr)
    class(subevt_expr_t), intent(inout), target :: expr
    if (.not. expr%var_list%contains (var_str ("@evt"))) then
      call var_list_append_subevt_ptr &
        (expr%var_list, &
        var_str ("@evt"), expr%subevt_t, &
        is_known = expr%subevt_filled, &
        locked = .true., verbose = .false., intrinsic=.true.)
    end if
  end subroutine subevt_expr_setup_var_self

```

Link a variable list to the local one. This could be done event by event, but before evaluating expressions.

```

<Subevt expr: subevt expr: TBP>+≡
  procedure :: link_var_list => subevt_expr_link_var_list

```

```

<Subvt expr: procedures>+≡
  subroutine subvt_expr_link_var_list (expr, var_list)
    class(subvt_expr_t), intent(inout) :: expr
    type(var_list_t), intent(in), target :: var_list
    call expr%var_list%link (var_list)
  end subroutine subvt_expr_link_var_list

```

Compile the selection expression. If there is no expression, the build method will not allocate the expression object.

```

<Subvt expr: subvt expr: TBP>+≡
  procedure :: setup_selection => subvt_expr_setup_selection

<Subvt expr: procedures>+≡
  subroutine subvt_expr_setup_selection (expr, ef_cuts)
    class(subvt_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_cuts
    call ef_cuts%build (expr%selection)
    if (allocated (expr%selection)) then
      call expr%setup_var_self ()
      call expr%selection%setup_lexpr (expr%var_list)
      expr%has_selection = .true.
    end if
  end subroutine subvt_expr_setup_selection

```

(De)activate color storage and evaluation for the expression. The subevent particles will have color information.

```

<Subvt expr: subvt expr: TBP>+≡
  procedure :: colorize => subvt_expr_colorize

<Subvt expr: procedures>+≡
  subroutine subvt_expr_colorize (expr, colorize_subvt)
    class(subvt_expr_t), intent(inout), target :: expr
    logical, intent(in) :: colorize_subvt
    expr%colorize_subvt = colorize_subvt
  end subroutine subvt_expr_colorize

```

30.1.3 Evaluation

Reset to initial state, i.e., mark the subvt as invalid.

```

<Subvt expr: subvt expr: TBP>+≡
  procedure :: reset_contents => subvt_expr_reset_contents
  procedure :: base_reset_contents => subvt_expr_reset_contents

<Subvt expr: procedures>+≡
  subroutine subvt_expr_reset_contents (expr)
    class(subvt_expr_t), intent(inout) :: expr
    expr%subvt_filled = .false.
  end subroutine subvt_expr_reset_contents

```

Evaluate the selection expression and return the result. There is also a deferred version: this should evaluate the remaining expressions if the event has passed.

```

<Subvt expr: subvt expr: TBP>+≡
  procedure :: base_evaluate => subvt_expr_evaluate

```

```

<Subvt expr: procedures>+≡
  subroutine subvt_expr_evaluate (expr, passed)
    class(subvt_expr_t), intent(inout) :: expr
    logical, intent(out) :: passed
    if (expr%has_selection) then
      call expr%selection%evaluate ()
      if (expr%selection%is_known ()) then
        passed = expr%selection%get_log ()
      else
        call msg_error ("Evaluate selection expression: result undefined")
        passed = .false.
      end if
    else
      passed = .true.
    end if
  end subroutine subvt_expr_evaluate

```

30.1.4 Implementation for partonic events

This implementation contains the expressions that we can evaluate for the partonic process during integration.

```

<Subvt expr: public>≡
  public :: parton_expr_t

<Subvt expr: types>+≡
  type, extends (subvt_expr_t) :: parton_expr_t
    integer, dimension(:), allocatable :: i_beam
    integer, dimension(:), allocatable :: i_in
    integer, dimension(:), allocatable :: i_out
    logical :: has_scale = .false.
    logical :: has_fac_scale = .false.
    logical :: has_ren_scale = .false.
    logical :: has_weight = .false.
    class(expr_t), allocatable :: scale
    class(expr_t), allocatable :: fac_scale
    class(expr_t), allocatable :: ren_scale
    class(expr_t), allocatable :: weight
  contains
    <Subvt expr: parton expr: TBP>
  end type parton_expr_t

```

Finalizer.

```

<Subvt expr: parton expr: TBP>≡
  procedure :: final => parton_expr_final

<Subvt expr: procedures>+≡
  subroutine parton_expr_final (object)
    class(parton_expr_t), intent(inout) :: object
    call object%base_final ()
    if (object%has_scale) then
      call object%scale%final ()
    end if
    if (object%has_fac_scale) then

```

```

        call object%fac_scale%final ()
    end if
    if (object%has_ren_scale) then
        call object%ren_scale%final ()
    end if
    if (object%has_weight) then
        call object%weight%final ()
    end if
end subroutine parton_expr_final

```

Output: continue writing the active expressions, after the common selection expression.

Note: the `prefix` argument is declared in the `write` method of the `subevt_t` base type. Here, it is unused.

(Subevt expr: parton expr: TBP)+≡

```

    procedure :: write => parton_expr_write

```

(Subevt expr: procedures)+≡

```

    subroutine parton_expr_write (object, unit, prefix, pacified)
    class(parton_expr_t), intent(in) :: object
    integer, intent(in), optional :: unit
    character(*), intent(in), optional :: prefix
    logical, intent(in), optional :: pacified
    integer :: u
    u = given_output_unit (unit)
    call object%base_write (u, pacified = pacified)
    if (object%subevt_filled) then
        if (object%has_scale) then
            call write_separator (u)
            write (u, "(1x,A)") "Scale expression:"
            call write_separator (u)
            call object%scale%write (u)
        end if
        if (object%has_fac_scale) then
            call write_separator (u)
            write (u, "(1x,A)") "Factorization scale expression:"
            call write_separator (u)
            call object%fac_scale%write (u)
        end if
        if (object%has_ren_scale) then
            call write_separator (u)
            write (u, "(1x,A)") "Renormalization scale expression:"
            call write_separator (u)
            call object%ren_scale%write (u)
        end if
        if (object%has_weight) then
            call write_separator (u)
            write (u, "(1x,A)") "Weight expression:"
            call write_separator (u)
            call object%weight%write (u)
        end if
    end if
end subroutine parton_expr_write

```

Define variables.

```

<Subevt expr: parton expr: TBP>+≡
  procedure :: setup_vars => parton_expr_setup_vars

<Subevt expr: procedures>+≡
  subroutine parton_expr_setup_vars (expr, sqrts)
    class(parton_expr_t), intent(inout), target :: expr
    real(default), intent(in) :: sqrts
    call expr%base_setup_vars (sqrts)
  end subroutine parton_expr_setup_vars

```

Compile the scale expressions. If a pointer is disassociated, there is no expression.

```

<Subevt expr: parton expr: TBP>+≡
  procedure :: setup_scale => parton_expr_setup_scale
  procedure :: setup_fac_scale => parton_expr_setup_fac_scale
  procedure :: setup_ren_scale => parton_expr_setup_ren_scale

<Subevt expr: procedures>+≡
  subroutine parton_expr_setup_scale (expr, ef_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_scale
    call ef_scale%build (expr%scale)
    if (allocated (expr%scale)) then
      call expr%setup_var_self ()
      call expr%scale%setup_expr (expr%var_list)
      expr%has_scale = .true.
    end if
  end subroutine parton_expr_setup_scale

  subroutine parton_expr_setup_fac_scale (expr, ef_fac_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_fac_scale
    call ef_fac_scale%build (expr%fac_scale)
    if (allocated (expr%fac_scale)) then
      call expr%setup_var_self ()
      call expr%fac_scale%setup_expr (expr%var_list)
      expr%has_fac_scale = .true.
    end if
  end subroutine parton_expr_setup_fac_scale

  subroutine parton_expr_setup_ren_scale (expr, ef_ren_scale)
    class(parton_expr_t), intent(inout), target :: expr
    class(expr_factory_t), intent(in) :: ef_ren_scale
    call ef_ren_scale%build (expr%ren_scale)
    if (allocated (expr%ren_scale)) then
      call expr%setup_var_self ()
      call expr%ren_scale%setup_expr (expr%var_list)
      expr%has_ren_scale = .true.
    end if
  end subroutine parton_expr_setup_ren_scale

```

Compile the weight expression.

```

<Subevt expr: parton expr: TBP>+≡

```



```

    procedure :: setup_weight => parton_expr_setup_weight
  <Subevt expr: procedures>+≡
    subroutine parton_expr_setup_weight (expr, ef_weight)
      class(parton_expr_t), intent(inout), target :: expr
      class(expr_factory_t), intent(in) :: ef_weight
      call ef_weight%build (expr%weight)
      if (allocated (expr%weight)) then
        call expr%setup_var_self ()
        call expr%weight%setup_expr (expr%var_list)
        expr%has_weight = .true.
      end if
    end subroutine parton_expr_setup_weight

```

Filling the partonic state consists of two parts. The first routine prepares the subevt without assigning momenta. It takes the particles from an `interaction_t`. It needs the indices and flavors for the beam, incoming, and outgoing particles.

We can assume that the particle content of the subevt does not change. Therefore, we set the event variables `n_in`, `n_out`, `n_tot` already in this initialization step.

```

  <Subevt expr: parton expr: TBP>+≡
    procedure :: setup_subevt => parton_expr_setup_subevt
  <Subevt expr: procedures>+≡
    subroutine parton_expr_setup_subevt (expr, int, &
      i_beam, i_in, i_out, f_beam, f_in, f_out)
      class(parton_expr_t), intent(inout) :: expr
      type(interaction_t), intent(in), target :: int
      integer, dimension(:), intent(in) :: i_beam, i_in, i_out
      type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
      allocate (expr%i_beam (size (i_beam)))
      allocate (expr%i_in (size (i_in)))
      allocate (expr%i_out (size (i_out)))
      expr%i_beam = i_beam
      expr%i_in = i_in
      expr%i_out = i_out
      call interaction_to_subevt (int, &
        expr%i_beam, expr%i_in, expr%i_out, expr%subevt_t)
      call subevt_set_pdg_beam (expr%subevt_t, f_beam%get_pdg ())
      call subevt_set_pdg_incoming (expr%subevt_t, f_in%get_pdg ())
      call subevt_set_pdg_outgoing (expr%subevt_t, f_out%get_pdg ())
      call subevt_set_p2_beam (expr%subevt_t, f_beam%get_mass () ** 2)
      call subevt_set_p2_incoming (expr%subevt_t, f_in%get_mass () ** 2)
      call subevt_set_p2_outgoing (expr%subevt_t, f_out%get_mass () ** 2)
      expr%n_in = size (i_in)
      expr%n_out = size (i_out)
      expr%n_tot = expr%n_in + expr%n_out
    end subroutine parton_expr_setup_subevt

```

Transfer PDG codes, masses (initialization) and momenta to a predefined subevent. We use the flavor assignment of the first branch in the interaction state matrix. Only incoming and outgoing particles are transferred. Switch momentum sign for incoming particles.

```

  <Subevt expr: interfaces>≡

```

```

interface interaction_momenta_to_subevt
  module procedure interaction_momenta_to_subevt_id
  module procedure interaction_momenta_to_subevt_tr
end interface

```

<Subevt expr: procedures>+≡

```

subroutine interaction_to_subevt (int, j_beam, j_in, j_out, subevt)
  type(interaction_t), intent(in), target :: int
  integer, dimension(:), intent(in) :: j_beam, j_in, j_out
  type(subevt_t), intent(out) :: subevt
  type(flavor_t), dimension(:), allocatable :: flv
  integer :: n_beam, n_in, n_out, i, j
  allocate (flv (int%get_n_tot ()))
  flv = quantum_numbers_get_flavor (int%get_quantum_numbers (1))
  n_beam = size (j_beam)
  n_in = size (j_in)
  n_out = size (j_out)
  call subevt_init (subevt, n_beam + n_in + n_out)
  do i = 1, n_beam
    j = j_beam(i)
    call subevt_set_beam (subevt, i, &
      flv(j)%get_pdg (), &
      vector4_null, &
      flv(j)%get_mass () ** 2)
  end do
  do i = 1, n_in
    j = j_in(i)
    call subevt_set_incoming (subevt, n_beam + i, &
      flv(j)%get_pdg (), &
      vector4_null, &
      flv(j)%get_mass () ** 2)
  end do
  do i = 1, n_out
    j = j_out(i)
    call subevt_set_outgoing (subevt, n_beam + n_in + i, &
      flv(j)%get_pdg (), &
      vector4_null, &
      flv(j)%get_mass () ** 2)
  end do
end subroutine interaction_to_subevt

subroutine interaction_momenta_to_subevt_id (int, j_beam, j_in, j_out, subevt)
  type(interaction_t), intent(in) :: int
  integer, dimension(:), intent(in) :: j_beam, j_in, j_out
  type(subevt_t), intent(inout) :: subevt
  call subevt_set_p_beam (subevt, - int%get_momenta (j_beam))
  call subevt_set_p_incoming (subevt, - int%get_momenta (j_in))
  call subevt_set_p_outgoing (subevt, int%get_momenta (j_out))
end subroutine interaction_momenta_to_subevt_id

subroutine interaction_momenta_to_subevt_tr &
  (int, j_beam, j_in, j_out, lt, subevt)
  type(interaction_t), intent(in) :: int
  integer, dimension(:), intent(in) :: j_beam, j_in, j_out

```

```

type(subevt_t), intent(inout) :: subevt
type(lorentz_transformation_t), intent(in) :: lt
call subevt_set_p_beam &
    (subevt, - lt * int%get_momenta (j_beam))
call subevt_set_p_incoming &
    (subevt, - lt * int%get_momenta (j_in))
call subevt_set_p_outgoing &
    (subevt, lt * int%get_momenta (j_out))
end subroutine interaction_momenta_to_subevt_tr

```

The second part takes the momenta from the interaction object and thus completes the subevt. The partonic energy can then be computed.

```

⟨Subevt expr: parton expr: TBP⟩+≡
    procedure :: fill_subevt => parton_expr_fill_subevt

⟨Subevt expr: procedures⟩+≡
    subroutine parton_expr_fill_subevt (expr, int)
    class(parton_expr_t), intent(inout) :: expr
    type(interaction_t), intent(in), target :: int
    call interaction_momenta_to_subevt (int, &
        expr%i_beam, expr%i_in, expr%i_out, expr%subevt_t)
    expr%sqrts_hat = subevt_get_sqrts_hat (expr%subevt_t)
    expr%subevt_filled = .true.
    end subroutine parton_expr_fill_subevt

```

Evaluate, if the event passes the selection. For absent expressions we take default values.

```

⟨Subevt expr: parton expr: TBP⟩+≡
    procedure :: evaluate => parton_expr_evaluate

⟨Subevt expr: procedures⟩+≡
    subroutine parton_expr_evaluate &
        (expr, passed, scale, fac_scale, ren_scale, weight, scale_forced, force_evaluation)
    class(parton_expr_t), intent(inout) :: expr
    logical, intent(out) :: passed
    real(default), intent(out) :: scale
    real(default), intent(out) :: fac_scale
    real(default), intent(out) :: ren_scale
    real(default), intent(out) :: weight
    real(default), intent(in), allocatable, optional :: scale_forced
    logical, intent(in), optional :: force_evaluation
    logical :: force_scale, force_eval
    force_scale = .false.; force_eval = .false.
    if (present (scale_forced)) force_scale = allocated (scale_forced)
    if (present (force_evaluation)) force_eval = force_evaluation
    call expr%base_evaluate (passed)
    if (passed .or. force_eval) then
        if (force_scale) then
            scale = scale_forced
        else if (expr%has_scale) then
            call expr%scale%evaluate ()
            if (expr%scale%is_known ()) then
                scale = expr%scale%get_real ()
            else

```

```

        call msg_error ("Evaluate scale expression: result undefined")
        scale = zero
    end if
else
    scale = expr%sqrts_hat
end if
if (force_scale) then
    fac_scale = scale_forced
else if (expr%has_fac_scale) then
    call expr%fac_scale%evaluate ()
    if (expr%fac_scale%is_known ()) then
        fac_scale = expr%fac_scale%get_real ()
    else
        call msg_error ("Evaluate factorization scale expression: &
            &result undefined")
        fac_scale = zero
    end if
else
    fac_scale = scale
end if
if (force_scale) then
    ren_scale = scale_forced
else if (expr%has_ren_scale) then
    call expr%ren_scale%evaluate ()
    if (expr%ren_scale%is_known ()) then
        ren_scale = expr%ren_scale%get_real ()
    else
        call msg_error ("Evaluate renormalization scale expression: &
            &result undefined")
        ren_scale = zero
    end if
else
    ren_scale = scale
end if
if (expr%has_weight) then
    call expr%weight%evaluate ()
    if (expr%weight%is_known ()) then
        weight = expr%weight%get_real ()
    else
        call msg_error ("Evaluate weight expression: result undefined")
        weight = zero
    end if
else
    weight = one
end if
else
    weight = zero
end if
end subroutine parton_expr_evaluate

```

Return the beam/incoming parton indices.

$\langle \text{Subevt expr: parton expr: TBP} \rangle + \equiv$

```
procedure :: get_beam_index => parton_expr_get_beam_index
```

```

    procedure :: get_in_index => parton_expr_get_in_index
  <Subvt expr: procedures>+≡
    subroutine parton_expr_get_beam_index (expr, i_beam)
      class(parton_expr_t), intent(in) :: expr
      integer, dimension(:), intent(out) :: i_beam
      i_beam = expr%i_beam
    end subroutine parton_expr_get_beam_index

    subroutine parton_expr_get_in_index (expr, i_in)
      class(parton_expr_t), intent(in) :: expr
      integer, dimension(:), intent(out) :: i_in
      i_in = expr%i_in
    end subroutine parton_expr_get_in_index

```

30.1.5 Implementation for full events

This implementation contains the expressions that we can evaluate for the full event. It also contains data that pertain to the event, suitable for communication with external event formats. These data simultaneously serve as pointer targets for the variable lists hidden in the expressions (eval trees).

Squared matrix element and weight values: when reading events from file, the `ref` value is the number in the file, while the `prc` value is the number that we calculate from the momenta in the file, possibly with different parameters. When generating events the first time, or if we do not recalculate, the numbers should coincide. Furthermore, the array of `alt` values is copied from an array of alternative event records. These values should represent calculated values.

```

  <Subvt expr: public>+≡
    public :: event_expr_t

  <Subvt expr: types>+≡
    type, extends (subvt_expr_t) :: event_expr_t
      logical :: has_reweight = .false.
      logical :: has_analysis = .false.
      class(expr_t), allocatable :: reweight
      class(expr_t), allocatable :: analysis
      logical :: has_id = .false.
      type(string_t) :: id
      logical :: has_num_id = .false.
      integer :: num_id = 0
      logical :: has_index = .false.
      integer :: index = 0
      logical :: has_sqme_ref = .false.
      real(default) :: sqme_ref = 0
      logical :: has_sqme_prc = .false.
      real(default) :: sqme_prc = 0
      logical :: has_weight_ref = .false.
      real(default) :: weight_ref = 0
      logical :: has_weight_prc = .false.
      real(default) :: weight_prc = 0
      logical :: has_excess_prc = .false.
      real(default) :: excess_prc = 0
      integer :: n_alt = 0

```

```

        logical :: has_sqme_alt = .false.
        real(default), dimension(:), allocatable :: sqme_alt
        logical :: has_weight_alt = .false.
        real(default), dimension(:), allocatable :: weight_alt
    contains
        <Subevt expr: event expr: TBP>
    end type event_expr_t

```

Finalizer for the expressions.

```

<Subevt expr: event expr: TBP>≡
    procedure :: final => event_expr_final
<Subevt expr: procedures>+≡
    subroutine event_expr_final (object)
        class(event_expr_t), intent(inout) :: object
        call object%base_final ()
        if (object%has_reweight) then
            call object%reweight%final ()
        end if
        if (object%has_analysis) then
            call object%analysis%final ()
        end if
    end subroutine event_expr_final

```

Output: continue writing the active expressions, after the common selection expression.

Note: the `prefix` argument is declared in the `write` method of the `subevt_t` base type. Here, it is unused.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: write => event_expr_write
<Subevt expr: procedures>+≡
    subroutine event_expr_write (object, unit, prefix, pacified)
        class(event_expr_t), intent(in) :: object
        integer, intent(in), optional :: unit
        character(*), intent(in), optional :: prefix
        logical, intent(in), optional :: pacified
        integer :: u
        u = given_output_unit (unit)
        call object%base_write (u, pacified = pacified)
        if (object%subevt_filled) then
            if (object%has_reweight) then
                call write_separator (u)
                write (u, "(1x,A)") "Reweighting expression:"
                call write_separator (u)
                call object%reweight%write (u)
            end if
            if (object%has_analysis) then
                call write_separator (u)
                write (u, "(1x,A)") "Analysis expression:"
                call write_separator (u)
                call object%analysis%write (u)
            end if
        end if
    end subroutine event_expr_write

```

```
end subroutine event_expr_write
```

Initializer. This is required only for the sqme_alt and weight_alt arrays.

```
<Subevt expr: event expr: TBP>+≡
  procedure :: init => event_expr_init

<Subevt expr: procedures>+≡
  subroutine event_expr_init (expr, n_alt)
    class(event_expr_t), intent(out) :: expr
    integer, intent(in), optional :: n_alt
    if (present (n_alt)) then
      expr%n_alt = n_alt
      allocate (expr%sqme_alt (n_alt), source = 0._default)
      allocate (expr%weight_alt (n_alt), source = 0._default)
    end if
  end subroutine event_expr_init
```

Define variables. We have the variables of the base type plus specific variables for full events. There is the event index.

```
<Subevt expr: event expr: TBP>+≡
  procedure :: setup_vars => event_expr_setup_vars

<Subevt expr: procedures>+≡
  subroutine event_expr_setup_vars (expr, sqrts)
    class(event_expr_t), intent(inout), target :: expr
    real(default), intent(in) :: sqrts
    call expr%base_setup_vars (sqrts)
    call var_list_append_string_ptr (expr%var_list, &
      var_str ("$_process_id"), expr%id, &
      is_known = expr%has_id, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_int_ptr (expr%var_list, &
      var_str ("process_num_id"), expr%num_id, &
      is_known = expr%has_num_id, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_real_ptr (expr%var_list, &
      var_str ("sqme"), expr%sqme_prc, &
      is_known = expr%has_sqme_prc, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_real_ptr (expr%var_list, &
      var_str ("sqme_ref"), expr%sqme_ref, &
      is_known = expr%has_sqme_ref, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_int_ptr (expr%var_list, &
      var_str ("event_index"), expr%index, &
      is_known = expr%has_index, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_real_ptr (expr%var_list, &
      var_str ("event_weight"), expr%weight_prc, &
      is_known = expr%has_weight_prc, &
      locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_real_ptr (expr%var_list, &
      var_str ("event_weight_ref"), expr%weight_ref, &
      is_known = expr%has_weight_ref, &
```

```

        locked = .true., verbose = .false., intrinsic = .true.)
    call var_list_append_real_ptr (expr%var_list, &
        var_str ("event_excess"), expr%excess_prc, &
        is_known = expr%has_excess_prc, &
        locked = .true., verbose = .false., intrinsic = .true.)
end subroutine event_expr_setup_vars

```

Compile the analysis expression. If the pointer is disassociated, there is no expression.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: setup_analysis => event_expr_setup_analysis

<Subevt expr: procedures>+≡
    subroutine event_expr_setup_analysis (expr, ef_analysis)
        class(event_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_analysis
        call ef_analysis%build (expr%analysis)
        if (allocated (expr%analysis)) then
            call expr%setup_var_self ()
            call expr%analysis%setup_lexpr (expr%var_list)
            expr%has_analysis = .true.
        end if
    end subroutine event_expr_setup_analysis

```

Compile the reweight expression.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: setup_reweight => event_expr_setup_reweight

<Subevt expr: procedures>+≡
    subroutine event_expr_setup_reweight (expr, ef_reweight)
        class(event_expr_t), intent(inout), target :: expr
        class(expr_factory_t), intent(in) :: ef_reweight
        call ef_reweight%build (expr%reweight)
        if (allocated (expr%reweight)) then
            call expr%setup_var_self ()
            call expr%reweight%setup_expr (expr%var_list)
            expr%has_reweight = .true.
        end if
    end subroutine event_expr_setup_reweight

```

Store the string or numeric process ID. This should be done during initialization.

```

<Subevt expr: event expr: TBP>+≡
    procedure :: set_process_id => event_expr_set_process_id
    procedure :: set_process_num_id => event_expr_set_process_num_id

<Subevt expr: procedures>+≡
    subroutine event_expr_set_process_id (expr, id)
        class(event_expr_t), intent(inout) :: expr
        type(string_t), intent(in) :: id
        expr%id = id
        expr%has_id = .true.
    end subroutine event_expr_set_process_id

```



```

subroutine event_expr_set_process_num_id (expr, num_id)
  class(event_expr_t), intent(inout) :: expr
  integer, intent(in) :: num_id
  expr%num_id = num_id
  expr%has_num_id = .true.
end subroutine event_expr_set_process_num_id

```

Reset / set the data that pertain to a particular event. The event index is reset unless explicitly told to keep it.

(Subevt expr: event expr: TBP)+≡

```

  procedure :: reset_contents => event_expr_reset_contents
  procedure :: set => event_expr_set

```

(Subevt expr: procedures)+≡

```

subroutine event_expr_reset_contents (expr)
  class(event_expr_t), intent(inout) :: expr
  call expr%base_reset_contents ()
  expr%has_sqme_ref = .false.
  expr%has_sqme_prc = .false.
  expr%has_sqme_alt = .false.
  expr%has_weight_ref = .false.
  expr%has_weight_prc = .false.
  expr%has_weight_alt = .false.
  expr%has_excess_prc = .false.
end subroutine event_expr_reset_contents

```

```

subroutine event_expr_set (expr, &
  weight_ref, weight_prc, weight_alt, &
  excess_prc, &
  sqme_ref, sqme_prc, sqme_alt)
  class(event_expr_t), intent(inout) :: expr
  real(default), intent(in), optional :: weight_ref, weight_prc
  real(default), intent(in), optional :: excess_prc
  real(default), intent(in), optional :: sqme_ref, sqme_prc
  real(default), dimension(:), intent(in), optional :: sqme_alt, weight_alt
  if (present (sqme_ref)) then
    expr%has_sqme_ref = .true.
    expr%sqme_ref = sqme_ref
  end if
  if (present (sqme_prc)) then
    expr%has_sqme_prc = .true.
    expr%sqme_prc = sqme_prc
  end if
  if (present (sqme_alt)) then
    expr%has_sqme_alt = .true.
    expr%sqme_alt = sqme_alt
  end if
  if (present (weight_ref)) then
    expr%has_weight_ref = .true.
    expr%weight_ref = weight_ref
  end if
  if (present (weight_prc)) then
    expr%has_weight_prc = .true.
    expr%weight_prc = weight_prc
  end if

```

```

end if
if (present (weight_alt)) then
  expr%has_weight_alt = .true.
  expr%weight_alt = weight_alt
end if
if (present (excess_prc)) then
  expr%has_excess_prc = .true.
  expr%excess_prc = excess_prc
end if
end subroutine event_expr_set

```

Access the subevent index.

```

<Subevt expr: event expr: TBP>+≡
  procedure :: has_event_index => event_expr_has_event_index
  procedure :: get_event_index => event_expr_get_event_index

<Subevt expr: procedures>+≡
  function event_expr_has_event_index (expr) result (flag)
    class(event_expr_t), intent(in) :: expr
    logical :: flag
    flag = expr%has_index
  end function event_expr_has_event_index

  function event_expr_get_event_index (expr) result (index)
    class(event_expr_t), intent(in) :: expr
    integer :: index
    if (expr%has_index) then
      index = expr%index
    else
      index = 0
    end if
  end function event_expr_get_event_index

```

Set/increment the subevent index. Initialize it if necessary.

```

<Subevt expr: event expr: TBP>+≡
  procedure :: set_event_index => event_expr_set_event_index
  procedure :: reset_event_index => event_expr_reset_event_index
  procedure :: increment_event_index => event_expr_increment_event_index

<Subevt expr: procedures>+≡
  subroutine event_expr_set_event_index (expr, index)
    class(event_expr_t), intent(inout) :: expr
    integer, intent(in) :: index
    expr%index = index
    expr%has_index = .true.
  end subroutine event_expr_set_event_index

  subroutine event_expr_reset_event_index (expr)
    class(event_expr_t), intent(inout) :: expr
    expr%has_index = .false.
  end subroutine event_expr_reset_event_index

  subroutine event_expr_increment_event_index (expr, offset)
    class(event_expr_t), intent(inout) :: expr

```

```

integer, intent(in), optional :: offset
if (expr%has_index) then
  expr%index = expr%index + 1
else if (present (offset)) then
  call expr%set_event_index (offset + 1)
else
  call expr%set_event_index (1)
end if
end subroutine event_expr_increment_event_index

```

Fill the event expression: take the particle data and kinematics from a `particle_set` object.

We allow the particle content to change for each event. Therefore, we set the event variables each time.

Also increment the event index; initialize it if necessary.

```

<Subevt expr: event expr: TBP>+≡
  procedure :: fill_subevt => event_expr_fill_subevt

<Subevt expr: procedures>+≡
  subroutine event_expr_fill_subevt (expr, particle_set)
    class(event_expr_t), intent(inout) :: expr
    type(particle_set_t), intent(in) :: particle_set
    call particle_set%to_subevt (expr%subevt_t, expr%colorize_subevt)
    expr%sqrts_hat = subevt_get_sqrts_hat (expr%subevt_t)
    expr%n_in = subevt_get_n_in (expr%subevt_t)
    expr%n_out = subevt_get_n_out (expr%subevt_t)
    expr%n_tot = expr%n_in + expr%n_out
    expr%subevt_filled = .true.
  end subroutine event_expr_fill_subevt

```

Evaluate, if the event passes the selection. For absent expressions we take default values.

```

<Subevt expr: event expr: TBP>+≡
  procedure :: evaluate => event_expr_evaluate

<Subevt expr: procedures>+≡
  subroutine event_expr_evaluate (expr, passed, reweight, analysis_flag)
    class(event_expr_t), intent(inout) :: expr
    logical, intent(out) :: passed
    real(default), intent(out) :: reweight
    logical, intent(out) :: analysis_flag
    call expr%base_evaluate (passed)
    if (passed) then
      if (expr%has_reweight) then
        call expr%reweight%evaluate ()
        if (expr%reweight%is_known ()) then
          reweight = expr%reweight%get_real ()
        else
          call msg_error ("Evaluate reweight expression: &
            &result undefined")
          reweight = 0
        end if
      else
        analysis_flag = .false.
      end if
    else
      passed = .false.
    end if
  end subroutine event_expr_evaluate

```

```

        reweight = 1
    end if
    if (expr%has_analysis) then
        call expr%analysis%evaluate ()
        if (expr%analysis%is_known ()) then
            analysis_flag = expr%analysis%get_log ()
        else
            call msg_error ("Evaluate analysis expression: &
                &result undefined")
            analysis_flag = .false.
        end if
    else
        analysis_flag = .true.
    end if
end if
end subroutine event_expr_evaluate

```

30.2 Parton states

A `parton_state_t` object contains the effective kinematics and dynamics of an elementary partonic interaction, with or without the beam/structure function state included. The type is abstract and has two distinct extensions. The `isolated_state_t` extension describes the isolated elementary interaction where the `int_eff` subobject contains the complex transition amplitude, exclusive in all quantum numbers. The particle content and kinematics describe the effective partonic state. The `connected_state_t` extension contains the partonic `subevt` and the expressions for cuts and scales which use it.

In the isolated state, the effective partonic interaction may either be identical to the hard interaction, in which case it is just a pointer to the latter. Or it may involve a rearrangement of partons, in which case we allocate it explicitly and flag this by `int_is_allocated`.

The `trace` evaluator contains the absolute square of the effective transition amplitude matrix, summed over final states. It is also summed over initial states, depending on the the beam setup allows. The result is used for integration.

The `matrix` evaluator is the counterpart of `trace` which is kept exclusive in all observable quantum numbers. The `flows` evaluator is furthermore exclusive in colors, but neglecting all color interference. The `matrix` and `flows` evaluators are filled only for sampling points that become part of physical events.

Note: It would be natural to make the evaluators allocatable. The extra `has_XXX` flags indicate whether evaluators are active, instead.

This module contains no unit tests. The tests are covered by the `processes` module below.

```

(parton_states.f90)≡
<File header>
module parton_states

    <Use kinds>
    <Use debug>
    use io_units

```

```

use format_utils, only: write_separator
use diagnostics
use lorentz
use subevents
use variables
use expr_base
use model_data
use flavors
use helicities
use colors
use quantum_numbers
use state_matrices
use polarizations
use interactions
use evaluators

use beams
use sf_base
use process_constants
use prc_core
use subvt_expr

<Standard module head>

<Parton states: public>

<Parton states: types>

contains

<Parton states: procedures>

end module parton_states

```

30.2.1 Abstract base type

The common part are the evaluators, one for the trace (summed over all quantum numbers), one for the transition matrix (summed only over unobservable quantum numbers), and one for the flow distribution (transition matrix without interferences, exclusive in color flow).

```

<Parton states: types>≡
type, abstract :: parton_state_t
  logical :: has_trace = .false.
  logical :: has_matrix = .false.
  logical :: has_flows = .false.
  type(evaluator_t) :: trace
  type(evaluator_t) :: matrix
  type(evaluator_t) :: flows
contains
  <Parton states: parton state: TBP>
end type parton_state_t

```

The `isolated_state_t` extension contains the `sf_chain_eff` object and the (hard) effective interaction `int_eff`, separately, both are implemented as a pointer. The evaluators (trace, matrix, flows) apply to the hard interaction only.

If the effective interaction differs from the hard interaction, the pointer is allocated explicitly. Analogously for `sf_chain_eff`.

```

(Parton states: public)≡
  public :: isolated_state_t

(Parton states: types)+≡
  type, extends (parton_state_t) :: isolated_state_t
    logical :: sf_chain_is_allocated = .false.
    type(sf_chain_instance_t), pointer :: sf_chain_eff => null ()
    logical :: int_is_allocated = .false.
    type(interaction_t), pointer :: int_eff => null ()
  contains
    (Parton states: isolated state: TBP)
  end type isolated_state_t

```

The `connected_state_t` extension contains all data that enable the evaluation of observables for the effective connected state. The evaluators connect the (effective) structure-function chain and hard interaction that were kept separate in the `isolated_state_t`.

The `flows_sf` evaluator is an extended copy of the structure-function

The `expr` subobject consists of the `subevt`, a simple event record, expressions for cuts etc. which refer to this record, and a `var_list` which contains event-specific variables, linked to the process variable list. Variables used within the expressions are looked up in `var_list`.

```

(Parton states: public)+≡
  public :: connected_state_t

(Parton states: types)+≡
  type, extends (parton_state_t) :: connected_state_t
    type(state_flv_content_t) :: state_flv
    logical :: has_flows_sf = .false.
    type(evaluator_t) :: flows_sf
    logical :: has_expr = .false.
    type(parton_expr_t) :: expr
  contains
    (Parton states: connected state: TBP)
  end type connected_state_t

```

Output: each evaluator is written only when it is active. The `sf_chain` is only written if it is explicitly allocated.

```

(Parton states: parton state: TBP)≡
  procedure :: write => parton_state_write

(Parton states: procedures)≡
  subroutine parton_state_write (state, unit, testflag)
    class(parton_state_t), intent(in) :: state
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u

```

```

u = given_output_unit (unit)
select type (state)
class is (isolated_state_t)
  if (state%sf_chain_is_allocated) then
    call write_separator (u)
    call state%sf_chain_eff%write (u)
  end if
  if (state%int_is_allocated) then
    call write_separator (u)
    write (u, "(1x,A)" &
           "Effective interaction:")
    call write_separator (u)
    call state%int_eff%basic_write (u, testflag = testflag)
  end if
class is (connected_state_t)
  if (state%has_flows_sf) then
    call write_separator (u)
    write (u, "(1x,A)" &
           "Evaluator (extension of the beam evaluator &
           &with color contractions):")
    call write_separator (u)
    call state%flows_sf%write (u, testflag = testflag)
  end if
end select
if (state%has_trace) then
  call write_separator (u)
  write (u, "(1x,A)" &
         "Evaluator (trace of the squared transition matrix):")
  call write_separator (u)
  call state%trace%write (u, testflag = testflag)
end if
if (state%has_matrix) then
  call write_separator (u)
  write (u, "(1x,A)" &
         "Evaluator (squared transition matrix):")
  call write_separator (u)
  call state%matrix%write (u, testflag = testflag)
end if
if (state%has_flows) then
  call write_separator (u)
  write (u, "(1x,A)" &
         "Evaluator (squared color-flow matrix):")
  call write_separator (u)
  call state%flows%write (u, testflag = testflag)
end if
select type (state)
class is (connected_state_t)
  if (state%has_expr) then
    call write_separator (u)
    call state%expr%write (u)
  end if
end select
end subroutine parton_state_write

```

Finalize interaction and evaluators, but only if allocated.

```

(Parton states: parton state: TBP)+≡
  procedure :: final => parton_state_final

(Parton states: procedures)+≡
  subroutine parton_state_final (state)
    class(parton_state_t), intent(inout) :: state
    if (state%has_flows) then
      call state%flows%final ()
      state%has_flows = .false.
    end if
    if (state%has_matrix) then
      call state%matrix%final ()
      state%has_matrix = .false.
    end if
    if (state%has_trace) then
      call state%trace%final ()
      state%has_trace = .false.
    end if
    select type (state)
    class is (connected_state_t)
      if (state%has_flows_sf) then
        call state%flows_sf%final ()
        state%has_flows_sf = .false.
      end if
      call state%expr%final ()
    class is (isolated_state_t)
      if (state%int_is_allocated) then
        call state%int_eff%final ()
        deallocate (state%int_eff)
        state%int_is_allocated = .false.
      end if
      if (state%sf_chain_is_allocated) then
        call state%sf_chain_eff%final ()
      end if
    end select
  end subroutine parton_state_final

```

30.2.2 Common Initialization

Initialize the isolated parton state. In this version, the effective structure-function chain `sf_chain_eff` and the effective interaction `int_eff` both are trivial pointers to the seed structure-function chain and to the hard interaction, respectively.

```

(Parton states: isolated state: TBP)≡
  procedure :: init => isolated_state_init

(Parton states: procedures)+≡
  subroutine isolated_state_init (state, sf_chain, int)
    class(isolated_state_t), intent(out) :: state
    type(sf_chain_instance_t), intent(in), target :: sf_chain
    type(interaction_t), intent(in), target :: int
    state%sf_chain_eff => sf_chain

```



```

state%int_eff => int
end subroutine isolated_state_init

```

30.2.3 Evaluator initialization: isolated state

Create an evaluator for the trace of the squared transition matrix. The trace goes over all outgoing quantum numbers. Whether we trace over incoming quantum numbers other than color, depends on the given `qn_mask.in`.

There are two options: explicitly computing the color factor table (`use_cf` false; `nc` defined), or taking the color factor table from the hard matrix element data.

```

(Parton states: isolated state: TBP)+≡
  procedure :: setup_square_trace => isolated_state_setup_square_trace

(Parton states: procedures)+≡
  subroutine isolated_state_setup_square_trace (state, core, &
    qn_mask_in, col, keep_fs_flavor)
    class(isolated_state_t), intent(inout), target :: state
    class(prc_core_t), intent(in) :: core
    type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask_in
    !!! Actually need allocatable attribute here for once because col might
    !!! enter the subroutine non-allocated.
    integer, intent(in), dimension(:), allocatable :: col
    logical, intent(in) :: keep_fs_flavor
    type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
    associate (data => core%data)
      allocate (qn_mask (data%n_in + data%n_out))
      qn_mask( : data%n_in) = &
        quantum_numbers_mask (.false., .true., .false.) &
        .or. qn_mask_in
      qn_mask(data%n_in + 1 : ) = &
        quantum_numbers_mask (.not. keep_fs_flavor, .true., .true.)
      if (core%use_color_factors) then
        call state%trace%init_square (state%int_eff, qn_mask, &
          col_flow_index = data%cf_index, &
          col_factor = data%color_factors, &
          col_index_hi = col, &
          nc = core%nc)
      else
        call state%trace%init_square (state%int_eff, qn_mask, nc = core%nc)
      end if
    end associate
    state%has_trace = .true.
  end subroutine isolated_state_setup_square_trace

```

Set up an identity-evaluator for the trace. This implies that `me` is considered to be a squared amplitude, as for example for BLHA matrix elements.

```

(Parton states: isolated state: TBP)+≡
  procedure :: setup_identity_trace => isolated_state_setup_identity_trace

```

<Parton states: procedures>+≡

```

subroutine isolated_state_setup_identity_trace (state, core, qn_mask_in, &
    keep_fs_flavors, keep_colors)
    class(isolated_state_t), intent(inout), target :: state
    class(prc_core_t), intent(in) :: core
    type(quantum_numbers_mask_t), intent(in), dimension(:) :: qn_mask_in
    logical, intent(in), optional :: keep_fs_flavors, keep_colors
    type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
    logical :: fs_flg_flag, col_flag
    fs_flg_flag = .true.; col_flag = .true.
    if (present(keep_fs_flavors)) fs_flg_flag = .not. keep_fs_flavors
    if (present(keep_colors)) col_flag = .not. keep_colors
    associate (data => core%data)
        allocate (qn_mask (data%n_in + data%n_out))
        qn_mask( : data%n_in) = &
            quantum_numbers_mask (.false., col_flag, .false.) .or. qn_mask_in
        qn_mask(data%n_in + 1 : ) = &
            quantum_numbers_mask (fs_flg_flag, col_flag, .true.)
    end associate
    call state%int_eff%set_mask (qn_mask)
    call state%trace%init_identity (state%int_eff)
    state%has_trace = .true.
end subroutine isolated_state_setup_identity_trace

```

Set up the evaluator for the transition matrix, exclusive in helicities where this is requested.

For all unstable final-state particles we keep polarization according to the applicable decay options. If the process is a decay itself, this applies also to the initial state.

For all polarized final-state particles, we keep polarization including off-diagonal entries. We drop helicity completely for unpolarized final-state particles.

For the initial state, if the particle has not been handled yet, we apply the provided `qn_mask_in` which communicates the beam properties.

<Parton states: isolated state: TBP>+≡

```

procedure :: setup_square_matrix => isolated_state_setup_square_matrix

```

<Parton states: procedures>+≡

```

subroutine isolated_state_setup_square_matrix &
    (state, core, model, qn_mask_in, col)
    class(isolated_state_t), intent(inout), target :: state
    class(prc_core_t), intent(in) :: core
    class(model_data_t), intent(in), target :: model
    type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
    integer, dimension(:), intent(in) :: col
    type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
    type(flavor_t), dimension(:), allocatable :: flv
    integer :: i
    logical :: helmask, helmask_hd
    associate (data => core%data)
        allocate (qn_mask (data%n_in + data%n_out))
        allocate (flv (data%n_flv))
        do i = 1, data%n_in + data%n_out

```

```

call flv%init (data%flv_state(i,:), model)
if ((data%n_in == 1 .or. i > data%n_in) &
    .and. any (.not. flv%is_stable ())) then
    helmask = all (flv%decays_isotropically ())
    helmask_hd = all (flv%decays_diagonal ())
    qn_mask(i) = quantum_numbers_mask (.false., .true., helmask, &
        mask_hd = helmask_hd)
else if (i > data%n_in) then
    helmask = all (.not. flv%is_polarized ())
    qn_mask(i) = quantum_numbers_mask (.false., .true., helmask)
else
    qn_mask(i) = quantum_numbers_mask (.false., .true., .false.) &
        .or. qn_mask_in(i)
end if
end do
if (core%use_color_factors) then
    call state%matrix%init_square (state%int_eff, qn_mask, &
        col_flow_index = data%cf_index, &
        col_factor = data%color_factors, &
        col_index_hi = col, &
        nc = core%nc)
else
    call state%matrix%init_square (state%int_eff, &
        qn_mask, &
        nc = core%nc)
end if
end associate
state%has_matrix = .true.
end subroutine isolated_state_setup_square_matrix

```

This procedure initializes the evaluator that computes the contributions to color flows, neglecting color interference. The incoming-particle mask can be used to sum over incoming flavor.

Helicity handling: see above.

(Parton states: isolated state: TBP)+≡

```
procedure :: setup_square_flows => isolated_state_setup_square_flows
```

(Parton states: procedures)+≡

```

subroutine isolated_state_setup_square_flows (state, core, model, qn_mask_in)
class(isolated_state_t), intent(inout), target :: state
class(prc_core_t), intent(in) :: core
class(model_data_t), intent(in), target :: model
type(quantum_numbers_mask_t), dimension(:), intent(in) :: qn_mask_in
type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
type(flavor_t), dimension(:), allocatable :: flv
integer :: i
logical :: helmask, helmask_hd
associate (data => core%data)
    allocate (qn_mask (data%n_in + data%n_out))
    allocate (flv (data%n_flv))
    do i = 1, data%n_in + data%n_out
        call flv%init (data%flv_state(i,:), model)
        if ((data%n_in == 1 .or. i > data%n_in) &
            .and. any (.not. flv%is_stable ())) then

```

```

        helmask = all (flv%decays_isotropically ())
        helmask_hd = all (flv%decays_diagonal ())
        qn_mask(i) = quantum_numbers_mask (.false., .false., helmask, &
            mask_hd = helmask_hd)
    else if (i > data%n_in) then
        helmask = all (.not. flv%is_polarized ())
        qn_mask(i) = quantum_numbers_mask (.false., .false., helmask)
    else
        qn_mask(i) = quantum_numbers_mask (.false., .false., .false.) &
            .or. qn_mask_in(i)
    end if
end do
call state%flows%init_square (state%int_eff, qn_mask, &
    expand_color_flows = .true.)
end associate
state%has_flows = .true.
end subroutine isolated_state_setup_square_flows

```

30.2.4 Evaluator initialization: connected state

Set up a trace evaluator as a product of two evaluators (incoming state, effective interaction). In the result, all quantum numbers are summed over.

If the optional `int` interaction is provided, use this for the first factor in the convolution. Otherwise, use the final interaction of the stored `sf_chain`.

The `resonant` flag applies if we want to construct a decay chain. The resonance property can propagate to the final event output.

If an extended structure function is required `requires_extended_sf`, we have to not consider `sub` as a quantum number.

```

(Parton states: connected state: TBP)≡
    procedure :: setup_connected_trace => connected_state_setup_connected_trace

(Parton states: procedures)+≡
    subroutine connected_state_setup_connected_trace &
        (state, isolated, int, resonant, undo_helicities, &
         keep_fs_flavors, requires_extended_sf)
    class(connected_state_t), intent(inout), target :: state
    type(isolated_state_t), intent(in), target :: isolated
    type(interaction_t), intent(in), optional, target :: int
    logical, intent(in), optional :: resonant
    logical, intent(in), optional :: undo_helicities
    logical, intent(in), optional :: keep_fs_flavors
    logical, intent(in), optional :: requires_extended_sf
    type(quantum_numbers_mask_t) :: mask
    type(interaction_t), pointer :: src_int, beam_int
    logical :: reduce, fs_flv_flag
    if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, &
        "connected_state_setup_connected_trace")
    reduce = .false.; fs_flv_flag = .true.
    if (present (undo_helicities)) reduce = undo_helicities
    if (present (keep_fs_flavors)) fs_flv_flag = .not. keep_fs_flavors
    mask = quantum_numbers_mask (fs_flv_flag, .true., .true.)
    if (present (int)) then

```

```

        src_int => int
    else
        src_int => isolated%sf_chain_eff%get_out_int_ptr ()
    end if

    if (debug2_active (D_PROCESS_INTEGRATION)) then
        call src_int%basic_write ()
    end if

    call state%trace%init_product (src_int, isolated%trace, &
        qn_mask_conn = mask, &
        qn_mask_rest = mask, &
        connections_are_resonant = resonant, &
        ignore_sub_for_qn = requires_extended_sf)

    if (reduce) then
        beam_int => isolated%sf_chain_eff%get_beam_int_ptr ()
        call undo_qn_hel (beam_int, mask, beam_int%get_n_tot ())
        call undo_qn_hel (src_int, mask, src_int%get_n_tot ())
        call beam_int%set_matrix_element (cmplx (1, 0, default))
        call src_int%set_matrix_element (cmplx (1, 0, default))
    end if

    state%has_trace = .true.
contains
    subroutine undo_qn_hel (int_in, mask, n_tot)
        type(interaction_t), intent(inout) :: int_in
        type(quantum_numbers_mask_t), intent(in) :: mask
        integer, intent(in) :: n_tot
        type(quantum_numbers_mask_t), dimension(n_tot) :: mask_in
        mask_in = mask
        call int_in%set_mask (mask_in)
    end subroutine undo_qn_hel
end subroutine connected_state_setup_connected_trace

```

Set up a matrix evaluator as a product of two evaluators (incoming state, effective interaction). In the intermediate state, color and helicity is summed over. In the final state, we keep the quantum numbers which are present in the original evaluators.

```

<Parton states: connected state: TBP>+≡
    procedure :: setup_connected_matrix => connected_state_setup_connected_matrix

<Parton states: procedures>+≡
    subroutine connected_state_setup_connected_matrix &
        (state, isolated, int, resonant, qn_filter_conn)
        class(connected_state_t), intent(inout), target :: state
        type(isolated_state_t), intent(in), target :: isolated
        type(interaction_t), intent(in), optional, target :: int
        logical, intent(in), optional :: resonant
        type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
        type(quantum_numbers_mask_t) :: mask
        type(interaction_t), pointer :: src_int
        mask = quantum_numbers_mask (.false., .true., .true.)
        if (present (int)) then

```

```

        src_int => int
    else
        src_int => isolated%sf_chain_eff%get_out_int_ptr ()
    end if
    call state%matrix%init_product &
        (src_int, isolated%matrix, mask, &
         qn_filter_conn = qn_filter_conn, &
         connections_are_resonant = resonant)
    state%has_matrix = .true.
end subroutine connected_state_setup_connected_matrix

```

Set up a matrix evaluator as a product of two evaluators (incoming state, effective interaction). In the intermediate state, only helicity is summed over. In the final state, we keep the quantum numbers which are present in the original evaluators.

If the optional `int` interaction is provided, use this for the first factor in the convolution. Otherwise, use the final interaction of the stored `sf_chain`, after creating an intermediate interaction that includes a correlated color state. We assume that for a caller-provided `int`, this is not necessary.

For fixed-order NLO differential distribution, we are interested at the partonic level, no parton showering takes place as this would demand for a proper matching. So, the flows in the `connected_state` are not needed, and the color part will be masked for the interaction coming from the `sf_chain`. The squared matrix elements coming from the OLP provider at the moment do not come with flows anyhow. This needs to be revised once the matching to the shower is completed.

```

(Parton states: connected state: TBP)+≡
    procedure :: setup_connected_flows => connected_state_setup_connected_flows

(Parton states: procedures)+≡
    subroutine connected_state_setup_connected_flows &
        (state, isolated, int, resonant, qn_filter_conn, mask_color)
    class(connected_state_t), intent(inout), target :: state
    type(isolated_state_t), intent(in), target :: isolated
    type(interaction_t), intent(in), optional, target :: int
    logical, intent(in), optional :: resonant, mask_color
    type(quantum_numbers_t), intent(in), optional :: qn_filter_conn
    type(quantum_numbers_mask_t) :: mask
    type(quantum_numbers_mask_t), dimension(:), allocatable :: mask_sf
    type(interaction_t), pointer :: src_int
    logical :: mask_c
    mask_c = .false.
    if (present (mask_color)) mask_c = mask_color
    mask = quantum_numbers_mask (.false., .false., .true.)
    if (present (int)) then
        src_int => int
    else
        src_int => isolated%sf_chain_eff%get_out_int_ptr ()
        call state%flows_sf%init_color_contractions (src_int)
        state%has_flows_sf = .true.
        src_int => state%flows_sf%interaction_t
        if (mask_c) then
            allocate (mask_sf (src_int%get_n_tot ()))

```

```

        mask_sf = quantum_numbers_mask (.false., .true., .false.)
        call src_int%reduce_state_matrix (mask_sf, keep_order = .true.)
    end if
end if
call state%flows%init_product (src_int, isolated%flows, mask, &
    qn_filter_conn = qn_filter_conn, &
    connections_are_resonant = resonant)
state%has_flows = .true.
end subroutine connected_state_setup_connected_flows

```

Determine and store the flavor content for the connected state. This queries the matrix evaluator component, which should hold the requested flavor information.

```

<Parton states: connected state: TBP>+≡
    procedure :: setup_state_flv => connected_state_setup_state_flv

<Parton states: procedures>+≡
    subroutine connected_state_setup_state_flv (state, n_out_hard)
        class(connected_state_t), intent(inout), target :: state
        integer, intent(in) :: n_out_hard
        call interaction_get_flv_content &
            (state%matrix%interaction_t, state%state_flv, n_out_hard)
    end subroutine connected_state_setup_state_flv

```

Return the current flavor state object.

```

<Parton states: connected state: TBP>+≡
    procedure :: get_state_flv => connected_state_get_state_flv

<Parton states: procedures>+≡
    function connected_state_get_state_flv (state) result (state_flv)
        class(connected_state_t), intent(in) :: state
        type(state_flv_content_t) :: state_flv
        state_flv = state%state_flv
    end function connected_state_get_state_flv

```

30.2.5 Cuts and expressions

Set up the `subevt` that corresponds to the connected interaction. The index arrays refer to the interaction.

We assign the particles as follows: the beam particles are the first two (decay process: one) entries in the trace evaluator. The incoming partons are identified by their link to the outgoing partons of the structure-function chain. The outgoing partons are those of the trace evaluator, which include radiated partons during the structure-function chain.

```

<Parton states: connected state: TBP>+≡
    procedure :: setup_subevt => connected_state_setup_subevt

<Parton states: procedures>+≡
    subroutine connected_state_setup_subevt (state, sf_chain, f_beam, f_in, f_out)
        class(connected_state_t), intent(inout), target :: state
        type(sf_chain_instance_t), intent(in), target :: sf_chain
        type(flavor_t), dimension(:), intent(in) :: f_beam, f_in, f_out
    end subroutine connected_state_setup_subevt

```

```

integer :: n_beam, n_in, n_out, n_vir, n_tot, i, j
integer, dimension(:), allocatable :: i_beam, i_in, i_out
integer :: sf_out_i
type(interaction_t), pointer :: sf_int
sf_int => sf_chain%get_out_int_ptr ()
n_beam = size (f_beam)
n_in = size (f_in)
n_out = size (f_out)
n_vir = state%trace%get_n_vir ()
n_tot = state%trace%get_n_tot ()
allocate (i_beam (n_beam), i_in (n_in), i_out (n_out))
i_beam = [(i, i = 1, n_beam)]
do j = 1, n_in
    sf_out_i = sf_chain%get_out_i (j)
    i_in(j) = interaction_find_link &
        (state%trace%interaction_t, sf_int, sf_out_i)
end do
i_out = [(i, i = n_vir + 1, n_tot)]
call state%expr%setup_subevt (state%trace%interaction_t, &
    i_beam, i_in, i_out, f_beam, f_in, f_out)
state%has_expr = .true.
end subroutine connected_state_setup_subevt

```

Initialize the variable list specific for this state/term. We insert event variables (`sqrts_hat`) and link the process variable list. The variable list acquires pointers to subobjects of `state`, which must therefore have a `target` attribute.

```

(Parton states: connected state: TBP)+≡
    procedure :: setup_var_list => connected_state_setup_var_list

(Parton states: procedures)+≡
    subroutine connected_state_setup_var_list (state, process_var_list, beam_data)
        class(connected_state_t), intent(inout), target :: state
        type(var_list_t), intent(in), target :: process_var_list
        type(beam_data_t), intent(in) :: beam_data
        call state%expr%setup_vars (beam_data%get_sqrts ())
        call state%expr%link_var_list (process_var_list)
    end subroutine connected_state_setup_var_list

```

Allocate the cut expression etc.

```

(Parton states: connected state: TBP)+≡
    procedure :: setup_cuts => connected_state_setup_cuts
    procedure :: setup_scale => connected_state_setup_scale
    procedure :: setup_fac_scale => connected_state_setup_fac_scale
    procedure :: setup_ren_scale => connected_state_setup_ren_scale
    procedure :: setup_weight => connected_state_setup_weight

(Parton states: procedures)+≡
    subroutine connected_state_setup_cuts (state, ef_cuts)
        class(connected_state_t), intent(inout), target :: state
        class(expr_factory_t), intent(in) :: ef_cuts
        call state%expr%setup_selection (ef_cuts)
    end subroutine connected_state_setup_cuts

    subroutine connected_state_setup_scale (state, ef_scale)

```



```

class(connected_state_t), intent(inout), target :: state
class(expr_factory_t), intent(in) :: ef_scale
call state%expr%setup_scale (ef_scale)
end subroutine connected_state_setup_scale

subroutine connected_state_setup_fac_scale (state, ef_fac_scale)
class(connected_state_t), intent(inout), target :: state
class(expr_factory_t), intent(in) :: ef_fac_scale
call state%expr%setup_fac_scale (ef_fac_scale)
end subroutine connected_state_setup_fac_scale

subroutine connected_state_setup_ren_scale (state, ef_ren_scale)
class(connected_state_t), intent(inout), target :: state
class(expr_factory_t), intent(in) :: ef_ren_scale
call state%expr%setup_ren_scale (ef_ren_scale)
end subroutine connected_state_setup_ren_scale

subroutine connected_state_setup_weight (state, ef_weight)
class(connected_state_t), intent(inout), target :: state
class(expr_factory_t), intent(in) :: ef_weight
call state%expr%setup_weight (ef_weight)
end subroutine connected_state_setup_weight

```

Reset the expression object: invalidate the subevt.

```

(Parton states: connected state: TBP) +=
  procedure :: reset_expressions => connected_state_reset_expressions

(Parton states: procedures) +=
  subroutine connected_state_reset_expressions (state)
    class(connected_state_t), intent(inout) :: state
    if (state%has_expr) call state%expr%reset_contents ()
  end subroutine connected_state_reset_expressions

```

30.2.6 Evaluation

Transfer momenta to the trace evaluator and fill the subevt with this effective kinematics, if applicable.

Note: we may want to apply a boost for the subevt.

```

(Parton states: parton state: TBP) +=
  procedure :: receive_kinematics => parton_state_receive_kinematics

(Parton states: procedures) +=
  subroutine parton_state_receive_kinematics (state)
    class(parton_state_t), intent(inout), target :: state
    if (state%has_trace) then
      call state%trace%receive_momenta ()
      select type (state)
        class is (connected_state_t)
          if (state%has_expr) then
            call state%expr%fill_subevt (state%trace%interaction_t)
          end if
        end select
    end if
  end subroutine parton_state_receive_kinematics

```

```

    end if
  end subroutine parton_state_receive_kinematics

```

Recover kinematics: We assume that the trace evaluator is filled with momenta. Send those momenta back to the sources, then fill the variables and subevent as above.

The incoming momenta of the connected state are not connected to the isolated state but to the beam interaction. Therefore, the incoming momenta within the isolated state do not become defined, yet. Instead, we reconstruct the beam (and ISR) momentum configuration.

```

(Parton states: parton state: TBP) +=
  procedure :: send_kinematics => parton_state_send_kinematics

(Parton states: procedures) +=
  subroutine parton_state_send_kinematics (state)
    class(parton_state_t), intent(inout), target :: state
    if (state%has_trace) then
      call interaction_send_momenta (state%trace%interaction_t)
      select type (state)
        class is (connected_state_t)
          call state%expr%fill_subevt (state%trace%interaction_t)
        end select
      end if
    end subroutine parton_state_send_kinematics

```

Evaluate the expressions. The routine evaluates first the cut expression. If the event passes, it evaluates the other expressions. Where no expressions are defined, default values are inserted.

```

(Parton states: connected state: TBP) +=
  procedure :: evaluate_expressions => connected_state_evaluate_expressions

(Parton states: procedures) +=
  subroutine connected_state_evaluate_expressions (state, passed, &
    scale, fac_scale, ren_scale, weight, scale_forced, force_evaluation)
    class(connected_state_t), intent(inout) :: state
    logical, intent(out) :: passed
    real(default), intent(out) :: scale, fac_scale, ren_scale, weight
    real(default), intent(in), allocatable, optional :: scale_forced
    logical, intent(in), optional :: force_evaluation
    if (state%has_expr) then
      call state%expr%evaluate (passed, scale, fac_scale, ren_scale, weight, &
        scale_forced, force_evaluation)
    end if
  end subroutine connected_state_evaluate_expressions

```

Evaluate the structure-function chain, if it is allocated explicitly. The argument is the factorization scale.

If the chain is merely a pointer, the chain should already be evaluated at this point.

```

(Parton states: isolated state: TBP) +=
  procedure :: evaluate_sf_chain => isolated_state_evaluate_sf_chain

```

```

⟨Parton states: procedures⟩+≡
  subroutine isolated_state_evaluate_sf_chain (state, fac_scale)
    class(isolated_state_t), intent(inout) :: state
    real(default), intent(in) :: fac_scale
    if (state%sf_chain_is_allocated) call state%sf_chain_eff%evaluate (fac_scale)
  end subroutine isolated_state_evaluate_sf_chain

```

Evaluate the trace.

```

⟨Parton states: parton state: TBP⟩+≡
  procedure :: evaluate_trace => parton_state_evaluate_trace

```

```

⟨Parton states: procedures⟩+≡
  subroutine parton_state_evaluate_trace (state)
    class(parton_state_t), intent(inout) :: state
    if (state%has_trace) call state%trace%evaluate ()
  end subroutine parton_state_evaluate_trace

```

```

⟨Parton states: parton state: TBP⟩+≡
  procedure :: evaluate_matrix => parton_state_evaluate_matrix

```

```

⟨Parton states: procedures⟩+≡
  subroutine parton_state_evaluate_matrix (state)
    class(parton_state_t), intent(inout) :: state
    if (state%has_matrix) call state%matrix%evaluate ()
  end subroutine parton_state_evaluate_matrix

```

Evaluate the extra evaluators that we need for physical events.

```

⟨Parton states: parton state: TBP⟩+≡
  procedure :: evaluate_event_data => parton_state_evaluate_event_data

```

```

⟨Parton states: procedures⟩+≡
  subroutine parton_state_evaluate_event_data (state, only_momenta)
    class(parton_state_t), intent(inout) :: state
    logical, intent(in), optional :: only_momenta
    logical :: only_mom
    only_mom = .false.; if (present (only_momenta)) only_mom = only_momenta
    select type (state)
    type is (connected_state_t)
      if (state%has_flows_sf) then
        call state%flows_sf%receive_momenta ()
        if (.not. only_mom) call state%flows_sf%evaluate ()
      end if
    end select
    if (state%has_matrix) then
      call state%matrix%receive_momenta ()
      if (.not. only_mom) call state%matrix%evaluate ()
    end if
    if (state%has_flows) then
      call state%flows%receive_momenta ()
      if (.not. only_mom) call state%flows%evaluate ()
    end if
  end subroutine parton_state_evaluate_event_data

```

Normalize the helicity density matrix by its trace, i.e., factor out the trace and put it into an overall normalization factor. The trace and flow evaluators are unchanged.

```

(Parton states: parton state: TBP)+≡
  procedure :: normalize_matrix_by_trace => &
    parton_state_normalize_matrix_by_trace

(Parton states: procedures)+≡
  subroutine parton_state_normalize_matrix_by_trace (state)
    class(parton_state_t), intent(inout) :: state
    if (state%has_matrix) call state%matrix%normalize_by_trace ()
  end subroutine parton_state_normalize_matrix_by_trace

```

30.2.7 Accessing the state

Three functions return a pointer to the event-relevant interactions.

```

(Parton states: parton state: TBP)+≡
  procedure :: get_trace_int_ptr => parton_state_get_trace_int_ptr
  procedure :: get_matrix_int_ptr => parton_state_get_matrix_int_ptr
  procedure :: get_flows_int_ptr => parton_state_get_flows_int_ptr

(Parton states: procedures)+≡
  function parton_state_get_trace_int_ptr (state) result (ptr)
    class(parton_state_t), intent(in), target :: state
    type(interaction_t), pointer :: ptr
    if (state%has_trace) then
      ptr => state%trace%interaction_t
    else
      ptr => null ()
    end if
  end function parton_state_get_trace_int_ptr

  function parton_state_get_matrix_int_ptr (state) result (ptr)
    class(parton_state_t), intent(in), target :: state
    type(interaction_t), pointer :: ptr
    if (state%has_matrix) then
      ptr => state%matrix%interaction_t
    else
      ptr => null ()
    end if
  end function parton_state_get_matrix_int_ptr

  function parton_state_get_flows_int_ptr (state) result (ptr)
    class(parton_state_t), intent(in), target :: state
    type(interaction_t), pointer :: ptr
    if (state%has_flows) then
      ptr => state%flows%interaction_t
    else
      ptr => null ()
    end if
  end function parton_state_get_flows_int_ptr

```

Return the indices of the beam particles and the outgoing particles within the trace (and thus, matrix and flows) evaluator, respectively.

```

(Parton states: connected state: TBP)+≡
  procedure :: get_beam_index => connected_state_get_beam_index
  procedure :: get_in_index => connected_state_get_in_index

(Parton states: procedures)+≡
  subroutine connected_state_get_beam_index (state, i_beam)
    class(connected_state_t), intent(in) :: state
    integer, dimension(:), intent(out) :: i_beam
    call state%expr%get_beam_index (i_beam)
  end subroutine connected_state_get_beam_index

  subroutine connected_state_get_in_index (state, i_in)
    class(connected_state_t), intent(in) :: state
    integer, dimension(:), intent(out) :: i_in
    call state%expr%get_in_index (i_in)
  end subroutine connected_state_get_in_index

(Parton states: public)+≡
  public :: refill_evaluator

(Parton states: procedures)+≡
  subroutine refill_evaluator (sqme, qn, flv_index, evaluator)
    complex(default), intent(in), dimension(:) :: sqme
    type(quantum_numbers_t), intent(in), dimension(:, :) :: qn
    integer, intent(in), dimension(:), optional :: flv_index
    type(evaluator_t), intent(inout) :: evaluator
    integer :: i, i_flv
    do i = 1, size (sqme)
      if (present (flv_index)) then
        i_flv = flv_index(i)
      else
        i_flv = i
      end if
      call evaluator%add_to_matrix_element (qn(:, i_flv), sqme(i), &
        match_only_flavor = .true.)
    end do
  end subroutine refill_evaluator

```

Return the number of outgoing (hard) particles for the state.

```

(Parton states: parton state: TBP)+≡
  procedure :: get_n_out => parton_state_get_n_out

(Parton states: procedures)+≡
  function parton_state_get_n_out (state) result (n)
    class(parton_state_t), intent(in), target :: state
    integer :: n
    n = state%trace%get_n_out ()
  end function parton_state_get_n_out

```

30.2.8 Unit tests

```
(parton_states_ut.f90)≡
  <File header>

  module parton_states_ut
    use unit_tests
    use parton_states_ut

  <Standard module head>

  <Parton states: public test>

  contains

  <Parton states: test driver>

  end module parton_states_ut
(parton_states_uti.f90)≡
  <File header>

  module parton_states_uti

  <Use kinds>
  <Use strings>
    use constants, only: zero
    use numeric_utils
    use flavors
    use colors
    use helicities
    use quantum_numbers
    use sf_base, only: sf_chain_instance_t
    use state_matrices, only: state_matrix_t
    use prc_template_me, only: prc_template_me_t
    use interactions, only: interaction_t
    use models, only: model_t, create_test_model
    use parton_states

  <Standard module head>

  <Parton states: test declarations>

  contains

  <Parton states: tests>

  end module parton_states_uti

  <Parton states: public test>≡
    public :: parton_states_test

  <Parton states: test driver>≡
    subroutine parton_states_test (u, results)
      integer, intent(in) :: u
      type(test_results_t), intent(inout) :: results
```

```

    <Parton states: execute tests>
end subroutine parton_states_test

```

Test a simple isolated state

```

<Parton states: execute tests>≡
    call test (parton_states_1, "parton_states_1", &
        "Create a 2 -> 2 isolated state and compute trace", &
        u, results)

<Parton states: test declarations>≡
    public :: parton_states_1

<Parton states: tests>≡
    subroutine parton_states_1 (u)
        integer, intent(in) :: u
        type(state_matrix_t), allocatable :: state
        type(flavor_t), dimension(2) :: flv_in
        type(flavor_t), dimension(2) :: flv_out1, flv_out2
        type(flavor_t), dimension(4) :: flv_tot
        type(helicity_t), dimension(4) :: hel
        type(color_t), dimension(4) :: col
        integer :: h1, h2, h3, h4
        integer :: f
        integer :: i
        type(quantum_numbers_t), dimension(4) :: qn
        type(prc_template_me_t) :: core
        type(sf_chain_instance_t), target :: sf_chain
        type(interaction_t), target :: int
        type(isolated_state_t) :: isolated_state
        integer :: n_states = 0
        integer, dimension(:), allocatable :: col_flow_index
        type(quantum_numbers_mask_t), dimension(2) :: qn_mask
        integer, dimension(8) :: i_allowed_states
        complex(default), dimension(8) :: me
        complex(default) :: me_check_tot, me_check_1, me_check_2, me2
        logical :: tmp1, tmp2
        type(model_t), pointer :: test_model => null ()

        write (u, "(A)") "* Test output: parton_states_1"
        write (u, "(A)") "* Purpose: Test the standard parton states"
        write (u, "(A)")

        call flv_in%init ([11, -11])
        call flv_out1%init ([1, -1])
        call flv_out2%init ([2, -2])

        write (u, "(A)") "* Using incoming flavors: "
        call flavor_write_array (flv_in, u)
        write (u, "(A)") "* Two outgoing flavor structures: "
        call flavor_write_array (flv_out1, u)
        call flavor_write_array (flv_out2, u)

```

```

write (u, "(A)") "* Initialize state matrix"
allocate (state)
call state%init ()

write (u, "(A)") "* Fill state matrix"
call col(3)%init ([1])
call col(4)%init ([-1])
do f = 1, 2
  do h1 = -1, 1, 2
    do h2 = -1, 1, 2
      do h3 = -1, 1, 2
        do h4 = -1, 1, 2
          n_states = n_states + 1
          call hel%init ([h1, h2, h3, h4], [h1, h2, h3, h4])
          if (f == 1) then
            flv_tot = [flv_in, flv_out1]
          else
            flv_tot = [flv_in, flv_out2]
          end if
          call qn%init (flv_tot, col, hel)
          call state%add_state (qn)
        end do
      end do
    end do
  end do
end do

!!! Two flavors, one color flow, 2 x 2 x 2 x 2 helicity configurations
!!! -> 32 states.
write (u, "(A)")
write (u, "(A,I2)") "* Generated number of states: ", n_states

call state%freeze ()

!!! Indices of the helicity configurations which are non-zero
i_allowed_states = [6, 7, 10, 11, 22, 23, 26, 27]
me = [cmplx (-1.89448E-5_default, 9.94456E-7_default, default), &
      cmplx (-8.37887E-2_default, 4.30842E-3_default, default), &
      cmplx (-1.99997E-1_default, -1.01985E-2_default, default), &
      cmplx (1.79717E-5_default, 9.27038E-7_default, default), &
      cmplx (-1.74859E-5_default, 8.78819E-7_default, default), &
      cmplx (1.67577E-1_default, -8.61683E-3_default, default), &
      cmplx (2.41331E-1_default, 1.23306E-2_default, default), &
      cmplx (-3.59435E-5_default, -1.85407E-6_default, default)]
me_check_tot = cmplx (zero, zero, default)
me_check_1 = cmplx (zero, zero, default)
me_check_2 = cmplx (zero, zero, default)
do i = 1, 8
  me2 = me(i) * conjg (me(i))
  me_check_tot = me_check_tot + me2
  if (i < 5) then
    me_check_1 = me_check_1 + me2
  else
    me_check_2 = me_check_2 + me2
  end if
end do

```



```

        end if
        call state%set_matrix_element (i_allowed_states(i), me(i))
    end do

    !!! Do not forget the color factor
    me_check_tot = 3._default * me_check_tot
    me_check_1 = 3._default * me_check_1
    me_check_2 = 3._default * me_check_2
    write (u, "(A)")

    write (u, "(A)") "* Setup interaction"
    call int%basic_init (2, 0, 2, set_relations = .true.)
    call int%set_state_matrix (state)

    core%data%n_in = 2; core%data%n_out = 2
    core%data%n_flv = 2
    allocate (core%data%flv_state (4, 2))
    core%data%flv_state (1, :) = [11, 11]
    core%data%flv_state (2, :) = [-11, -11]
    core%data%flv_state (3, :) = [1, 2]
    core%data%flv_state (4, :) = [-1, -2]
    core%use_color_factors = .false.
    core%nc = 3

    write (u, "(A)") "* Init isolated state"
    call isolated_state%init (sf_chain, int)
    !!! There is only one color flow.
    allocate (col_flow_index (n_states)); col_flow_index = 1
    call qn_mask%init (.false., .false., .true., mask_cg = .false.)
    write (u, "(A)") "* Give a trace to the isolated state"
    call isolated_state%setup_square_trace (core, qn_mask, col_flow_index, .false.)
    call isolated_state%evaluate_trace ()
    write (u, "(A)")
    write (u, "(A)", advance = "no") "* Squared matrix element correct: "
    write (u, "(L1)") nearly_equal (me_check_tot, &
        isolated_state%trace%get_matrix_element (1), rel_smallness = 0.00001_default)

    write (u, "(A)") "* Give a matrix to the isolated state"
    call create_test_model (var_str ("SM"), test_model)
    call isolated_state%setup_square_matrix (core, test_model, qn_mask, col_flow_index)
    call isolated_state%evaluate_matrix ()

    write (u, "(A)") "* Sub-matrixelements correct: "
    tmp1 = nearly_equal (me_check_1, &
        isolated_state%matrix%get_matrix_element (1), rel_smallness = 0.00001_default)
    tmp2 = nearly_equal (me_check_2, &
        isolated_state%matrix%get_matrix_element (2), rel_smallness = 0.00001_default)
    write (u, "(A,L1,A,L1)") "* 1: ", tmp1, ", 2: ", tmp2

    write (u, "(A)") "* Test output end: parton_states_1"
end subroutine parton_states_1

```

30.3 Process component management

This module contains tools for managing and combining process components and matrix-element code and values, acting at a level below the actual process definition.

30.3.1 Abstract base type

The types introduced here are abstract base types.

`<pcm_base.f90>`≡

<File header>

`module pcm_base`

<Use kinds>

`use io_units`

`use diagnostics`

`use format_utils, only: write_integer_array`

`use format_utils, only: write_separator`

`use physics_defs, only: BORN, NLO_REAL`

<Use strings>

`use os_interface, only: os_data_t`

`use process_libraries, only: process_component_def_t`

`use process_libraries, only: process_library_t`

`use prc_core_def`

`use prc_core`

`use variables, only: var_list_t`

`use mappings, only: mapping_defaults_t`

`use phs_base, only: phs_config_t`

`use phs_forests, only: phs_parameters_t`

`use mci_base, only: mci_t`

`use model_data, only: model_data_t`

`use models, only: model_t`

`use blha_config, only: blha_master_t`

`use blha_olp_interfaces, only: blha_template_t`

`use process_config`

`use process_mci, only: process_mci_entry_t`

<Standard module head>

<PCM base: public>

<PCM base: parameters>

<PCM base: types>

<PCM base: interfaces>

`contains`

```
<PCM base: procedures>
```

```
end module pcm_base
```

30.3.2 Core management

This object holds information about the cores used by the components and allocates the corresponding manager instance.

i_component is the index of the process component which this core belongs to. The pointer to the core definition is a convenient help in configuring the core itself.

We allow for a **blha_config** configuration object that covers BLHA cores. The BLHA standard is suitable generic to warrant support outside of specific type extension (i.e., applies to LO and NLO if requested). The BLHA configuration is allocated only if the core requires it.

```
<PCM base: public>≡
```

```
public :: core_entry_t
```

```
<PCM base: types>≡
```

```
type :: core_entry_t
  integer :: i_component = 0
  logical :: active = .false.
  class(prc_core_def_t), pointer :: core_def => null ()
  type(blha_template_t), allocatable :: blha_config
  class(prc_core_t), allocatable :: core
contains
  <PCM base: core entry: TBP>
end type core_entry_t
```

```
<PCM base: core entry: TBP>≡
```

```
procedure :: get_core_ptr => core_entry_get_core_ptr
```

```
<PCM base: procedures>≡
```

```
function core_entry_get_core_ptr (core_entry) result (core)
  class(core_entry_t), intent(in), target :: core_entry
  class(prc_core_t), pointer :: core
  if (allocated (core_entry%core)) then
    core => core_entry%core
  else
    core => null ()
  end if
end function core_entry_get_core_ptr
```

Configure the core object after allocation with correct type. The **core_def** object pointer and the index **i_component** of the associated process component are already there.

```
<PCM base: core entry: TBP>+≡
```

```
procedure :: configure => core_entry_configure
```

```

<PCM base: procedures>+≡
  subroutine core_entry_configure (core_entry, lib, id)
    class(core_entry_t), intent(inout) :: core_entry
    type(process_library_t), intent(in), target :: lib
    type(string_t), intent(in) :: id
    call core_entry%core%init &
      (core_entry%core_def, lib, id, core_entry%i_component)
  end subroutine core_entry_configure

```

30.3.3 Process component manager

The process-component manager `pcm` is the master component of the `process_t` object. It serves two purposes:

1. It holds configuration data which allow us to centrally manage the components, terms, etc. of the process object.
2. It implements the methods that realize the algorithm for constructing the process object and computing an integral. This algorithm makes use of the data stored within `pcm`.

To this end, the object is abstract and polymorphic. The two extensions that we support, implement (a) default tree-level calculation, optionally including a sum over sub-processes with different particle content, or (b) the FKS-NLO subtraction algorithm for QCD-corrected processes. In both cases, the type extensions may hold suitable further data.

Data included in the base type:

The number of components determines the `component_selected` array.

`i_phs_config` is a lookup table that holds the PHS configuration index for a given component index.

`i_core` is a lookup table that holds the core-entry index for a given component index.

`i_mci` is a lookup table that holds the integrator (MCI) index for a given component index.

```

<PCM base: public>+≡
  public :: pcm_t

```

```

<PCM base: types>+≡
  type, abstract :: pcm_t
    logical :: initialized = .false.
    logical :: has_pdfs = .false.
    integer :: n_components = 0
    integer :: n_cores = 0
    integer :: n_mci = 0
    logical, dimension(:), allocatable :: component_selected
    logical, dimension(:), allocatable :: component_active
    integer, dimension(:), allocatable :: i_phs_config
    integer, dimension(:), allocatable :: i_core
    integer, dimension(:), allocatable :: i_mci
    type(blha_template_t) :: blha_defaults
    logical :: uses_blha = .false.
    type(os_data_t) :: os_data

```

```

contains
  <PCM base: pcm: TBP>
end type pcm_t

```

The factory method. We use the `inout` intent, so calling this again is an error.

```

<PCM base: pcm: TBP>≡
  procedure(pcm_allocate_workspace), deferred :: allocate_workspace

<PCM base: interfaces>≡
  abstract interface
    subroutine pcm_allocate_workspace (pcm, work)
      import
      class(pcm_t), intent(in) :: pcm
      class(pcm_workspace_t), intent(inout), allocatable :: work
    end subroutine pcm_allocate_workspace
  end interface

```

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_is_nlo), deferred :: is_nlo

<PCM base: interfaces>+≡
  abstract interface
    function pcm_is_nlo (pcm) result (is_nlo)
      import
      logical :: is_nlo
      class(pcm_t), intent(in) :: pcm
    end function pcm_is_nlo
  end interface

```

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_final), deferred :: final

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_final (pcm)
      import
      class(pcm_t), intent(inout) :: pcm
    end subroutine pcm_final
  end interface

```

30.3.4 Initialization methods

The PCM has the duty to coordinate and configure the process-object components.

Initialize the PCM configuration itself, using environment data.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_init), deferred :: init

```

```

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_init (pcm, env, meta)
      import
      class(pcm_t), intent(out) :: pcm
      type(process_environment_t), intent(in) :: env
      type(process_metadata_t), intent(in) :: meta
    end subroutine pcm_init
  end interface

```

Initialize the BLHA configuration block, the component-independent default settings. This is to be called by `pcm_init`. We use the provided variable list.

This block is filled regardless of whether BLHA is actually used, because why not? We use a default value for the scheme (not set in unit tests).

```

<PCM base: pcm: TBP>+≡
  procedure :: set_blha_defaults => pcm_set_blha_defaults

<PCM base: procedures>+≡
  subroutine pcm_set_blha_defaults (pcm, polarized_beams, var_list)
    class(pcm_t), intent(inout) :: pcm
    type(var_list_t), intent(in) :: var_list
    logical, intent(in) :: polarized_beams
    logical :: muon_yukawa_off
    real(default) :: top_yukawa
    type(string_t) :: ew_scheme
    muon_yukawa_off = &
      var_list%get_lval (var_str ("?openloops_switch_off_muon_yukawa"))
    top_yukawa = &
      var_list%get_rval (var_str ("blha_top_yukawa"))
    ew_scheme = &
      var_list%get_sval (var_str ("$blha_ew_scheme"))
    if (ew_scheme == "") ew_scheme = "Gmu"
    call pcm%blha_defaults%init &
      (polarized_beams, muon_yukawa_off, top_yukawa, ew_scheme)
  end subroutine pcm_set_blha_defaults

```

Read the method settings from the variable list and store them in the BLHA master. The details depend on the `pcm` concrete type.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_set_blha_methods), deferred :: set_blha_methods

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_set_blha_methods (pcm, blha_master, var_list)
      import
      class(pcm_t), intent(inout) :: pcm
      type(blha_master_t), intent(inout) :: blha_master
      type(var_list_t), intent(in) :: var_list
    end subroutine pcm_set_blha_methods
  end interface

```

Produce the LO and NLO flavor-state tables (as far as available), as appropriate for BLHA configuration. We may inspect either the PCM itself or the array of process cores.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_get_blha_flv_states), deferred :: get_blha_flv_states
<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_get_blha_flv_states (pcm, core_entry, flv_born, flv_real)
      import
      class(pcm_t), intent(in) :: pcm
      type(core_entry_t), dimension(:), intent(in) :: core_entry
      integer, dimension(:,:), allocatable, intent(out) :: flv_born
      integer, dimension(:,:), allocatable, intent(out) :: flv_real
    end subroutine pcm_get_blha_flv_states
  end interface

```

Allocate the right number of process components. The number is also stored in the process meta. Initially, all components are active but none are selected.

```

<PCM base: pcm: TBP>+≡
  procedure :: allocate_components => pcm_allocate_components
<PCM base: procedures>+≡
  subroutine pcm_allocate_components (pcm, comp, meta)
    class(pcm_t), intent(inout) :: pcm
    type(process_component_t), dimension(:), allocatable, intent(out) :: comp
    type(process_metadata_t), intent(in) :: meta
    pcm%n_components = meta%n_components
    allocate (comp (pcm%n_components))
    allocate (pcm%component_selected (pcm%n_components), source = .false.)
    allocate (pcm%component_active (pcm%n_components), source = .true.)
  end subroutine pcm_allocate_components

```

Each process component belongs to a category/type, which we identify by a universal integer constant. The categories can be taken from the process definition. For easy lookup, we store the categories in an array.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_categorize_components), deferred :: categorize_components
<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_categorize_components (pcm, config)
      import
      class(pcm_t), intent(inout) :: pcm
      type(process_config_data_t), intent(in) :: config
    end subroutine pcm_categorize_components
  end interface

```

Allocate the right number and type(s) of process-core objects, i.e., the interface object between the process and matrix-element code.

Within the `pcm` block, also associate cores with components and store relevant configuration data, including the `i_core` lookup table.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_allocate_cores), deferred :: allocate_cores

```

```

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_allocate_cores (pcm, config, core_entry)
      import
      class(pcm_t), intent(inout) :: pcm
      type(process_config_data_t), intent(in) :: config
      type(core_entry_t), dimension(:), allocatable, intent(out) :: core_entry
    end subroutine pcm_allocate_cores
  end interface

```

Generate and interface external code for a single core, if this is required.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_prepare_any_external_code), deferred :: &
    prepare_any_external_code

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_prepare_any_external_code &
      (pcm, core_entry, i_core, libname, model, var_list)
      import
      class(pcm_t), intent(in) :: pcm
      type(core_entry_t), intent(inout) :: core_entry
      integer, intent(in) :: i_core
      type(string_t), intent(in) :: libname
      type(model_data_t), intent(in), target :: model
      type(var_list_t), intent(in) :: var_list
    end subroutine pcm_prepare_any_external_code
  end interface

```

Prepare the BLHA configuration for a core object that requires it. This does not affect the core object, which may not yet be allocated.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_setup_blha), deferred :: setup_blha

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_setup_blha (pcm, core_entry)
      import
      class(pcm_t), intent(in) :: pcm
      type(core_entry_t), intent(inout) :: core_entry
    end subroutine pcm_setup_blha
  end interface

```

Configure the BLHA interface for a core object that requires it. This is separate from the previous method, assuming that the pcm has to allocate the actual cores and acquire some data in-between.

```

<PCM base: pcm: TBP>+≡
  procedure(pcm_prepare_blha_core), deferred :: prepare_blha_core

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_prepare_blha_core (pcm, core_entry, model)
      import

```



```

        class(pcm_t), intent(in) :: pcm
        type(core_entry_t), intent(inout) :: core_entry
        class(model_data_t), intent(in), target :: model
    end subroutine pcm_prepare_blha_core
end interface

```

Allocate and configure the MCI (multi-channel integrator) records and their relation to process components, appropriate for the algorithm implemented by pcm.

Create a `mci_t` template: the procedure `dispatch_mci` is called as a factory method for allocating the `mci_t` object with a specific concrete type. The call may depend on the concrete `pcm` type.

```

<PCM base: public>+≡
    public :: dispatch_mci_proc

<PCM base: interfaces>+≡
    abstract interface
        subroutine dispatch_mci_proc (mci, var_list, process_id, is_nlo)
            import
            class(mci_t), allocatable, intent(out) :: mci
            type(var_list_t), intent(in) :: var_list
            type(string_t), intent(in) :: process_id
            logical, intent(in), optional :: is_nlo
        end subroutine dispatch_mci_proc
    end interface

    <PCM base: pcm: TBP>+≡
        procedure(pcm_setup_mci), deferred :: setup_mci
        procedure(pcm_call_dispatch_mci), deferred :: call_dispatch_mci

    <PCM base: interfaces>+≡
        abstract interface
            subroutine pcm_setup_mci (pcm, mci_entry)
                import
                class(pcm_t), intent(inout) :: pcm
                type(process_mci_entry_t), &
                    dimension(:), allocatable, intent(out) :: mci_entry
            end subroutine pcm_setup_mci
        end interface

        abstract interface
            subroutine pcm_call_dispatch_mci (pcm, &
                dispatch_mci, var_list, process_id, mci_template)
                import
                class(pcm_t), intent(inout) :: pcm
                procedure(dispatch_mci_proc) :: dispatch_mci
                type(var_list_t), intent(in) :: var_list
                type(string_t), intent(in) :: process_id
                class(mci_t), intent(out), allocatable :: mci_template
            end subroutine pcm_call_dispatch_mci
        end interface

```

Proceed with PCM configuration based on the core and component configuration data. Base version is empty.

```

<PCM base: pcm: TBP>+≡
    procedure(pcm_complete_setup), deferred :: complete_setup

<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_complete_setup (pcm, core_entry, component, model)
            import
            class(pcm_t), intent(inout) :: pcm
            type(core_entry_t), dimension(:), intent(in) :: core_entry
            type(process_component_t), dimension(:), intent(inout) :: component
            type(model_t), intent(in), target :: model
        end subroutine pcm_complete_setup
    end interface

```

Retrieve information

Return the core index that belongs to a particular component.

```

<PCM base: pcm: TBP>+≡
    procedure :: get_i_core => pcm_get_i_core

<PCM base: procedures>+≡
    function pcm_get_i_core (pcm, i_component) result (i_core)
        class(pcm_t), intent(in) :: pcm
        integer, intent(in) :: i_component
        integer :: i_core
        if (allocated (pcm%i_core)) then
            i_core = pcm%i_core(i_component)
        else
            i_core = 0
        end if
    end function pcm_get_i_core

```

Phase-space configuration

Allocate and initialize the right number and type(s) of phase-space configuration entries. The `i_phs_config` lookup table must be set accordingly.

```

<PCM base: pcm: TBP>+≡
    procedure(pcm_init_phs_config), deferred :: init_phs_config

<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_init_phs_config &
            (pcm, phs_entry, meta, env, phs_par, mapping_defs)
            import
            class(pcm_t), intent(inout) :: pcm
            type(process_phs_config_t), &
                dimension(:), allocatable, intent(out) :: phs_entry
            type(process_metadata_t), intent(in) :: meta
            type(process_environment_t), intent(in) :: env
            type(mapping_defaults_t), intent(in) :: mapping_defs

```

```

        type(phs_parameters_t), intent(in) :: phs_par
    end subroutine pcm_init_phs_config
end interface

```

Initialize a single component. We require all process-configuration blocks, and specific templates for the phase-space and integrator configuration.

We also provide the current component index `i` and the `active` flag.

```

<PCM base: pcm: TBP>+≡
    procedure(pcm_init_component), deferred :: init_component

<PCM base: interfaces>+≡
    abstract interface
        subroutine pcm_init_component &
            (pcm, component, i, active, phs_config, env, meta, config)
        import
        class(pcm_t), intent(in) :: pcm
        type(process_component_t), intent(out) :: component
        integer, intent(in) :: i
        logical, intent(in) :: active
        class(phs_config_t), allocatable, intent(in) :: phs_config
        type(process_environment_t), intent(in) :: env
        type(process_metadata_t), intent(in) :: meta
        type(process_config_data_t), intent(in) :: config
    end subroutine pcm_init_component
    end interface

```

Record components in the process meta data if they have turned out to be inactive.

```

<PCM base: pcm: TBP>+≡
    procedure :: record_inactive_components => pcm_record_inactive_components

<PCM base: procedures>+≡
    subroutine pcm_record_inactive_components (pcm, component, meta)
        class(pcm_t), intent(inout) :: pcm
        type(process_component_t), dimension(:), intent(in) :: component
        type(process_metadata_t), intent(inout) :: meta
        integer :: i
        pcm%component_active = component%active
        do i = 1, pcm%n_components
            if (.not. component(i)%active) call meta%deactivate_component (i)
        end do
    end subroutine pcm_record_inactive_components

```

30.3.5 Manager workspace

This object deals with the actual (squared) matrix element values. It holds any central data that are generated and/or used when calculating a particular phase-space point.

Since phase-space points are associated with an integrator, we expect the instances of this type to correspond to MCI instances.

```

<PCM base: public>+≡
    public :: pcm_workspace_t

```

```

<PCM base: types>+≡
  type, abstract :: pcm_workspace_t
  !      class(pcm_t), pointer :: config => null ()
        logical :: bad_point = .false.
  contains
  <PCM base: pcm instance: TBP>
  end type pcm_workspace_t

<PCM base: pcm instance: TBP>≡
  procedure(pcm_work_final), deferred :: final

<PCM base: interfaces>+≡
  abstract interface
    subroutine pcm_work_final (pcm_work)
      import
      class(pcm_workspace_t), intent(inout) :: pcm_work
    end subroutine pcm_work_final
  end interface

<PCM base: pcm instance: TBP>+≡
  procedure(pcm_work_is_nlo), deferred :: is_nlo

<PCM base: interfaces>+≡
  abstract interface
    function pcm_work_is_nlo (pcm_work) result (is_nlo)
      import
      logical :: is_nlo
      class(pcm_workspace_t), intent(inout) :: pcm_work
    end function pcm_work_is_nlo
  end interface

<XXX PCM base: pcm instance: TBP>≡
  procedure :: link_config => pcm_work_link_config

<XXX PCM base: procedures>≡
  subroutine pcm_work_link_config (pcm_work, config)
    class(pcm_workspace_t), intent(inout) :: pcm_work
    class(pcm_t), intent(in), target :: config
    pcm_work%config => config
  end subroutine pcm_work_link_config

<PCM base: pcm instance: TBP>+≡
  procedure :: is_valid => pcm_work_is_valid

<PCM base: procedures>+≡
  function pcm_work_is_valid (pcm_work) result (valid)
    logical :: valid
    class(pcm_workspace_t), intent(in) :: pcm_work
    valid = .not. pcm_work%bad_point
  end function pcm_work_is_valid

<PCM base: pcm instance: TBP>+≡
  procedure :: set_bad_point => pcm_work_set_bad_point

```

```

⟨PCM base: procedures⟩+≡
  pure subroutine pcm_work_set_bad_point (pcm_work, bad_point)
    class(pcm_workspace_t), intent(inout) :: pcm_work
    logical, intent(in) :: bad_point
    pcm_work%bad_point = pcm_work%bad_point .or. bad_point
  end subroutine pcm_work_set_bad_point

```

30.4 The process object

```

⟨process.f90⟩≡
  ⟨File header⟩

  module process

    ⟨Use kinds⟩
    ⟨Use strings⟩
    ⟨Use debug⟩
    use io_units
    use format_utils, only: write_separator
    use constants
    use diagnostics
    use numeric_utils
    use lorentz
    use cputime
    use md5
    use rng_base
    use dispatch_rng, only: dispatch_rng_factory
    use dispatch_rng, only: update_rng_seed_in_var_list
    use os_interface
    use sm_qcd
    use integration_results
    use mci_base
    use flavors
    use model_data
    use models
    use physics_defs
    use process_libraries
    use process_constants
    use particles
    use variables
    use beam_structures
    use beams
    use interactions
    use pdg_arrays
    use expr_base
    use sf_base
    use sf_mappings
    use resonances, only: resonance_history_t, resonance_history_set_t

    use prc_test_core, only: test_t
    use prc_core_def, only: prc_core_def_t
    use prc_core, only: prc_core_t, helicity_selection_t

```

```

use prc_external, only: prc_external_t
use prc_recola, only: prc_recola_t
use blha_olp_interfaces, only: prc_blha_t, blha_template_t
use prc_threshold, only: prc_threshold_t
use phs_fks, only: phs_fks_config_t

use phs_base
use mappings, only: mapping_defaults_t
use phs_forests, only: phs_parameters_t
use phs_wood, only: phs_wood_config_t
use dispatch_phase_space, only: dispatch_phs
use blha_config, only: blha_master_t
use nlo_data, only: FKS_DEFAULT, FKS_RESONANCES

use parton_states, only: connected_state_t
use pcm_base
use pcm
use process_counter
use process_config
use process_mci

<Standard module head>

<Process: public>

<Process: public parameters>

<Process: types>

<Process: interfaces>

contains

<Process: procedures>

end module process

```

30.4.1 Process status

Store counter and status information in a process object.

```

<Process: types>≡
  type :: process_status_t
  private
  end type process_status_t

```

30.4.2 Process status

Store integration results in a process object.

```

<Process: types>+≡
  type :: process_results_t
  private

```

```
end type process_results_t
```

30.4.3 The process type

NOTE: The description below represents the intended structure after refactoring and disentangling the FKS-NLO vs. LO algorithm dependencies.

A **process** object is the internal representation of integration-run methods and data, as they are controlled by the user via a Sindarin script. The process object provides access to matrix elements (the actual “process” definitions that the user has provided before), it defines the separation into individually integrable components, and it manages phase-space construction, the actual integration over phase space, and the accumulation of results.

As a workspace for individual sampling calls, we introduce an associated **process_instance** object type elsewhere. The **process** object contains data that either define the configuration or accumulate results from a complete integration pass.

After successful phase-space integration, subsequent event generation is not actually represented by the **process** object. However, any event generation refers to an existing **process** object which represents a specific integration pass, and it uses a fresh **process_instance** workspace for calculations.

The process object consists of several subobjects with their specific purposes. The corresponding types are defined below. (Technically, the subobject type definitions have to come before the process type definition, but with NOWEB magic we reverse this order here.)

The **meta** object describes the process globally. All contents become fixed when the object is initialized. Similarly, the **env** component captures the (Sindarin) environment at the point where the process object is initialized.

The **config** object holds physical and technical configuration data that are collected and derived from the environment during process initialization, and which are common to all process components.

The **pcm** object (process-component manager) is polymorphic. This is an object which holds data which represent the process-object structure and breakdown, and it contains the methods that implement the algorithm of managing this structure, accumulating partial results, and finally collecting the pieces. Depending on the generic process type, the contents of **pcm** do vary. In particular, there is some base-type data content and a simple (default) extension which is designed for traditional O’MEGA matrix elements and tree-level integration, possibly with several sub-processes to sum over. The second extension is designed for the FKS phase-space and subtraction algorithm for NLO QCD, which interfaces external one-loop providers.

The **component** subobjects are, first of all, interfaces to the original process-component definitions that have been provided by the user, which the program has already taken to produce matrix-element code and interfaces. The management of those components is deferred by **pcm**, which contains the information that defines the role of each component. In particular, in the default (LO) version, process components correspond to distinct particle combinations which have been included in the original process definition. In the FKS-NLO version, the breakdown of a NLO process into Born, real, virtual, etc. components determines the setup.

The `phs_config` subobjects hold data that allow and implement the construction of phase-space configurations. The type `process_phs_config_t` is a wrapper type around the concrete polymorphic `phs_config_t` object type, which manages phase-space construction, including some bookkeeping required for setting up multi-channel integration. In the LO case, we expect a separate entry for each independent sub-process. For the FKS-NLO algorithm, we expect several entries: a default-type entry which implements the underlying Born phase space, and additional entries which enable the construction of various real-radiation and subtraction kinematics configurations.

A `core_entry` is the interface to existing matrix-element and interaction code. Depending on the process and its components, there may be various distinct matrix elements to compute.

The `mci_entry` objects configure distinct MC input parameter sets and their associated (multi-channel) integrators.

The `rng_factory` object is a single objects which constructs individual random-number generators for various tasks, in a uniform and well-defined way.

The `beam_config` object describes the incoming particles, either the decay mother or the scattering beams. It also contains the spectrum- and structure-function setup, which has to interact with the phase-space and integrator facilities.

The `term` subobjects break down the process in its smallest parts which appear in the calculation. For LO processes, the correspondence between terms and components is one-to-one. The FKS-NLO algorithm requires not just separation of Born, real, and virtual components but also subtraction terms, and a decomposition of the real phase space into singular regions. The general idea is that the integration results of distinct sets of terms are summed over to provide the results of individual components. This is also controlled by the `pcm` subobject.

The `process_status` object is a bookkeeping device that allows us to query the status of an ongoing calculation.

The `process_results` object collects the integration results for external use, including integration history information.

```

(Process: public)≡
    public :: process_t

(Process: types)+≡
    type :: process_t
    private
    type(process_metadata_t) :: &
        meta
    type(process_environment_t) :: &
        env
    type(process_config_data_t) :: &
        config
    class(pcm_t), allocatable :: &
        pcm
    type(process_component_t), dimension(:), allocatable :: &
        component
    type(process_phs_config_t), dimension(:), allocatable :: &
        phs_entry
    type(core_entry_t), dimension(:), allocatable :: &
        core_entry

```



```

type(process_mci_entry_t), dimension(:), allocatable :: &
    mci_entry
class(rng_factory_t), allocatable :: &
    rng_factory
type(process_beam_config_t) :: &
    beam_config
type(process_term_t), dimension(:), allocatable :: &
    term
type(process_status_t) :: &
    status
type(process_results_t) :: &
    result
contains
    <Process: process: TBP>
end type process_t

```

30.4.4 Process pointer

Wrapper type for storing pointers to process objects in arrays.

```

<Process: public>+≡
    public :: process_ptr_t

<Process: types>+≡
    type :: process_ptr_t
        type(process_t), pointer :: p => null ()
    end type process_ptr_t

```

30.4.5 Output

This procedure is an important debugging and inspection tool; it is not used during normal operation. The process object is written to a file (identified by unit, which may also be standard output). Optional flags determine whether we show everything or just the interesting parts.

The shorthand as a traditional TBP.

```

<Process: process: TBP>≡
    procedure :: write => process_write

<Process: procedures>≡
    subroutine process_write (process, screen, unit, &
        show_os_data, show_var_list, show_rng, show_expressions, pacify)
        class(process_t), intent(in) :: process
        logical, intent(in) :: screen
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_os_data
        logical, intent(in), optional :: show_var_list
        logical, intent(in), optional :: show_rng
        logical, intent(in), optional :: show_expressions
        logical, intent(in), optional :: pacify
        integer :: u, iostat
        character(0) :: iomsg
        integer, dimension(:), allocatable :: v_list
    end subroutine process_write

```

```

u = given_output_unit (unit)
allocate (v_list (0))
call set_flag (v_list, F_SHOW_OS_DATA, show_os_data)
call set_flag (v_list, F_SHOW_VAR_LIST, show_var_list)
call set_flag (v_list, F_SHOW_RNG, show_rng)
call set_flag (v_list, F_SHOW_EXPRESSIONS, show_expressions)
call set_flag (v_list, F_PACIFY, pacify)
if (screen) then
    call process%write_formatted (u, "LISTDIRECTED", v_list, iostat, iomsg)
else
    call process%write_formatted (u, "DT", v_list, iostat, iomsg)
end if
end subroutine process_write

```

Standard DTIO procedure with binding.

For the particular application, the screen format is triggered by the LISTDIRECTED option for the iotype format editor string. The other options activate when the particular parameter value is found in v_list.

NOTE: The DTIO generic binding is supported by gfortran since 7.0.

TODO wk 2018: The default could be to show everything, and we should have separate switches for all major parts. Currently, there are only a few.

(Process: process: TBP)+≡

```

! generic :: write (formatted) => write_formatted
procedure :: write_formatted => process_write_formatted

```

(Process: procedures)+≡

```

subroutine process_write_formatted (dtv, unit, iotype, v_list, iostat, iomsg)
    class(process_t), intent(in) :: dtv
    integer, intent(in) :: unit
    character(*), intent(in) :: iotype
    integer, dimension(:), intent(in) :: v_list
    integer, intent(out) :: iostat
    character(*), intent(inout) :: iomsg
    integer :: u
    logical :: screen
    logical :: var_list
    logical :: rng_factory
    logical :: expressions
    logical :: counters
    logical :: os_data
    logical :: model
    logical :: pacify
    integer :: i
    u = unit
    select case (iotype)
    case ("LISTDIRECTED")
        screen = .true.
    case default
        screen = .false.
    end select
    var_list = flagged (v_list, F_SHOW_VAR_LIST)
    rng_factory = flagged (v_list, F_SHOW_RNG, .true.)
    expressions = flagged (v_list, F_SHOW_EXPRESSIONS)

```

```

counters = .true.
os_data = flagged (v_list, F_SHOW_OS_DATA)
model = .false.
pacify = flagged (v_list, F_PACIFY)
associate (process => dtv)
  if (screen) then
    write (msg_buffer, "(A)") repeat ("-", 72)
    call msg_message ()
  else
    call write_separator (u, 2)
  end if
  call process%meta%write (u, screen)
  if (var_list) then
    call process%env%write (u, show_var_list=var_list, &
      show_model=.false., show_lib=.false., &
      show_os_data=os_data)
  else if (.not. screen) then
    write (u, "(1x,A)") "Variable list: [not shown]"
  end if
  if (process%meta%type == PRC_UNKNOWN) then
    call write_separator (u, 2)
    return
  else if (screen) then
    return
  end if
  call write_separator (u)
  call process%config%write (u, counters, model, expressions)
  if (rng_factory) then
    if (allocated (process%rng_factory)) then
      call write_separator (u)
      call process%rng_factory%write (u)
    end if
  end if
  call write_separator (u, 2)
  if (allocated (process%component)) then
    write (u, "(1x,A)") "Process component configuration:"
    do i = 1, size (process%component)
      call write_separator (u)
      call process%component(i)%write (u)
    end do
  else
    write (u, "(1x,A)") "Process component configuration: [undefined]"
  end if
  call write_separator (u, 2)
  if (allocated (process%term)) then
    write (u, "(1x,A)") "Process term configuration:"
    do i = 1, size (process%term)
      call write_separator (u)
      call process%term(i)%write (u)
    end do
  else
    write (u, "(1x,A)") "Process term configuration: [undefined]"
  end if
  call write_separator (u, 2)

```

```

call process%beam_config%write (u)
call write_separator (u, 2)
if (allocated (process%mc_entry)) then
  write (u, "(1x,A)") "Multi-channel integrator configurations:"
  do i = 1, size (process%mc_entry)
    call write_separator (u)
    write (u, "(1x,A,I0,A)") "MCI #", i, ":"
    call process%mc_entry(i)%write (u, pacify)
  end do
end if
call write_separator (u, 2)
end associate
iostat = 0
iomsg = ""
end subroutine process_write_formatted

```

<Process: process: TBP>+≡

```

procedure :: write_meta => process_write_meta

```

<Process: procedures>+≡

```

subroutine process_write_meta (process, unit, testflag)
  class(process_t), intent(in) :: process
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  integer :: u, i
  u = given_output_unit (unit)
  select case (process%meta%type)
  case (PRC_UNKNOWN)
    write (u, "(1x,A)") "Process instance [undefined]"
    return
  case (PRC_DECAY)
    write (u, "(1x,A)", advance="no") "Process instance [decay]:"
  case (PRC_SCATTERING)
    write (u, "(1x,A)", advance="no") "Process instance [scattering]:"
  case default
    call msg_bug ("process_instance_write: undefined process type")
  end select
  write (u, "(1x,A,A,A)") "'", char (process%meta%id), "'"
  write (u, "(3x,A,A,A)") "Run ID = '", char (process%meta%run_id), "'"
  if (allocated (process%meta%component_id)) then
    write (u, "(3x,A)") "Process components:"
    do i = 1, size (process%meta%component_id)
      if (process%pcm%component_selected(i)) then
        write (u, "(3x,'*')", advance="no")
      else
        write (u, "(4x)", advance="no")
      end if
      write (u, "(1x,I0,9A)") i, ": '", &
        char (process%meta%component_id (i)), "' : ", &
        char (process%meta%component_description (i))
    end do
  end if
end subroutine process_write_meta

```

Screen output. Write a short account of the process configuration and the current results. The verbose version lists the components, the short version just the results.

```

(Process: process: TBP)+≡
  procedure :: show => process_show

(Process: procedures)+≡
  subroutine process_show (object, unit, verbose)
    class(process_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u
    logical :: verb
    real(default) :: err_percent
    u = given_output_unit (unit)
    verb = .true.; if (present (verbose)) verb = verbose
    if (verb) then
      call object%meta%show (u, object%config%model%get_name ())
      select case (object%meta%type)
        case (PRC_DECAY)
          write (u, "(2x,A)", advance="no") "Computed width ="
        case (PRC_SCATTERING)
          write (u, "(2x,A)", advance="no") "Computed cross section ="
        case default; return
      end select
    else
      if (object%meta%run_id /= "") then
        write (u, "('Run',1x,A,':',1x)", advance="no") &
          char (object%meta%run_id)
      end if
      write (u, "(A)", advance="no") char (object%meta%id)
      select case (object%meta%num_id)
        case (0)
          write (u, "(::)")
        case default
          write (u, "(1x,'(,IO,')','::')" object%meta%num_id)
      end select
      write (u, "(2x)", advance="no")
    end if
    if (object%has_integral_tot ()) then
      write (u, "(ES14.7,1x,'+-',ES9.2)", advance="no") &
        object%get_integral_tot (), object%get_error_tot ()
      select case (object%meta%type)
        case (PRC_DECAY)
          write (u, "(1x,A)", advance="no") "GeV"
        case (PRC_SCATTERING)
          write (u, "(1x,A)", advance="no") "fb "
        case default
          write (u, "(1x,A)", advance="no") " "
      end select
      if (object%get_integral_tot () /= 0) then
        err_percent = abs (100 &
          * object%get_error_tot () / object%get_integral_tot ())
      else

```

```

        err_percent = 0
    end if
    if (err_percent == 0) then
        write (u, "(1x,'(,F4.0,4x,')')") err_percent
    else if (err_percent < 0.1) then
        write (u, "(1x,'(,F7.3,1x,')')") err_percent
    else if (err_percent < 1) then
        write (u, "(1x,'(,F6.2,2x,')')") err_percent
    else if (err_percent < 10) then
        write (u, "(1x,'(,F5.1,3x,')')") err_percent
    else
        write (u, "(1x,'(,F4.0,4x,')')") err_percent
    end if
else
    write (u, "(A)") "[integral undefined]"
end if
end subroutine process_show

```

Finalizer. Explicitly iterate over all subobjects that may contain allocated pointers.

TODO wk 2018 (workaround): The finalizer for the `config_data` component is not called. The reason is that this deletes model data local to the process, but these could be referenced by pointers (flavor objects) from some persistent event record. Obviously, such side effects should be avoided, but this requires refactoring the event-handling procedures.

```

(Process: process: TBP)+≡
    procedure :: final => process_final

(Process: procedures)+≡
    subroutine process_final (process)
        class(process_t), intent(inout) :: process
        integer :: i
        ! call process%meta%final ()
        call process%env%final ()
        ! call process%config%final ()
        if (allocated (process%component)) then
            do i = 1, size (process%component)
                call process%component(i)%final ()
            end do
        end if
        if (allocated (process%term)) then
            do i = 1, size (process%term)
                call process%term(i)%final ()
            end do
        end if
        call process%beam_config%final ()
        if (allocated (process%mci_entry)) then
            do i = 1, size (process%mci_entry)
                call process%mci_entry(i)%final ()
            end do
        end if
        if (allocated (process%pcm)) then
            call process%pcm%final ()
        end if
    end subroutine process_final

```

```

        deallocate (process%pcm)
    end if
end subroutine process_final

```

Process setup

Initialize a process. We need a process library `lib` and the process identifier `proc_id` (string). We will fetch the current run ID from the variable list `var_list`.

We collect all important data from the environment and store them in the appropriate places. OS data, model, and variable list are copied into `env` (true snapshot), also the process library (pointer only).

The `meta` subobject is initialized with process ID and attributes taken from the process library.

We initialize the `config` subobject with all data that are relevant for this run, using the settings from `env`. These data determine the MD5 sum for this run, which allows us to identify the setup and possibly skips in a later re-run.

We also allocate and initialize the embedded RNG factory. We take the seed from the `var_list`, and we should return the `var_list` to the caller with a new seed.

Finally, we allocate the process component manager `pcm`, which implements the chosen algorithm for process integration. The first task of the manager is to allocate the component array and to determine the component categories (e.g., Born/Virtual etc.).

TODO wk 2018: The `pcm` dispatcher should be provided by the caller, if we eventually want to eliminate dependencies on concrete `pcm_t` extensions.

```

(Process: process: TBP)+≡
    procedure :: init => process_init

(Process: procedures)+≡
    subroutine process_init &
        (process, proc_id, lib, os_data, model, var_list, beam_structure)
        class(process_t), intent(out) :: process
        type(string_t), intent(in) :: proc_id
        type(process_library_t), intent(in), target :: lib
        type(os_data_t), intent(in) :: os_data
        class(model_t), intent(in), target :: model
        type(var_list_t), intent(inout), target, optional :: var_list
        type(beam_structure_t), intent(in), optional :: beam_structure
        integer :: next_rng_seed
        if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, "process_init")
        associate &
            (meta => process%meta, env => process%env, config => process%config)
            call env%init &
                (model, lib, os_data, var_list, beam_structure)
            call meta%init &
                (proc_id, lib, env%get_var_list_ptr ())
            call config%init &
                (meta, env)
            call dispatch_rng_factory &
                (process%rng_factory, env%get_var_list_ptr (), next_rng_seed)
        end associate
    end subroutine process_init

```

```

    call update_rng_seed_in_var_list (var_list, next_rng_seed)
    call dispatch_pcm &
      (process%pcm, config%process_def%is_nlo ())
    associate (pcm => process%pcm)
      call pcm%init (env, meta)
      call pcm%allocate_components (process%component, meta)
      call pcm%categorize_components (config)
    end associate
  end associate
end subroutine process_init

```

30.4.6 Process component manager

The pcm (read: process-component manager) takes the responsibility of steering the actual algorithm of configuration and integration. Depending on the concrete type, different algorithms can be implemented.

The first version of this supports just two implementations: leading-order (tree-level) integration and event generation, and NLO (QCD/FKS subtraction). We thus can start with a single logical for steering the dispatcher.

TODO wk 2018: Eventually, we may eliminate all references to the extensions of pcm_t from this module and therefore move this outside the module as well.

```

<Process: procedures>+≡
  subroutine dispatch_pcm (pcm, is_nlo)
    class(pcm_t), allocatable, intent(out) :: pcm
    logical, intent(in) :: is_nlo
    if (.not. is_nlo) then
      allocate (pcm_default_t :: pcm)
    else
      allocate (pcm_nlo_t :: pcm)
    end if
  end subroutine dispatch_pcm

```

This step is performed after phase-space and core objects are done: collect all missing information and prepare the process component manager for the appropriate integration algorithm.

```

<Process: process: TBP>+≡
  procedure :: complete_pcm_setup => process_complete_pcm_setup

<Process: procedures>+≡
  subroutine process_complete_pcm_setup (process)
    class(process_t), intent(inout) :: process
    call process%pcm%complete_setup &
      (process%core_entry, process%component, process%env%get_model_ptr ())
  end subroutine process_complete_pcm_setup

```

30.4.7 Core management

Allocate cores (interface objects to matrix-element code).

The `dispatch_core` procedure is taken as an argument, so we do not depend on the implementation, and thus on the specific core types.

The `helicity_selection` object collects data that the matrix-element code needs for configuring the appropriate behavior.

After the cores have been allocated, and assuming the phs initial configuration has been done before, we proceed with computing the `pcm` internal data.

```

(Process: process: TBP)+≡
  procedure :: setup_cores => process_setup_cores

(Process: procedures)+≡
  subroutine process_setup_cores (process, dispatch_core, &
    helicity_selection, use_color_factors, has_beam_pol)
    class(process_t), intent(inout) :: process
    procedure(dispatch_core_proc) :: dispatch_core
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    logical, intent(in), optional :: use_color_factors
    logical, intent(in), optional :: has_beam_pol
    integer :: i
    associate (pcm => process%pcm)
      call pcm%allocate_cores (process%config, process%core_entry)
      do i = 1, size (process%core_entry)
        call dispatch_core (process%core_entry(i)%core, &
          process%core_entry(i)%core_def, &
          process%config%model, &
          helicity_selection, &
          process%config%qcd, &
          use_color_factors, &
          has_beam_pol)
        call process%core_entry(i)%configure &
          (process%env%get_lib_ptr (), process%meta%id)
        if (process%core_entry(i)%core%uses_blha ()) then
          call pcm%setup_blha (process%core_entry(i))
        end if
      end do
    end associate
  end subroutine process_setup_cores

(Process: interfaces)≡
  abstract interface
    subroutine dispatch_core_proc (core, core_def, model, &
      helicity_selection, qcd, use_color_factors, has_beam_pol)
    import
    class(prc_core_t), allocatable, intent(inout) :: core
    class(prc_core_def_t), intent(in) :: core_def
    class(model_data_t), intent(in), target, optional :: model
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    type(qcd_t), intent(in), optional :: qcd
    logical, intent(in), optional :: use_color_factors
    logical, intent(in), optional :: has_beam_pol
  end subroutine dispatch_core_proc
end interface

```

Use the `pcm` to initialize the BLHA interface for each core which requires it.

```

(Process: process: TBP)+≡
  procedure :: prepare_blha_cores => process_prepare_blha_cores

(Process: procedures)+≡
  subroutine process_prepare_blha_cores (process)
    class(process_t), intent(inout), target :: process
    integer :: i
    associate (pcm => process%pcm)
      do i = 1, size (process%core_entry)
        associate (core_entry => process%core_entry(i))
          if (core_entry%core%uses_blha ()) then
            pcm%uses_blha = .true.
            call pcm%prepare_blha_core (core_entry, process%config%model)
          end if
        end associate
      end do
    end associate
  end subroutine process_prepare_blha_cores

```

Create the BLHA interface data, using PCM for specific data, and write the BLHA contract file(s).

We take various configuration data and copy them to the `blha_master` record, which then creates and writes the contracts.

For assigning the QCD/EW coupling powers, we inspect the first process component only. The other parameters are taken as-is from the process environment variables.

```

(Process: process: TBP)+≡
  procedure :: create_blha_interface => process_create_blha_interface

(Process: procedures)+≡
  subroutine process_create_blha_interface (process)
    class(process_t), intent(inout) :: process
    integer :: alpha_power, alphas_power
    integer :: openloops_phs_tolerance, openloops_stability_log
    logical :: use_cms
    type(string_t) :: ew_scheme, correction_type
    type(string_t) :: openloops_extra_cmd
    type(blha_master_t) :: blha_master
    integer, dimension(:,:), allocatable :: flv_born, flv_real
    if (process%pcm%uses_blha) then
      call collect_configuration_parameters (process%get_var_list_ptr ())
      call process%component(1)%config%get_coupling_powers &
        (alpha_power, alphas_power)
      associate (pcm => process%pcm)
        call pcm%set_blha_methods (blha_master, process%get_var_list_ptr ())
        call blha_master%set_ew_scheme (ew_scheme)
        call blha_master%allocate_config_files ()
        call blha_master%set_correction_type (correction_type)
        call blha_master%setup_additional_features ( &
          openloops_phs_tolerance, &
          use_cms, &
          openloops_stability_log, &
          extra_cmd = openloops_extra_cmd, &
          beam_structure = process%env%get_beam_structure ())
      end associate
    end if
  end subroutine process_create_blha_interface

```

```

        call pcm%get_blha_flv_states (process%core_entry, flv_born, flv_real)
        call blha_master%set_photon_characteristics (flv_born, process%config%n_in)
        call blha_master%generate (process%meta%id, &
            process%config%model, process%config%n_in, &
            alpha_power, alphas_power, &
            flv_born, flv_real)
        call blha_master%write_olp (process%meta%id)
    end associate
end if
contains
subroutine collect_configuration_parameters (var_list)
    type(var_list_t), intent(in) :: var_list
    openloops_phs_tolerance = &
        var_list%get_ival (var_str ("openloops_phs_tolerance"))
    openloops_stability_log = &
        var_list%get_ival (var_str ("openloops_stability_log"))
    use_cms = &
        var_list%get_lval (var_str ("?openloops_use_cms"))
    ew_scheme = &
        var_list%get_sval (var_str ("$blha_ew_scheme"))
    correction_type = &
        var_list%get_sval (var_str ("$nlo_correction_type"))
    openloops_extra_cmd = &
        var_list%get_sval (var_str ("$openloops_extra_cmd"))
end subroutine collect_configuration_parameters
end subroutine process_create_blha_interface

```

Initialize the process components, one by one. We require templates for the `mci` (integrator) and `phs_config` (phase-space) configuration data.

The `active` flag is set if the component has an associated matrix element, so we can compute it. The case of no core is a unit-test case.

The specifics depend on the algorithm and are delegated to the `pcm` process-component manager.

The optional `phs_config` overrides a pre-generated config array (for unit test).

```

<Process: process: TBP>+≡
    procedure :: init_components => process_init_components

<Process: procedures>+≡
    subroutine process_init_components (process, phs_config)
        class(process_t), intent(inout), target :: process
        class(phs_config_t), allocatable, intent(in), optional :: phs_config
        integer :: i, i_core
        class(prc_core_t), pointer :: core
        logical :: active
        associate (pcm => process%pcm)
            do i = 1, pcm%n_components
                i_core = pcm%get_i_core(i)
                if (i_core > 0) then
                    core => process%get_core_ptr (i_core)
                    active = core%has_matrix_element ()
                else
                    active = .true.
                end if
            end do
        end associate
    end subroutine

```

```

end if
select type (pcm => process%pcm)
type is (pcm_nlo_t)
    if (pcm%use_real_partition .and. .not. pcm%use_real_singular) then
        if (pcm%component_type(i) == COMP_REAL_SING) then
            active = .false.
        end if
    end if
end select
if (present (phs_config)) then
    call pcm%init_component (process%component(i), &
        i, &
        active, &
        phs_config, &
        process%env, process%meta, process%config)
else
    call pcm%init_component (process%component(i), &
        i, &
        active, &
        process%phs_entry(pcm%i_phs_config(i))%phs_config, &
        process%env, process%meta, process%config)
end if
end do
end associate
end subroutine process_init_components

```

If process components have turned out to be inactive, this has to be recorded in the meta block. Delegate to the pcm.

```

<Process: process: TBP>+≡
    procedure :: record_inactive_components => process_record_inactive_components

<Process: procedures>+≡
    subroutine process_record_inactive_components (process)
        class(process_t), intent(inout) :: process
        associate (pcm => process%pcm)
            call pcm%record_inactive_components (process%component, process%meta)
        end associate
    end subroutine process_record_inactive_components

```

Determine the process terms for each process component.

```

<Process: process: TBP>+≡
    procedure :: setup_terms => process_setup_terms

<Process: procedures>+≡
    subroutine process_setup_terms (process, with_beams)
        class(process_t), intent(inout), target :: process
        logical, intent(in), optional :: with_beams
        class(model_data_t), pointer :: model
        integer :: i, j, k, i_term
        integer, dimension(:), allocatable :: n_entry
        integer :: n_components, n_tot
        integer :: i_sub
        type(string_t) :: subtraction_method
        class(prc_core_t), pointer :: core => null ()
    end subroutine process_setup_terms

```

```

logical :: setup_subtraction_component, singular_real
logical :: requires_spin_correlations
integer :: nlo_type_to_fetch, n_emitters
i_sub = 0
model => process%config%model
n_components = process%meta%n_components
allocate (n_entry (n_components), source = 0)
do i = 1, n_components
  associate (component => process%component(i))
    if (component%active) then
      n_entry(i) = 1
      if (component%get_nlo_type () == NLO_REAL) then
        select type (pcm => process%pcm)
          type is (pcm_nlo_t)
            if (component%component_type /= COMP_REAL_FIN) &
              n_entry(i) = n_entry(i) + pcm%region_data%get_n_phs ()
          end select
        end select
      end if
    end if
  end associate
end do
n_tot = sum (n_entry)
allocate (process%term (n_tot))
k = 0
if (process%is_nlo_calculation ()) then
  i_sub = process%component(1)%config%get_associated_subtraction ()
  subtraction_method = process%component(i_sub)%config%get_me_method ()
  if (debug_on) call msg_debug2 &
    (D_PROCESS_INTEGRATION, "process_setup_terms: ", subtraction_method)
end if

do i = 1, n_components
  associate (component => process%component(i))
    if (.not. component%active) cycle
    allocate (component%i_term (n_entry(i)))
    do j = 1, n_entry(i)
      singular_real = component%get_nlo_type () == NLO_REAL &
        .and. component%component_type /= COMP_REAL_FIN
      setup_subtraction_component = singular_real .and. j == n_entry(i)
      i_term = k + j
      component%i_term(j) = i_term
      if (singular_real) then
        process%term(i_term)%i_sub = k + n_entry(i)
      else
        process%term(i_term)%i_sub = 0
      end if
      if (setup_subtraction_component) then
        select type (pcm => process%pcm)
          class is (pcm_nlo_t)
            process%term(i_term)%i_core = pcm%i_core(pcm%i_sub)
          end select
        else
          process%term(i_term)%i_core = process%pcm%get_i_core(i)
        end if
      end if
    end do
  end associate
end do

```

```

if (process%term(i_term)%i_core == 0) then
  call msg_bug ("Process '" // char (process%get_id ()) &
    // "': core not found!")
end if
core => process%get_core_term (i_term)
if (i_sub > 0) then
  select type (pcm => process%pcm)
  type is (pcm_nlo_t)
    requires_spin_correlations = &
      pcm%region_data%requires_spin_correlations ()
    n_emitters = pcm%region_data%get_n_emitters_sc ()
  class default
    requires_spin_correlations = .false.
    n_emitters = 0
  end select
  if (requires_spin_correlations) then
    call process%term(i_term)%init ( &
      i_term, i, j, core, model, &
      nlo_type = component%config%get_nlo_type (), &
      use_beam_pol = with_beams, &
      subtraction_method = subtraction_method, &
      has_pdfs = process%pcm%has_pdfs, &
      n_emitters = n_emitters)
  else
    call process%term(i_term)%init ( &
      i_term, i, j, core, model, &
      nlo_type = component%config%get_nlo_type (), &
      use_beam_pol = with_beams, &
      subtraction_method = subtraction_method, &
      has_pdfs = process%pcm%has_pdfs)
  end if
else
  call process%term(i_term)%init ( &
    i_term, i, j, core, model, &
    nlo_type = component%config%get_nlo_type (), &
    use_beam_pol = with_beams, &
    subtraction_method = subtraction_method, &
    has_pdfs = process%pcm%has_pdfs)
end if
end do
end associate
k = k + n_entry(i)
end do
process%config%n_terms = n_tot
end subroutine process_setup_terms

```

Initialize the beam setup. This is the trivial version where the incoming state of the matrix element coincides with the initial state of the process. For a scattering process, we need the c.m. energy, all other variables are set to their default values (no polarization, lab frame and c.m. frame coincide, etc.)

We assume that all components consistently describe a scattering process, i.e., two incoming particles.

Note: The current layout of the `beam_data_t` record requires that the fla-

vor for each beam is unique. For processes with multiple flavors in the initial state, one has to set up beams explicitly. This restriction could be removed by extending the code in the `beams` module.

```

(Process: process: TBP)+≡
  procedure :: setup_beams_sqrts => process_setup_beams_sqrts

(Process: procedures)+≡
  subroutine process_setup_beams_sqrts (process, sqrts, beam_structure, i_core)
    class(process_t), intent(inout) :: process
    real(default), intent(in) :: sqrts
    type(beam_structure_t), intent(in), optional :: beam_structure
    integer, intent(in), optional :: i_core
    type(pdg_array_t), dimension(:,,:), allocatable :: pdg_in
    integer, dimension(2) :: pdg_scattering
    type(flavor_t), dimension(2) :: flv_in
    integer :: i, i0, ic
    allocate (pdg_in (2, process%meta%n_components))
    i0 = 0
    do i = 1, process%meta%n_components
      if (process%component(i)%active) then
        if (present (i_core)) then
          ic = i_core
        else
          ic = process%pcm%get_i_core (i)
        end if
        associate (core => process%core_entry(ic)%core)
          pdg_in(:,i) = core%data%get_pdg_in ()
        end associate
        if (i0 == 0) i0 = i
      end if
    end do
    do i = 1, process%meta%n_components
      if (.not. process%component(i)%active) then
        pdg_in(:,i) = pdg_in(:,i0)
      end if
    end do
    if (all (pdg_array_get_length (pdg_in) == 1) .and. &
        all (pdg_in(1,:) == pdg_in(1,i0)) .and. &
        all (pdg_in(2,:) == pdg_in(2,i0))) then
      pdg_scattering = pdg_array_get (pdg_in(:,i0), 1)
      call flv_in%init (pdg_scattering, process%config%model)
      call process%beam_config%init_scattering (flv_in, sqrts, beam_structure)
    else
      call msg_fatal ("Setting up process '" // char (process%meta%id) // "':", &
        [var_str ("-----"), &
        var_str ("Inconsistent initial state. This happens if either "), &
        var_str ("several processes with non-matching initial states "), &
        var_str ("have been added, or for a single process with an "), &
        var_str ("initial state flavor sum. In that case, please set beams "), &
        var_str ("explicitly [singling out a flavor / structure function.]")])
    end if
  end subroutine process_setup_beams_sqrts

```

This is the version that applies to decay processes. The energy is the particle

mass, hence no extra argument.

```

(Process: process: TBP)+≡
  procedure :: setup_beams_decay => process_setup_beams_decay

(Process: procedures)+≡
  subroutine process_setup_beams_decay (process, rest_frame, beam_structure, i_core)
    class(process_t), intent(inout), target :: process
    logical, intent(in), optional :: rest_frame
    type(beam_structure_t), intent(in), optional :: beam_structure
    integer, intent(in), optional :: i_core
    type(pdg_array_t), dimension(:,,:), allocatable :: pdg_in
    integer, dimension(1) :: pdg_decay
    type(flavor_t), dimension(1) :: flv_in
    integer :: i, i0, ic
    allocate (pdg_in (1, process%meta%n_components))
    i0 = 0
    do i = 1, process%meta%n_components
      if (process%component(i)%active) then
        if (present (i_core)) then
          ic = i_core
        else
          ic = process%pcm%get_i_core (i)
        end if
        associate (core => process%core_entry(ic)%core)
          pdg_in(:,i) = core%data%get_pdg_in ()
        end associate
        if (i0 == 0) i0 = i
      end if
    end do
    do i = 1, process%meta%n_components
      if (.not. process%component(i)%active) then
        pdg_in(:,i) = pdg_in(:,i0)
      end if
    end do
    if (all (pdg_array_get_length (pdg_in) == 1) &
        .and. all (pdg_in(1,:) == pdg_in(1,i0))) then
      pdg_decay = pdg_array_get (pdg_in(:,i0), 1)
      call flv_in%init (pdg_decay, process%config%model)
      call process%beam_config%init_decay (flv_in, rest_frame, beam_structure)
    else
      call msg_fatal ("Setting up decay '" &
                     // char (process%meta%id) // "' : decaying particle not unique")
    end if
  end subroutine process_setup_beams_decay

```

We have to make sure that the masses of the various flavors in a given position in the particle string coincide.

```

(Process: process: TBP)+≡
  procedure :: check_masses => process_check_masses

(Process: procedures)+≡
  subroutine process_check_masses (process)
    class(process_t), intent(in) :: process
    type(flavor_t), dimension(:), allocatable :: flv

```



```

real(default), dimension(:), allocatable :: mass
integer :: i, j
integer :: i_component
class(prc_core_t), pointer :: core
do i = 1, process%get_n_terms ()
  i_component = process%term(i)%i_component
  if (.not. process%component(i_component)%active) cycle
  core => process%get_core_term (i)
  associate (data => core%data)
    allocate (flv (data%n_flv), mass (data%n_flv))
    do j = 1, data%n_in + data%n_out
      call flv%init (data%flv_state(j,:), process%config%model)
      mass = flv%get_mass ()
      if (any (.not. nearly_equal(mass, mass(1)))) then
        call msg_fatal ("Process '" // char (process%meta%id) // "': " &
          // "mass values in flavor combination do not coincide. ")
      end if
    end do
    deallocate (flv, mass)
  end associate
end do
end subroutine process_check_masses

```

Set up index mapping for `region_data` for singular regions equivalent w.r.t. their amplitudes. Has to be called after `region_data` AND the `core` are fully set up. For processes with structure function, subprocesses which lead to the same amplitude for the hard interaction can differ if structure functions are applied. In this case we remap flavor structures to themselves if the equivalent hard interaction flavor structure has no identical initial state.

(Process: process: TBP)+≡

```

procedure :: optimize_nlo_singular_regions => process_optimize_nlo_singular_regions

```

(Process: procedures)+≡

```

subroutine process_optimize_nlo_singular_regions (process)
  class(process_t), intent(inout) :: process
  class(prc_core_t), pointer :: core, core_sub
  integer, dimension(:), allocatable :: eqv_flv_index_born
  integer, dimension(:), allocatable :: eqv_flv_index_real
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  integer :: i_flv, i_flv2, n_in, i
  integer :: i_component, i_core, i_core_sub
  logical :: fetched_born, fetched_real
  logical :: optimize
  fetched_born = .false.; fetched_real = .false.
  select type (pcm => process%pcm)
  type is (pcm_nlo_t)
    optimize = pcm%settings%reuse_amplitudes_fks
    if (optimize) then
      do i_component = 1, pcm%n_components
        i_core = pcm%get_i_core(i_component)
        core => process%get_core_ptr (i_core)
        if (.not. core%data_known) cycle
        associate (data => core%data)
          if (pcm%nlo_type_core(i_core) == NLO_REAL .and. &

```

```

        .not. pcm%component_type(i_component) == COMP_SUB) then
    if (allocated (core%data%eqv_flv_index)) then
        eqv_flv_index_real = core%get_equivalent_flv_index ()
        fetched_real = .true.
    end if
    i_core_sub = pcm%get_i_core (pcm%i_sub)
    core_sub => process%get_core_ptr (i_core_sub)
    if (allocated (core_sub%data%eqv_flv_index)) then
        eqv_flv_index_born = core_sub%get_equivalent_flv_index ()
        fetched_born = .true.
    end if
    if (fetched_born .and. fetched_real) exit
end if
end associate
end do
if (.not. fetched_born .or. .not. fetched_real) then
    call msg_warning('Failed to fetch flavor equivalence indices. &
        &Disabling singular region optimization')
    optimize = .false.
    eqv_flv_index_born = [(i, i = 1, pcm%region_data%n_flv_born)]
    eqv_flv_index_real = [(i, i = 1, pcm%region_data%n_flv_real)]
end if
if (optimize .and. pcm%has_pdfs) then
    flv_born = pcm%region_data%get_flv_states_born ()
    flv_real = pcm%region_data%get_flv_states_real ()
    n_in = pcm%region_data%n_in
    do i_flv = 1, size (eqv_flv_index_born)
        do i_flv2 = 1, i_flv
            if (any (flv_born(1:n_in, eqv_flv_index_born(i_flv)) /= &
                flv_born(1:n_in, i_flv))) then
                eqv_flv_index_born(i_flv) = i_flv
                exit
            end if
        end do
    end do
    do i_flv = 1, size (eqv_flv_index_real)
        do i_flv2 = 1, i_flv
            if (any (flv_real(1:n_in, eqv_flv_index_real(i_flv)) /= &
                flv_real(1:n_in, i_flv))) then
                eqv_flv_index_real(i_flv) = i_flv
                exit
            end if
        end do
    end do
end if
else
    eqv_flv_index_born = [(i, i = 1, pcm%region_data%n_flv_born)]
    eqv_flv_index_real = [(i, i = 1, pcm%region_data%n_flv_real)]
end if
pcm%region_data%eqv_flv_index_born = eqv_flv_index_born
pcm%region_data%eqv_flv_index_real = eqv_flv_index_real
call pcm%region_data%find_eqv_regions (optimize)
end select
end subroutine process_optimize_nlo_singular_regions

```

For some structure functions we need to get the list of initial state flavors. This is a two-dimensional array. The first index is the beam index, the second index is the component index. Each array element is itself a PDG array object, which consists of the list of incoming PDG values for this beam and component.

```

(Process: process: TBP)+≡
  procedure :: get_pdg_in => process_get_pdg_in

(Process: procedures)+≡
  subroutine process_get_pdg_in (process, pdg_in)
    class(process_t), intent(in), target :: process
    type(pdg_array_t), dimension(:,,:), allocatable, intent(out) :: pdg_in
    integer :: i, i_core
    allocate (pdg_in (process%config%n_in, process%meta%n_components))
    do i = 1, process%meta%n_components
      if (process%component(i)%active) then
        i_core = process%pcm%get_i_core (i)
        associate (core => process%core_entry(i_core)%core)
          pdg_in(:,i) = core%data%get_pdg_in ()
        end associate
      end if
    end do
  end subroutine process_get_pdg_in

```

The phase-space configuration object, in case we need it separately.

```

(Process: process: TBP)+≡
  procedure :: get_phs_config => process_get_phs_config

(Process: procedures)+≡
  function process_get_phs_config (process, i_component) result (phs_config)
    class(phs_config_t), pointer :: phs_config
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_component
    if (allocated (process%component)) then
      phs_config => process%component(i_component)%phs_config
    else
      phs_config => null ()
    end if
  end function process_get_phs_config

```

The resonance history set can be extracted from the phase-space configuration. However, this is only possible if the default phase-space method (wood) has been chosen. If `include_trivial` is set, we include the resonance history with no resonances in the set.

```

(Process: process: TBP)+≡
  procedure :: extract_resonance_history_set &
    => process_extract_resonance_history_set

(Process: procedures)+≡
  subroutine process_extract_resonance_history_set &
    (process, res_set, include_trivial, i_component)
    class(process_t), intent(in), target :: process
    type(resonance_history_set_t), intent(out) :: res_set

```

```

logical, intent(in), optional :: include_trivial
integer, intent(in), optional :: i_component
integer :: i
i = 1; if (present (i_component)) i = i_component
select type (phs_config => process%get_phs_config (i))
class is (phs_wood_config_t)
    call phs_config%extract_resonance_history_set (res_set, include_trivial)
class default
    call msg_error ("process '" // char (process%get_id ()) &
        // "' : extract resonance histories: phase-space method must be &
        &'wood'. No resonances can be determined.")
end select
end subroutine process_extract_resonance_history_set

```

Initialize from a complete beam setup. If the beam setup does not apply directly to the process, choose a fallback option as a straight scattering or decay process.

```

(Process: process: TBP)+≡
    procedure :: setup_beams_beam_structure => process_setup_beams_beam_structure

(Process: procedures)+≡
    subroutine process_setup_beams_beam_structure &
        (process, beam_structure, sqrts, decay_rest_frame)
    class(process_t), intent(inout) :: process
    type(beam_structure_t), intent(in) :: beam_structure
    real(default), intent(in) :: sqrts
    logical, intent(in), optional :: decay_rest_frame
    integer :: n_in
    logical :: applies
    n_in = process%get_n_in ()
    call beam_structure%check_against_n_in (process%get_n_in (), applies)
    if (applies) then
        call process%beam_config%init_beam_structure &
            (beam_structure, sqrts, process%get_model_ptr (), decay_rest_frame)
    else if (n_in == 2) then
        call process%setup_beams_sqrts (sqrts, beam_structure)
    else
        call process%setup_beams_decay (decay_rest_frame, beam_structure)
    end if
end subroutine process_setup_beams_beam_structure

```

Notify the user about beam setup.

```

(Process: process: TBP)+≡
    procedure :: beams_startup_message => process_beams_startup_message

(Process: procedures)+≡
    subroutine process_beams_startup_message (process, unit, beam_structure)
    class(process_t), intent(in) :: process
    integer, intent(in), optional :: unit
    type(beam_structure_t), intent(in), optional :: beam_structure
    call process%beam_config%startup_message (unit, beam_structure)
end subroutine process_beams_startup_message

```

Initialize phase-space configuration by reading out the environment variables. We return the rebuild flags and store parameters in the blocks `phs_par` and `mapping_defs`.

The phase-space configuration object(s) are allocated by `pcm`.

```

(Process: process: TBP)+≡
  procedure :: init_phs_config => process_init_phs_config

(Process: procedures)+≡
  subroutine process_init_phs_config (process)
    class(process_t), intent(inout) :: process

    type(var_list_t), pointer :: var_list
    type(phs_parameters_t) :: phs_par
    type(mapping_defaults_t) :: mapping_defs

    var_list => process%env%get_var_list_ptr ()

    phs_par%m_threshold_s = &
      var_list%get_rval (var_str ("phs_threshold_s"))
    phs_par%m_threshold_t = &
      var_list%get_rval (var_str ("phs_threshold_t"))
    phs_par%off_shell = &
      var_list%get_ival (var_str ("phs_off_shell"))
    phs_par%keep_nonresonant = &
      var_list%get_lval (var_str ("?phs_keep_nonresonant"))
    phs_par%t_channel = &
      var_list%get_ival (var_str ("phs_t_channel"))

    mapping_defs%energy_scale = &
      var_list%get_rval (var_str ("phs_e_scale"))
    mapping_defs%invariant_mass_scale = &
      var_list%get_rval (var_str ("phs_m_scale"))
    mapping_defs%momentum_transfer_scale = &
      var_list%get_rval (var_str ("phs_q_scale"))
    mapping_defs%step_mapping = &
      var_list%get_lval (var_str ("?phs_step_mapping"))
    mapping_defs%step_mapping_exp = &
      var_list%get_lval (var_str ("?phs_step_mapping_exp"))
    mapping_defs%enable_s_mapping = &
      var_list%get_lval (var_str ("?phs_s_mapping"))

    associate (pcm => process%pcm)
      call pcm%init_phs_config (process%phs_entry, &
        process%meta, process%env, phs_par, mapping_defs)
    end associate

  end subroutine process_init_phs_config

```

We complete the kinematics configuration after the beam setup, but before we configure the chain of structure functions. The reason is that we need the total energy `sqrts` for the kinematics, but the structure-function setup requires the number of channels, which depends on the kinematics configuration. For instance, the kinematics module may return the need for parameterizing an

s-channel resonance.

```

(Process: process: TBP)+≡
  procedure :: configure_phs => process_configure_phs
(Process: procedures)+≡
  subroutine process_configure_phs (process, rebuild, ignore_mismatch, &
    combined_integration, subdir)
    class(process_t), intent(inout) :: process
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    logical, intent(in), optional :: combined_integration
    type(string_t), intent(in), optional :: subdir
    real(default) :: sqrts
    integer :: i, i_born, nlo_type
    class(phs_config_t), pointer :: phs_config_born
    sqrts = process%get_sqrts ()
    do i = 1, process%meta%n_components
      associate (component => process%component(i))
        if (component%active) then
          select type (pcm => process%pcm)
            type is (pcm_default_t)
              call component%configure_phs (sqrts, process%beam_config, &
                rebuild, ignore_mismatch, subdir)
            class is (pcm_nlo_t)
              nlo_type = component%config%get_nlo_type ()
              select case (nlo_type)
                case (BORN, NLO_VIRTUAL, NLO_SUBTRACTION)
                  call component%configure_phs (sqrts, process%beam_config, &
                    rebuild, ignore_mismatch, subdir)
                  call check_and_extend_phs (component)
                case (NLO_REAL, NLO_MISMATCH, NLO_DGLAP)
                  i_born = component%config%get_associated_born ()
                  if (component%component_type /= COMP_REAL_FIN) &
                    call check_and_extend_phs (component)
                  call process%component(i_born)%get_phs_config &
                    (phs_config_born)
                  select type (config => component%phs_config)
                    type is (phs_fks_config_t)
                      select type (phs_config_born)
                        type is (phs_wood_config_t)
                          config%md5sum_born_config = &
                            phs_config_born%md5sum_phs_config
                          call config%set_born_config (phs_config_born)
                          call config%set_mode (component%config%get_nlo_type ())
                        end select
                      end select
                  call component%configure_phs (sqrts, &
                    process%beam_config, rebuild, ignore_mismatch, subdir)
                end select
              class default
                call msg_bug ("process_configure_phs: unsupported PCM type")
              end select
            end if
          end associate
        end do

```

```

contains
  subroutine check_and_extend_phs (component)
    type(process_component_t), intent(inout) :: component
    if (combined_integration) then
      select type (phs_config => component%phs_config)
        class is (phs_wood_config_t)
          phs_config%is_combined_integration = .true.
          call phs_config%increase_n_par ()
        end select
      end if
    end subroutine check_and_extend_phs
  end subroutine process_configure_phs

<Process: process: TBP>+≡
  procedure :: print_phs_startup_message => process_print_phs_startup_message

<Process: procedures>+≡
  subroutine process_print_phs_startup_message (process)
    class(process_t), intent(in) :: process
    integer :: i_component
    do i_component = 1, process%meta%n_components
      associate (component => process%component(i_component))
        if (component%active) then
          call component%phs_config%startup_message ()
        end if
      end associate
    end do
  end subroutine process_print_phs_startup_message

```

Insert the structure-function configuration data. First allocate the storage, then insert data one by one. The third procedure declares a mapping (of the MC input parameters) for a specific channel and structure-function combination.

We take the number of channels from the corresponding entry in the `config.data` section.

Otherwise, these are simple wrapper routines. The extra level in the call tree may allow for simple addressing of multiple concurrent beam configurations, not implemented currently.

If we do not want structure functions, we simply do not call those procedures.

```

<Process: process: TBP>+≡
  procedure :: init_sf_chain => process_init_sf_chain
  generic :: set_sf_channel => set_sf_channel_single
  procedure :: set_sf_channel_single => process_set_sf_channel
  generic :: set_sf_channel => set_sf_channel_array
  procedure :: set_sf_channel_array => process_set_sf_channel_array

<Process: procedures>+≡
  subroutine process_init_sf_chain (process, sf_config, sf_trace_file)
    class(process_t), intent(inout) :: process
    type(sf_config_t), dimension(:), intent(in) :: sf_config
    type(string_t), intent(in), optional :: sf_trace_file
    type(string_t) :: file
    if (present (sf_trace_file)) then
      if (sf_trace_file /= "") then

```

```

        file = sf_trace_file
    else
        file = process%get_id () // "_sftrace.dat"
    end if
    call process%beam_config%init_sf_chain (sf_config, file)
else
    call process%beam_config%init_sf_chain (sf_config)
end if
end subroutine process_init_sf_chain

subroutine process_set_sf_channel (process, c, sf_channel)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: c
    type(sf_channel_t), intent(in) :: sf_channel
    call process%beam_config%set_sf_channel (c, sf_channel)
end subroutine process_set_sf_channel

subroutine process_set_sf_channel_array (process, sf_channel)
    class(process_t), intent(inout) :: process
    type(sf_channel_t), dimension(:), intent(in) :: sf_channel
    integer :: c
    call process%beam_config%allocate_sf_channels (size (sf_channel))
    do c = 1, size (sf_channel)
        call process%beam_config%set_sf_channel (c, sf_channel(c))
    end do
end subroutine process_set_sf_channel_array

```

Notify about the structure-function setup.

```

(Process: process: TBP)+≡
    procedure :: sf_startup_message => process_sf_startup_message

(Process: procedures)+≡
    subroutine process_sf_startup_message (process, sf_string, unit)
        class(process_t), intent(in) :: process
        type(string_t), intent(in) :: sf_string
        integer, intent(in), optional :: unit
        call process%beam_config%sf_startup_message (sf_string, unit)
    end subroutine process_sf_startup_message

```

As soon as both the kinematics configuration and the structure-function setup are complete, we match parameterizations (channels) for both. The matching entries are (re)set in the component phase-space configuration, while the structure-function configuration is left intact.

```

(Process: process: TBP)+≡
    procedure :: collect_channels => process_collect_channels

(Process: procedures)+≡
    subroutine process_collect_channels (process, coll)
        class(process_t), intent(inout) :: process
        type(phs_channel_collection_t), intent(inout) :: coll
        integer :: i
        do i = 1, process%meta%n_components
            associate (component => process%component(i))
                if (component%active) &

```



```

        call component%collect_channels (coll)
    end associate
end do
end subroutine process_collect_channels

```

Independently, we should be able to check if any component does not contain phase-space parameters. Such a process can only be integrated if there are structure functions.

```

(Process: process: TBP)+≡
    procedure :: contains_trivial_component => process_contains_trivial_component

(Process: procedures)+≡
    function process_contains_trivial_component (process) result (flag)
        class(process_t), intent(in) :: process
        logical :: flag
        integer :: i
        flag = .true.
        do i = 1, process%meta%n_components
            associate (component => process%component(i))
                if (component%active) then
                    if (component%get_n_phs_par () == 0) return
                end if
            end associate
        end do
        flag = .false.
    end function process_contains_trivial_component

(Process: process: TBP)+≡
    procedure :: get_master_component => process_get_master_component

(Process: procedures)+≡
    function process_get_master_component (process, i_mci) result (i_component)
        integer :: i_component
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
        integer :: i
        i_component = 0
        do i = 1, size (process%component)
            if (process%component(i)%i_mci == i_mci) then
                i_component = i
                return
            end if
        end do
    end function process_get_master_component

```

Determine the MC parameter set structure and the MCI configuration for each process component. We need data from the structure-function and phase-space setup, so those should be complete before this is called. We also make a random-number generator instance for each MCI group.

```

(Process: process: TBP)+≡
    procedure :: setup_mci => process_setup_mci

```

```

(Process: procedures)+≡
subroutine process_setup_mci (process, dispatch_mci)
  class(process_t), intent(inout) :: process
  procedure(dispatch_mci_proc) :: dispatch_mci
  class(mci_t), allocatable :: mci_template
  integer :: i, i_mci
  if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, "process_setup_mci")
  associate (pcm => process%pcm)
    call pcm%call_dispatch_mci (dispatch_mci, &
      process%get_var_list_ptr (), process%meta%id, mci_template)
    call pcm%setup_mci (process%mci_entry)
    process%config%n_mci = pcm%n_mci
    process%component(:)%i_mci = pcm%i_mci(:)
    do i = 1, pcm%n_components
      i_mci = process%pcm%i_mci(i)
      if (i_mci > 0) then
        associate (component => process%component(i), &
          mci_entry => process%mci_entry(i_mci))
          call mci_entry%configure (mci_template, &
            process%meta%type, &
            i_mci, i, component, process%beam_config%n_sfpar, &
            process%rng_factory)
          call mci_entry%set_parameters (process%get_var_list_ptr ())
        end associate
      end if
    end do
  end associate
end subroutine process_setup_mci

```

Set cuts. This is a parse node, namely the right-hand side of the `cut` assignment. When creating an instance, we compile this into an evaluation tree. The parse node may be null.

```

(Process: process: TBP)+≡
  procedure :: set_cuts => process_set_cuts

(Process: procedures)+≡
subroutine process_set_cuts (process, ef_cuts)
  class(process_t), intent(inout) :: process
  class(expr_factory_t), intent(in) :: ef_cuts
  allocate (process%config%ef_cuts, source = ef_cuts)
end subroutine process_set_cuts

```

Analogously for the other expressions.

```

(Process: process: TBP)+≡
  procedure :: set_scale => process_set_scale
  procedure :: set_fac_scale => process_set_fac_scale
  procedure :: set_ren_scale => process_set_ren_scale
  procedure :: set_weight => process_set_weight

(Process: procedures)+≡
subroutine process_set_scale (process, ef_scale)
  class(process_t), intent(inout) :: process
  class(expr_factory_t), intent(in) :: ef_scale
  allocate (process%config%ef_scale, source = ef_scale)

```

```

end subroutine process_set_scale

subroutine process_set_fac_scale (process, ef_fac_scale)
  class(process_t), intent(inout) :: process
  class(expr_factory_t), intent(in) :: ef_fac_scale
  allocate (process%config%ef_fac_scale, source = ef_fac_scale)
end subroutine process_set_fac_scale

subroutine process_set_ren_scale (process, ef_ren_scale)
  class(process_t), intent(inout) :: process
  class(expr_factory_t), intent(in) :: ef_ren_scale
  allocate (process%config%ef_ren_scale, source = ef_ren_scale)
end subroutine process_set_ren_scale

subroutine process_set_weight (process, ef_weight)
  class(process_t), intent(inout) :: process
  class(expr_factory_t), intent(in) :: ef_weight
  allocate (process%config%ef_weight, source = ef_weight)
end subroutine process_set_weight

```

MD5 sum

The MD5 sum of the process object should reflect the state completely, including integration results. It is used for checking the integrity of event files. This global checksum includes checksums for the various parts. In particular, the MCI object receives a checksum that includes the configuration of all configuration parts relevant for an individual integration. This checksum is used for checking the integrity of integration grids.

We do not need MD5 sums for the process terms, since these are generated from the component definitions.

```

(Process: process: TBP)+≡
  procedure :: compute_md5sum => process_compute_md5sum

(Process: procedures)+≡
  subroutine process_compute_md5sum (process)
    class(process_t), intent(inout) :: process
    integer :: i
    call process%config%compute_md5sum ()
    do i = 1, process%config%n_components
      associate (component => process%component(i))
        if (component%active) then
          call component%compute_md5sum ()
        end if
      end associate
    end do
    call process%beam_config%compute_md5sum ()
    do i = 1, process%config%n_mci
      call process%mci_entry(i)%compute_md5sum &
        (process%config, process%component, process%beam_config)
    end do
  end subroutine process_compute_md5sum

```

```

(Process: process: TBP)+≡
    procedure :: sampler_test => process_sampler_test

(Process: procedures)+≡
    subroutine process_sampler_test (process, sampler, n_calls, i_mci)
        class(process_t), intent(inout) :: process
        class(mci_sampler_t), intent(inout) :: sampler
        integer, intent(in) :: n_calls, i_mci
        call process%mci_entry(i_mci)%sampler_test (sampler, n_calls)
    end subroutine process_sampler_test

```

The finalizer should be called after all integration passes have been completed. It will, for instance, write a summary of the integration results.

`integrate_dummy` does a “dummy” integration in the sense that nothing is done but just empty integration results appended.

```

(Process: process: TBP)+≡
    procedure :: final_integration => process_final_integration
    procedure :: integrate_dummy => process_integrate_dummy

(Process: procedures)+≡
    subroutine process_final_integration (process, i_mci)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        call process%mci_entry(i_mci)%final_integration ()
    end subroutine process_final_integration

    subroutine process_integrate_dummy (process)
        class(process_t), intent(inout) :: process
        type(integration_results_t) :: results
        integer :: u_log
        u_log = logfile_unit ()
        call results%init (process%meta%type)
        call results%display_init (screen = .true., unit = u_log)
        call results%new_pass ()
        call results%record (1, 0, 0._default, 0._default, 0._default)
        call results%display_final ()
    end subroutine process_integrate_dummy

```

```

(Process: process: TBP)+≡
    procedure :: integrate => process_integrate

(Process: procedures)+≡
    subroutine process_integrate (process, i_mci, mci_work, &
        mci_sampler, n_it, n_calls, adapt_grids, adapt_weights, final, &
        pacify, nlo_type)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(mci_work_t), intent(inout) :: mci_work
        class(mci_sampler_t), intent(inout) :: mci_sampler
        integer, intent(in) :: n_it, n_calls
        logical, intent(in), optional :: adapt_grids, adapt_weights
        logical, intent(in), optional :: final
        logical, intent(in), optional :: pacify
        integer, intent(in), optional :: nlo_type

```

```

        associate (mci_entry => process%mci_entry(i_mci))
            call mci_entry%integrate (mci_work%mci, mci_sampler, n_it, n_calls, &
                adapt_grids, adapt_weights, final, pacify, &
                nlo_type = nlo_type)
            call mci_entry%results%display_pass (pacify)
        end associate
    end subroutine process_integrate

```

```

<Process: process: TBP>+≡
    procedure :: generate_weighted_event => process_generate_weighted_event

```

```

<Process: procedures>+≡
    subroutine process_generate_weighted_event (process, i_mci, mci_work, &
        mci_sampler, keep_failed_events)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(mci_work_t), intent(inout) :: mci_work
        class(mci_sampler_t), intent(inout) :: mci_sampler
        logical, intent(in) :: keep_failed_events
        associate (mci_entry => process%mci_entry(i_mci))
            call mci_entry%generate_weighted_event (mci_work%mci, &
                mci_sampler, keep_failed_events)
        end associate
    end subroutine process_generate_weighted_event

```

```

<Process: process: TBP>+≡
    procedure :: generate_unweighted_event => process_generate_unweighted_event

```

```

<Process: procedures>+≡
    subroutine process_generate_unweighted_event (process, i_mci, &
        mci_work, mci_sampler)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        type(mci_work_t), intent(inout) :: mci_work
        class(mci_sampler_t), intent(inout) :: mci_sampler
        associate (mci_entry => process%mci_entry(i_mci))
            call mci_entry%generate_unweighted_event &
                (mci_work%mci, mci_sampler)
        end associate
    end subroutine process_generate_unweighted_event

```

Display the final results for the sum of all components. This is useful, obviously, only if there is more than one component and not if a combined integration of all components together has been performed.

```

<Process: process: TBP>+≡
    procedure :: display_summed_results => process_display_summed_results

```

```

<Process: procedures>+≡
    subroutine process_display_summed_results (process, pacify)
        class(process_t), intent(inout) :: process
        logical, intent(in) :: pacify
        type(integration_results_t) :: results
        integer :: u_log
        u_log = logfile_unit ()

```

```

call results%init (process%meta%type)
call results%display_init (screen = .true., unit = u_log)
call results%new_pass ()
call results%record (1, 0, &
    process%get_integral (), &
    process%get_error (), &
    process%get_efficiency (), suppress = pacify)
select type (pcm => process%pcm)
class is (pcm_nlo_t)
    !!! Check that Born integral is there
    if (.not. pcm%settings%combined_integration .and. &
        process%component_can_be_integrated (1)) then
        call results%record_correction (process%get_correction (), &
            process%get_correction_error ())
    end if
end select
call results%display_final ()
end subroutine process_display_summed_results

```

Run LaTeX/Metapost to generate a ps/pdf file for the integration history. We (re)write the driver file – just in case it has been missed before – then we compile it.

```

(Process: process: TBP)+≡
    procedure :: display_integration_history => &
        process_display_integration_history
(Process: procedures)+≡
    subroutine process_display_integration_history &
        (process, i_mci, filename, os_data, eff_reset)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(string_t), intent(in) :: filename
    type(os_data_t), intent(in) :: os_data
    logical, intent(in), optional :: eff_reset
    call integration_results_write_driver &
        (process%pci_entry(i_mci)%results, filename, eff_reset)
    call integration_results_compile_driver &
        (process%pci_entry(i_mci)%results, filename, os_data)
    end subroutine process_display_integration_history

```

Write a complete logfile (with hardcoded name based on the process ID). We do not write internal data.

```

(Process: process: TBP)+≡
    procedure :: write_logfile => process_write_logfile
(Process: procedures)+≡
    subroutine process_write_logfile (process, i_mci, filename)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(string_t), intent(in) :: filename
    type(time_t) :: time
    integer :: unit, u
    unit = free_unit ()
    open (unit = unit, file = char (filename), action = "write", &

```

```

        status = "replace")
u = given_output_unit (unit)
write (u, "(A)") repeat ("#", 79)
call process%meta%write (u, .false.)
write (u, "(A)") repeat ("#", 79)
write (u, "(3x,A,ES17.10)") "Integral   = ", &
    process%mci_entry(i_mci)%get_integral ()
write (u, "(3x,A,ES17.10)") "Error      = ", &
    process%mci_entry(i_mci)%get_error ()
write (u, "(3x,A,ES17.10)") "Accuracy   = ", &
    process%mci_entry(i_mci)%get_accuracy ()
write (u, "(3x,A,ES17.10)") "Chi2       = ", &
    process%mci_entry(i_mci)%get_chi2 ()
write (u, "(3x,A,ES17.10)") "Efficiency = ", &
    process%mci_entry(i_mci)%get_efficiency ()
call process%mci_entry(i_mci)%get_time (time, 10000)
if (time%is_known ()) then
    write (u, "(3x,A,1x,A)") "T(10k evt) = ", char (time%to_string_dhms ())
else
    write (u, "(3x,A)") "T(10k evt) = [undefined]"
end if
call process%mci_entry(i_mci)%results%write (u)
write (u, "(A)") repeat ("#", 79)
call process%mci_entry(i_mci)%results%write_chain_weights (u)
write (u, "(A)") repeat ("#", 79)
call process%mci_entry(i_mci)%counter%write (u)
write (u, "(A)") repeat ("#", 79)
call process%mci_entry(i_mci)%mci%write_log_entry (u)
write (u, "(A)") repeat ("#", 79)
call process%beam_config%data%write (u)
write (u, "(A)") repeat ("#", 79)
if (allocated (process%config%ef_cuts)) then
    write (u, "(3x,A)") "Cut expression:"
    call process%config%ef_cuts%write (u)
else
    write (u, "(3x,A)") "No cuts used."
end if
call write_separator (u)
if (allocated (process%config%ef_scale)) then
    write (u, "(3x,A)") "Scale expression:"
    call process%config%ef_scale%write (u)
else
    write (u, "(3x,A)") "No scale expression was given."
end if
call write_separator (u)
if (allocated (process%config%ef_fac_scale)) then
    write (u, "(3x,A)") "Factorization scale expression:"
    call process%config%ef_fac_scale%write (u)
else
    write (u, "(3x,A)") "No factorization scale expression was given."
end if
call write_separator (u)
if (allocated (process%config%ef_ren_scale)) then
    write (u, "(3x,A)") "Renormalization scale expression:"

```

```

        call process%config%ef_ren_scale%write (u)
    else
        write (u, "(3x,A)") "No renormalization scale expression was given."
    end if
    call write_separator (u)
    if (allocated (process%config%ef_weight)) then
        call write_separator (u)
        write (u, "(3x,A)") "Weight expression:"
        call process%config%ef_weight%write (u)
    else
        write (u, "(3x,A)") "No weight expression was given."
    end if
    write (u, "(A)") repeat ("#", 79)
    write (u, "(1x,A)") "Summary of quantum-number states:"
    write (u, "(1x,A)") " + sign: allowed and contributing"
    write (u, "(1x,A)") " no + : switched off at runtime"
    call process%write_state_summary (u)
    write (u, "(A)") repeat ("#", 79)
    call process%env%write (u, show_var_list=.true., &
        show_model=.false., show_lib=.false., show_os_data=.false.)
    write (u, "(A)") repeat ("#", 79)
    close (u)
end subroutine process_write_logfile

```

Display the quantum-number combinations of the process components, and their current status (allowed or switched off).

```

<Process: process: TBP>+≡
    procedure :: write_state_summary => process_write_state_summary

<Process: procedures>+≡
    subroutine process_write_state_summary (process, unit)
        class(process_t), intent(in) :: process
        integer, intent(in), optional :: unit
        integer :: i, i_component, u
        u = given_output_unit (unit)
        do i = 1, size (process%term)
            call write_separator (u)
            i_component = process%term(i)%i_component
            if (i_component /= 0) then
                call process%term(i)%write_state_summary &
                    (process%get_core_term(i), unit)
            end if
        end do
    end subroutine process_write_state_summary

```

Prepare event generation for the specified MCI entry. This implies, in particular, checking the phase-space file.

```

<Process: process: TBP>+≡
    procedure :: prepare_simulation => process_prepare_simulation

<Process: procedures>+≡
    subroutine process_prepare_simulation (process, i_mci)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
    end subroutine process_prepare_simulation

```



```

        call process%mci_entry(i_mci)%prepare_simulation ()
    end subroutine process_prepare_simulation

```

Retrieve process data

Tell whether integral (and error) are known.

```

(Process: process: TBP) +=
    generic :: has_integral => has_integral_tot, has_integral_mci
    procedure :: has_integral_tot => process_has_integral_tot
    procedure :: has_integral_mci => process_has_integral_mci

(Process: procedures) +=
    function process_has_integral_mci (process, i_mci) result (flag)
        logical :: flag
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
        if (allocated (process%mci_entry)) then
            flag = process%mci_entry(i_mci)%has_integral ()
        else
            flag = .false.
        end if
    end function process_has_integral_mci

    function process_has_integral_tot (process) result (flag)
        logical :: flag
        class(process_t), intent(in) :: process
        integer :: i, j, i_component
        if (allocated (process%mci_entry)) then
            flag = .true.
            do i = 1, size (process%mci_entry)
                do j = 1, size (process%mci_entry(i)%i_component)
                    i_component = process%mci_entry(i)%i_component(j)
                    if (process%component_can_be_integrated (i_component)) &
                        flag = flag .and. process%mci_entry(i)%has_integral ()
                end do
            end do
        else
            flag = .false.
        end if
    end function process_has_integral_tot

```

Return the current integral and error obtained by the integrator *i_mci*.

```

(Process: process: TBP) +=
    generic :: get_integral => get_integral_tot, get_integral_mci
    generic :: get_error => get_error_tot, get_error_mci
    generic :: get_efficiency => get_efficiency_tot, get_efficiency_mci
    procedure :: get_integral_tot => process_get_integral_tot
    procedure :: get_integral_mci => process_get_integral_mci
    procedure :: get_error_tot => process_get_error_tot
    procedure :: get_error_mci => process_get_error_mci
    procedure :: get_efficiency_tot => process_get_efficiency_tot
    procedure :: get_efficiency_mci => process_get_efficiency_mci

```

<Process: procedures>+≡

```

function process_get_integral_mci (process, i_mci) result (integral)
    real(default) :: integral
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
    integral = process%mci_entry(i_mci)%get_integral ()
end function process_get_integral_mci

function process_get_error_mci (process, i_mci) result (error)
    real(default) :: error
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
    error = process%mci_entry(i_mci)%get_error ()
end function process_get_error_mci

function process_get_efficiency_mci (process, i_mci) result (efficiency)
    real(default) :: efficiency
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_mci
    efficiency = process%mci_entry(i_mci)%get_efficiency ()
end function process_get_efficiency_mci

function process_get_integral_tot (process) result (integral)
    real(default) :: integral
    class(process_t), intent(in) :: process
    integer :: i, j, i_component
    integral = zero
    if (allocated (process%mci_entry)) then
        do i = 1, size (process%mci_entry)
            do j = 1, size (process%mci_entry(i)%i_component)
                i_component = process%mci_entry(i)%i_component(j)
                if (process%component_can_be_integrated(i_component)) &
                    integral = integral + process%mci_entry(i)%get_integral ()
            end do
        end do
    end if
end function process_get_integral_tot

function process_get_error_tot (process) result (error)
    real(default) :: variance
    class(process_t), intent(in) :: process
    real(default) :: error
    integer :: i, j, i_component
    variance = zero
    if (allocated (process%mci_entry)) then
        do i = 1, size (process%mci_entry)
            do j = 1, size (process%mci_entry(i)%i_component)
                i_component = process%mci_entry(i)%i_component(j)
                if (process%component_can_be_integrated(i_component)) &
                    variance = variance + process%mci_entry(i)%get_error () ** 2
            end do
        end do
    end if
    error = sqrt (variance)
end function process_get_error_tot

```

```

end function process_get_error_tot

function process_get_efficiency_tot (process) result (efficiency)
  real(default) :: efficiency
  class(process_t), intent(in) :: process
  real(default) :: den, eff, int
  integer :: i, j, i_component
  den = zero
  if (allocated (process%mci_entry)) then
    do i = 1, size (process%mci_entry)
      do j = 1, size (process%mci_entry(i)%i_component)
        i_component = process%mci_entry(i)%i_component(j)
        if (process%component_can_be_integrated(i_component)) then
          int = process%get_integral (i)
          if (int > 0) then
            eff = process%mci_entry(i)%get_efficiency ()
            if (eff > 0) then
              den = den + int / eff
            else
              efficiency = 0
              return
            end if
          end if
        end if
      end do
    end do
  end if
  if (den > 0) then
    efficiency = process%get_integral () / den
  else
    efficiency = 0
  end if
end function process_get_efficiency_tot

```

Let us call the ratio of the NLO and the LO result $\iota = I_{NLO}/I_{LO}$. Then usual error propagation gives

$$\sigma_{\iota}^2 = \left(\frac{\partial \iota}{\partial I_{LO}} \right)^2 \sigma_{I_{LO}}^2 + \left(\frac{\partial \iota}{\partial I_{NLO}} \right)^2 \sigma_{I_{NLO}}^2 = \frac{I_{NLO}^2 \sigma_{I_{LO}}^2}{I_{LO}^4} + \frac{\sigma_{I_{NLO}}^2}{I_{LO}^2}.$$

```

(Process: process: TBP)+≡
  procedure :: get_correction => process_get_correction
  procedure :: get_correction_error => process_get_correction_error

(Process: procedures)+≡
  function process_get_correction (process) result (ratio)
    real(default) :: ratio
    class(process_t), intent(in) :: process
    integer :: i_mci, i_component
    real(default) :: int_born, int_nlo
    int_nlo = zero
    int_born = process%mci_entry(1)%get_integral ()
    i_mci = 2
    do i_component = 2, size (process%component)

```

```

        if (process%component_can_be_integrated (i_component)) then
            int_nlo = int_nlo + process%mci_entry(i_mci)%get_integral ()
            i_mci = i_mci + 1
        end if
    end do
    ratio = int_nlo / int_born * 100
end function process_get_correction

function process_get_correction_error (process) result (error)
    real(default) :: error
    class(process_t), intent(in) :: process
    real(default) :: int_born, sum_int_nlo
    real(default) :: err_born, err2
    integer :: i_mci, i_component
    sum_int_nlo = zero; err2 = zero
    int_born = process%mci_entry(1)%get_integral ()
    err_born = process%mci_entry(1)%get_error ()
    i_mci = 2
    do i_component = 2, size (process%component)
        if (process%component_can_be_integrated (i_component)) then
            sum_int_nlo = sum_int_nlo + process%mci_entry(i_mci)%get_integral ()
            err2 = err2 + process%mci_entry(i_mci)%get_error()**2
            i_mci = i_mci + 1
        end if
    end do
    error = sqrt (err2 / int_born**2 + sum_int_nlo**2 * err_born**2 / int_born**4) * 100
end function process_get_correction_error

```

```

<Process: process: TBP>+≡
    procedure :: lab_is_cm => process_lab_is_cm

<Process: procedures>+≡
    pure function process_lab_is_cm (process) result (lab_is_cm)
        logical :: lab_is_cm
        class(process_t), intent(in) :: process
        lab_is_cm = process%beam_config%lab_is_cm
        ! This asks beam_config for the frame
    end function process_lab_is_cm

```

```

<Process: process: TBP>+≡
    procedure :: get_component_ptr => process_get_component_ptr

<Process: procedures>+≡
    function process_get_component_ptr (process, i) result (component)
        type(process_component_t), pointer :: component
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i
        component => process%component(i)
    end function process_get_component_ptr

```

```

<Process: process: TBP>+≡
    procedure :: get_qcd => process_get_qcd

```

```

(Process: procedures)+≡
function process_get_qcd (process) result (qcd)
    type(qcd_t) :: qcd
    class(process_t), intent(in) :: process
    qcd = process%config%get_qcd ()
end function process_get_qcd

(Process: process: TBP)+≡
generic :: get_component_type => get_component_type_single
procedure :: get_component_type_single => process_get_component_type_single

(Process: procedures)+≡
elemental function process_get_component_type_single &
    (process, i_component) result (comp_type)
    integer :: comp_type
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    comp_type = process%component(i_component)%component_type
end function process_get_component_type_single

(Process: process: TBP)+≡
generic :: get_component_type => get_component_type_all
procedure :: get_component_type_all => process_get_component_type_all

(Process: procedures)+≡
function process_get_component_type_all &
    (process) result (comp_type)
    integer, dimension(:), allocatable :: comp_type
    class(process_t), intent(in) :: process
    allocate (comp_type (size (process%component)))
    comp_type = process%component%component_type
end function process_get_component_type_all

(Process: process: TBP)+≡
procedure :: get_component_i_terms => process_get_component_i_terms

(Process: procedures)+≡
function process_get_component_i_terms (process, i_component) result (i_term)
    integer, dimension(:), allocatable :: i_term
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    allocate (i_term (size (process%component(i_component)%i_term)))
    i_term = process%component(i_component)%i_term
end function process_get_component_i_terms

(Process: process: TBP)+≡
procedure :: get_n_allowed_born => process_get_n_allowed_born

(Process: procedures)+≡
function process_get_n_allowed_born (process, i_born) result (n_born)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_born
    integer :: n_born
    n_born = process%term(i_born)%n_allowed

```

```
end function process_get_n_allowed_born
```

Workaround getter. Would be better to remove this.

```

(Process: process: TBP)+≡
  procedure :: get_pcm_ptr => process_get_pcm_ptr

(Process: procedures)+≡
  function process_get_pcm_ptr (process) result (pcm)
    class(pcm_t), pointer :: pcm
    class(process_t), intent(in), target :: process
    pcm => process%pcm
  end function process_get_pcm_ptr

(Process: process: TBP)+≡
  generic :: component_can_be_integrated => component_can_be_integrated_single
  generic :: component_can_be_integrated => component_can_be_integrated_all
  procedure :: component_can_be_integrated_single => process_component_can_be_integrated_single

(Process: procedures)+≡
  function process_component_can_be_integrated_single (process, i_component) &
    result (active)
    logical :: active
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    logical :: combined_integration
    select type (pcm => process%pcm)
    type is (pcm_nlo_t)
      combined_integration = pcm%settings%combined_integration
    class default
      combined_integration = .false.
    end select
    associate (component => process%component(i_component))
      active = component%can_be_integrated ()
      if (combined_integration) &
        active = active .and. component%component_type <= COMP_MASTER
    end associate
  end function process_component_can_be_integrated_single

(Process: process: TBP)+≡
  procedure :: component_can_be_integrated_all => process_component_can_be_integrated_all

(Process: procedures)+≡
  function process_component_can_be_integrated_all (process) result (val)
    logical, dimension(:), allocatable :: val
    class(process_t), intent(in) :: process
    integer :: i
    allocate (val (size (process%component)))
    do i = 1, size (process%component)
      val(i) = process%component_can_be_integrated (i)
    end do
  end function process_component_can_be_integrated_all

(Process: process: TBP)+≡
  procedure :: reset_selected_cores => process_reset_selected_cores

```

```

<Process: procedures>+≡
  pure subroutine process_reset_selected_cores (process)
    class(process_t), intent(inout) :: process
    process%pcm%component_selected = .false.
  end subroutine process_reset_selected_cores

<Process: process: TBP>+≡
  procedure :: select_components => process_select_components

<Process: procedures>+≡
  pure subroutine process_select_components (process, indices)
    class(process_t), intent(inout) :: process
    integer, dimension(:), intent(in) :: indices
    associate (pcm => process%pcm)
      pcm%component_selected(indices) = .true.
    end associate
  end subroutine process_select_components

<Process: process: TBP>+≡
  procedure :: component_is_selected => process_component_is_selected

<Process: procedures>+≡
  pure function process_component_is_selected (process, index) result (val)
    logical :: val
    class(process_t), intent(in) :: process
    integer, intent(in) :: index
    associate (pcm => process%pcm)
      val = pcm%component_selected(index)
    end associate
  end function process_component_is_selected

<Process: process: TBP>+≡
  procedure :: get_coupling_powers => process_get_coupling_powers

<Process: procedures>+≡
  pure subroutine process_get_coupling_powers (process, alpha_power, alphas_power)
    class(process_t), intent(in) :: process
    integer, intent(out) :: alpha_power, alphas_power
    call process%component(1)%config%get_coupling_powers (alpha_power, alphas_power)
  end subroutine process_get_coupling_powers

<Process: process: TBP>+≡
  procedure :: get_real_component => process_get_real_component

<Process: procedures>+≡
  function process_get_real_component (process) result (i_real)
    integer :: i_real
    class(process_t), intent(in) :: process
    integer :: i_component
    type(process_component_def_t), pointer :: config => null ()
    i_real = 0
    do i_component = 1, size (process%component)
      config => process%get_component_def_ptr (i_component)
      if (config%get_nlo_type () == NLO_REAL) then

```

```

        i_real = i_component
        exit
    end if
end do
end function process_get_real_component

```

```

<Process: process: TBP>+≡
    procedure :: extract_active_component_mci => process_extract_active_component_mci

```

```

<Process: procedures>+≡
    function process_extract_active_component_mci (process) result (i_active)
        integer :: i_active
        class(process_t), intent(in) :: process
        integer :: i_mci, j, i_component, n_active
        call count_n_active ()
        if (n_active /= 1) i_active = 0
    contains
        subroutine count_n_active ()
            n_active = 0
            do i_mci = 1, size (process%mci_entry)
                associate (mci_entry => process%mci_entry(i_mci))
                    do j = 1, size (mci_entry%i_component)
                        i_component = mci_entry%i_component(j)
                        associate (component => process%component (i_component))
                            if (component%can_be_integrated ()) then
                                i_active = i_mci
                                n_active = n_active + 1
                            end if
                        end associate
                    end do
                end associate
            end do
        end subroutine count_n_active
    end function process_extract_active_component_mci

```

```

<Process: process: TBP>+≡
    procedure :: uses_real_partition => process_uses_real_partition

```

```

<Process: procedures>+≡
    function process_uses_real_partition (process) result (val)
        logical :: val
        class(process_t), intent(in) :: process
        val = any (process%mci_entry%real_partition_type /= REAL_FULL)
    end function process_uses_real_partition

```

Return the MD5 sums that summarize the process component definitions. These values should be independent of parameters, beam details, expressions, etc. They can be used for checking the integrity of a process when reusing an old event file.

```

<Process: process: TBP>+≡
    procedure :: get_md5sum_prc => process_get_md5sum_prc

```



```

(Process: procedures)+≡
function process_get_md5sum_prc (process, i_component) result (md5sum)
  character(32) :: md5sum
  class(process_t), intent(in) :: process
  integer, intent(in) :: i_component
  if (process%component(i_component)%active) then
    md5sum = process%component(i_component)%config%get_md5sum ()
  else
    md5sum = ""
  end if
end function process_get_md5sum_prc

```

Return the MD5 sums that summarize the state of the MCI integrators. These values should encode all process data, integration and phase space configuration, etc., and the integration results. They can thus be used for checking the integrity of an event-generation setup when reusing an old event file.

```

(Process: process: TBP)+≡
procedure :: get_md5sum_mci => process_get_md5sum_mci

(Process: procedures)+≡
function process_get_md5sum_mci (process, i_mci) result (md5sum)
  character(32) :: md5sum
  class(process_t), intent(in) :: process
  integer, intent(in) :: i_mci
  md5sum = process%pci_entry(i_mci)%get_md5sum ()
end function process_get_md5sum_mci

```

Return the MD5 sum of the process configuration. This should encode the process setup, data, and expressions, but no integration results.

```

(Process: process: TBP)+≡
procedure :: get_md5sum_cfg => process_get_md5sum_cfg

(Process: procedures)+≡
function process_get_md5sum_cfg (process) result (md5sum)
  character(32) :: md5sum
  class(process_t), intent(in) :: process
  md5sum = process%config%md5sum
end function process_get_md5sum_cfg

```

```

(Process: process: TBP)+≡
procedure :: get_n_cores => process_get_n_cores

(Process: procedures)+≡
function process_get_n_cores (process) result (n)
  integer :: n
  class(process_t), intent(in) :: process
  n = process%pcm%n_cores
end function process_get_n_cores

```

```

(Process: process: TBP)+≡
procedure :: get_base_i_term => process_get_base_i_term

```

```

<Process: procedures>+≡
function process_get_base_i_term (process, i_component) result (i_term)
    integer :: i_term
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    i_term = process%component(i_component)%i_term(1)
end function process_get_base_i_term

<Process: process: TBP>+≡
procedure :: get_core_term => process_get_core_term

<Process: procedures>+≡
function process_get_core_term (process, i_term) result (core)
    class(prc_core_t), pointer :: core
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_term
    integer :: i_core
    i_core = process%term(i_term)%i_core
    core => process%core_entry(i_core)%get_core_ptr ()
end function process_get_core_term

<Process: process: TBP>+≡
procedure :: get_core_ptr => process_get_core_ptr

<Process: procedures>+≡
function process_get_core_ptr (process, i_core) result (core)
    class(prc_core_t), pointer :: core
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_core
    if (allocated (process%core_entry)) then
        core => process%core_entry(i_core)%get_core_ptr ()
    else
        core => null ()
    end if
end function process_get_core_ptr

<Process: process: TBP>+≡
procedure :: get_term_ptr => process_get_term_ptr

<Process: procedures>+≡
function process_get_term_ptr (process, i) result (term)
    type(process_term_t), pointer :: term
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i
    term => process%term(i)
end function process_get_term_ptr

<Process: process: TBP>+≡
procedure :: get_i_term => process_get_i_term

<Process: procedures>+≡
function process_get_i_term (process, i_core) result (i_term)
    integer :: i_term
    class(process_t), intent(in) :: process

```

```

integer, intent(in) :: i_core
do i_term = 1, process%get_n_terms ()
    if (process%term(i_term)%i_core == i_core) return
end do
i_term = -1
end function process_get_i_term

<Process: process: TBP>+≡
    procedure :: get_i_core => process_get_i_core

<Process: procedures>+≡
    integer function process_get_i_core (process, i_term) result (i_core)
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_term
        i_core = process%term(i_term)%i_core
    end function process_get_i_core

<Process: process: TBP>+≡
    procedure :: set_i_mci_work => process_set_i_mci_work

<Process: procedures>+≡
    subroutine process_set_i_mci_work (process, i_mci)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_mci
        process%mci_entry(i_mci)%i_mci = i_mci
    end subroutine process_set_i_mci_work

<Process: process: TBP>+≡
    procedure :: get_i_mci_work => process_get_i_mci_work

<Process: procedures>+≡
    pure function process_get_i_mci_work (process, i_mci) result (i_mci_work)
        integer :: i_mci_work
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
        i_mci_work = process%mci_entry(i_mci)%i_mci
    end function process_get_i_mci_work

<Process: process: TBP>+≡
    procedure :: get_i_sub => process_get_i_sub

<Process: procedures>+≡
    elemental function process_get_i_sub (process, i_term) result (i_sub)
        integer :: i_sub
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_term
        i_sub = process%term(i_term)%i_sub
    end function process_get_i_sub

<Process: process: TBP>+≡
    procedure :: get_i_term_virtual => process_get_i_term_virtual

```

```

<Process: procedures>+=
  elemental function process_get_i_term_virtual (process) result (i_term)
    integer :: i_term
    class(process_t), intent(in) :: process
    integer :: i_component
    i_term = 0
    do i_component = 1, size (process%component)
      if (process%component(i_component)%get_nlo_type () == NLO_VIRTUAL) &
        i_term = process%component(i_component)%i_term(1)
    end do
  end function process_get_i_term_virtual

<Process: process: TBP>+=
  generic :: component_is_active => component_is_active_single
  procedure :: component_is_active_single => process_component_is_active_single

<Process: procedures>+=
  elemental function process_component_is_active_single (process, i_comp) result (val)
    logical :: val
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_comp
    val = process%component(i_comp)%is_active ()
  end function process_component_is_active_single

<Process: process: TBP>+=
  generic :: component_is_active => component_is_active_all
  procedure :: component_is_active_all => process_component_is_active_all

<Process: procedures>+=
  pure function process_component_is_active_all (process) result (val)
    logical, dimension(:), allocatable :: val
    class(process_t), intent(in) :: process
    allocate (val (size (process%component)))
    val = process%component%is_active ()
  end function process_component_is_active_all

```

30.4.8 Default iterations

If the user does not specify the passes and iterations for integration, we should be able to give reasonable defaults. These depend on the process, therefore we implement the following procedures as methods of the process object. The algorithm is not very sophisticated yet, it may be improved by looking at the process in more detail.

We investigate only the first process component, assuming that it characterizes the complexity of the process reasonable well.

The number of passes is limited to two: one for adaption, one for integration.

```

<Process: process: TBP>+=
  procedure :: get_n_pass_default => process_get_n_pass_default
  procedure :: adapt_grids_default => process_adapt_grids_default
  procedure :: adapt_weights_default => process_adapt_weights_default

```

<Process: procedures>+≡

```
function process_get_n_pass_default (process) result (n_pass)
  class(process_t), intent(in) :: process
  integer :: n_pass
  integer :: n_eff
  type(process_component_def_t), pointer :: config
  config => process%component(1)%config
  n_eff = config%get_n_tot () - 2
  select case (n_eff)
  case (1)
    n_pass = 1
  case default
    n_pass = 2
  end select
end function process_get_n_pass_default

function process_adapt_grids_default (process, pass) result (flag)
  class(process_t), intent(in) :: process
  integer, intent(in) :: pass
  logical :: flag
  integer :: n_eff
  type(process_component_def_t), pointer :: config
  config => process%component(1)%config
  n_eff = config%get_n_tot () - 2
  select case (n_eff)
  case (1)
    flag = .false.
  case default
    select case (pass)
    case (1); flag = .true.
    case (2); flag = .false.
    case default
      call msg_bug ("adapt grids default: impossible pass index")
    end select
  end select
end function process_adapt_grids_default

function process_adapt_weights_default (process, pass) result (flag)
  class(process_t), intent(in) :: process
  integer, intent(in) :: pass
  logical :: flag
  integer :: n_eff
  type(process_component_def_t), pointer :: config
  config => process%component(1)%config
  n_eff = config%get_n_tot () - 2
  select case (n_eff)
  case (1)
    flag = .false.
  case default
    select case (pass)
    case (1); flag = .true.
    case (2); flag = .false.
    case default
      call msg_bug ("adapt weights default: impossible pass index")
    end select
  end select
end function process_adapt_weights_default
```

```

        end select
    end select
end function process_adapt_weights_default

```

The number of iterations and calls per iteration depends on the number of outgoing particles.

```

(Process: process: TBP)+≡
    procedure :: get_n_it_default => process_get_n_it_default
    procedure :: get_n_calls_default => process_get_n_calls_default

(Process: procedures)+≡
    function process_get_n_it_default (process, pass) result (n_it)
        class(process_t), intent(in) :: process
        integer, intent(in) :: pass
        integer :: n_it
        integer :: n_eff
        type(process_component_def_t), pointer :: config
        config => process%component(1)%config
        n_eff = config%get_n_tot () - 2
        select case (pass)
        case (1)
            select case (n_eff)
            case (1);    n_it = 1
            case (2);    n_it = 3
            case (3);    n_it = 5
            case (4:5);  n_it = 10
            case (6);    n_it = 15
            case (7:);   n_it = 20
            end select
        case (2)
            select case (n_eff)
            case (:3);   n_it = 3
            case (4:);   n_it = 5
            end select
        end select
    end function process_get_n_it_default

    function process_get_n_calls_default (process, pass) result (n_calls)
        class(process_t), intent(in) :: process
        integer, intent(in) :: pass
        integer :: n_calls
        integer :: n_eff
        type(process_component_def_t), pointer :: config
        config => process%component(1)%config
        n_eff = config%get_n_tot () - 2
        select case (pass)
        case (1)
            select case (n_eff)
            case (1);    n_calls = 100
            case (2);    n_calls = 1000
            case (3);    n_calls = 5000
            case (4);    n_calls = 10000
            case (5);    n_calls = 20000
            case (6:);   n_calls = 50000
            end select
        end select
    end function process_get_n_calls_default

```

```

        end select
    case (2)
        select case (n_eff)
            case (:3); n_calls = 10000
            case (4);  n_calls = 20000
            case (5);  n_calls = 50000
            case (6);  n_calls = 100000
            case (7:); n_calls = 200000
        end select
    end select
end function process_get_n_calls_default

```

30.4.9 Constant process data

Manually set the Run ID (unit test only).

```

(Process: process: TBP)+≡
    procedure :: set_run_id => process_set_run_id

(Process: procedures)+≡
    subroutine process_set_run_id (process, run_id)
        class(process_t), intent(inout) :: process
        type(string_t), intent(in) :: run_id
        process%meta%run_id = run_id
    end subroutine process_set_run_id

```

The following methods return basic process data that stay constant after initialization.

The process and IDs.

```

(Process: process: TBP)+≡
    procedure :: get_id => process_get_id
    procedure :: get_num_id => process_get_num_id
    procedure :: get_run_id => process_get_run_id
    procedure :: get_library_name => process_get_library_name

(Process: procedures)+≡
    function process_get_id (process) result (id)
        class(process_t), intent(in) :: process
        type(string_t) :: id
        id = process%meta%id
    end function process_get_id

    function process_get_num_id (process) result (id)
        class(process_t), intent(in) :: process
        integer :: id
        id = process%meta%num_id
    end function process_get_num_id

    function process_get_run_id (process) result (id)
        class(process_t), intent(in) :: process
        type(string_t) :: id
        id = process%meta%run_id
    end function process_get_run_id

```

```

function process_get_library_name (process) result (id)
  class(process_t), intent(in) :: process
  type(string_t) :: id
  id = process%meta%lib_name
end function process_get_library_name

```

The number of incoming particles.

```

(Process: process: TBP)+≡
  procedure :: get_n_in => process_get_n_in
(Process: procedures)+≡
  function process_get_n_in (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
    n = process%config%n_in
  end function process_get_n_in

```

The number of MCI data sets.

```

(Process: process: TBP)+≡
  procedure :: get_n_mci => process_get_n_mci
(Process: procedures)+≡
  function process_get_n_mci (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
    n = process%config%n_mci
  end function process_get_n_mci

```

The number of process components, total.

```

(Process: process: TBP)+≡
  procedure :: get_n_components => process_get_n_components
(Process: procedures)+≡
  function process_get_n_components (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
    n = process%meta%n_components
  end function process_get_n_components

```

The number of process terms, total.

```

(Process: process: TBP)+≡
  procedure :: get_n_terms => process_get_n_terms
(Process: procedures)+≡
  function process_get_n_terms (process) result (n)
    class(process_t), intent(in) :: process
    integer :: n
    n = process%config%n_terms
  end function process_get_n_terms

```

Return the indices of the components that belong to a specific MCI entry.

```

(Process: process: TBP)+≡
  procedure :: get_i_component => process_get_i_component

```



```

(Process: procedures)+≡
subroutine process_get_i_component (process, i_mci, i_component)
  class(process_t), intent(in) :: process
  integer, intent(in) :: i_mci
  integer, dimension(:), intent(out), allocatable :: i_component
  associate (mci_entry => process%mci_entry(i_mci))
    allocate (i_component (size (mci_entry%i_component)))
    i_component = mci_entry%i_component
  end associate
end subroutine process_get_i_component

```

Return the ID of a specific component.

```

(Process: process: TBP)+≡
  procedure :: get_component_id => process_get_component_id

(Process: procedures)+≡
function process_get_component_id (process, i_component) result (id)
  class(process_t), intent(in) :: process
  integer, intent(in) :: i_component
  type(string_t) :: id
  id = process%meta%component_id(i_component)
end function process_get_component_id

```

Return a pointer to the definition of a specific component.

```

(Process: process: TBP)+≡
  procedure :: get_component_def_ptr => process_get_component_def_ptr

(Process: procedures)+≡
function process_get_component_def_ptr (process, i_component) result (ptr)
  type(process_component_def_t), pointer :: ptr
  class(process_t), intent(in) :: process
  integer, intent(in) :: i_component
  ptr => process%config%process_def%get_component_def_ptr (i_component)
end function process_get_component_def_ptr

```

These procedures extract and restore (by transferring the allocation) the process core. This is useful for changing process parameters from outside this module.

```

(Process: process: TBP)+≡
  procedure :: extract_core => process_extract_core
  procedure :: restore_core => process_restore_core

(Process: procedures)+≡
subroutine process_extract_core (process, i_term, core)
  class(process_t), intent(inout) :: process
  integer, intent(in) :: i_term
  class(prc_core_t), intent(inout), allocatable :: core
  integer :: i_core
  i_core = process%term(i_term)%i_core
  call move_alloc (from = process%core_entry(i_core)%core, to = core)
end subroutine process_extract_core

subroutine process_restore_core (process, i_term, core)
  class(process_t), intent(inout) :: process

```

```

integer, intent(in) :: i_term
class(prc_core_t), intent(inout), allocatable :: core
integer :: i_core
i_core = process%term(i_term)%i_core
call move_alloc (from = core, to = process%core_entry(i_core)%core)
end subroutine process_restore_core

```

The block of process constants.

```

(Process: process: TBP)+≡
  procedure :: get_constants => process_get_constants

(Process: procedures)+≡
  function process_get_constants (process, i_core) result (data)
    type(process_constants_t) :: data
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_core
    data = process%core_entry(i_core)%core%data
  end function process_get_constants

```

```

(Process: process: TBP)+≡
  procedure :: get_config => process_get_config

(Process: procedures)+≡
  function process_get_config (process) result (config)
    type(process_config_data_t) :: config
    class(process_t), intent(in) :: process
    config = process%config
  end function process_get_config

```

Construct an MD5 sum for the constant data, including the NLO type.

For the NLO type `NLO_MISMATCH`, we pretend that this was `NLO_SUBTRACTION` instead.

TODO wk 2018: should not depend explicitly on NLO data.

```

(Process: process: TBP)+≡
  procedure :: get_md5sum_constants => process_get_md5sum_constants

(Process: procedures)+≡
  function process_get_md5sum_constants (process, i_component, &
    type_string, nlo_type) result (this_md5sum)
    character(32) :: this_md5sum
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    type(string_t), intent(in) :: type_string
    integer, intent(in) :: nlo_type
    type(process_constants_t) :: data
    integer :: unit
    call process%env%fill_process_constants (process%meta%id, i_component, data)
    unit = data%fill_unit_for_md5sum (.false.)
    write (unit, '(A)') char(type_string)
    select case (nlo_type)
    case (NLO_MISMATCH)
      write (unit, '(IO)') NLO_SUBTRACTION
    case default

```

```

        write (unit, '(I0)') nlo_type
    end select
    rewind (unit)
    this_md5sum = md5sum (unit)
    close (unit)
end function process_get_md5sum_constants

```

Return the set of outgoing flavors that are associated with a particular term. We deduce this from the effective interaction.

```

(Process: process: TBP)+≡
    procedure :: get_term_flv_out => process_get_term_flv_out

(Process: procedures)+≡
    subroutine process_get_term_flv_out (process, i_term, flv)
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i_term
        type(flavor_t), dimension(:,:), allocatable, intent(out) :: flv
        type(interaction_t), pointer :: int
        int => process%term(i_term)%int_eff
        if (.not. associated (int)) int => process%term(i_term)%int
        call interaction_get_flv_out (int, flv)
    end subroutine process_get_term_flv_out

```

Return true if there is any unstable particle in any of the process terms. We decide this based on the provided model instance, not the one that is stored in the process object.

```

(Process: process: TBP)+≡
    procedure :: contains_unstable => process_contains_unstable

(Process: procedures)+≡
    function process_contains_unstable (process, model) result (flag)
        class(process_t), intent(in) :: process
        class(model_data_t), intent(in), target :: model
        logical :: flag
        integer :: i_term
        type(flavor_t), dimension(:,:), allocatable :: flv
        flag = .false.
        do i_term = 1, process%get_n_terms ()
            call process%get_term_flv_out (i_term, flv)
            call flv%set_model (model)
            flag = .not. all (flv%is_stable ())
            deallocate (flv)
            if (flag) return
        end do
    end function process_contains_unstable

```

The nominal process energy.

```

(Process: process: TBP)+≡
    procedure :: get_sqrts => process_get_sqrts

(Process: procedures)+≡
    function process_get_sqrts (process) result (sqrts)
        class(process_t), intent(in) :: process

```

```

    real(default) :: sqrts
    sqrts = process%beam_config%data%get_sqrts ()
end function process_get_sqrts

```

The lab-frame beam energy/energies..

```

(Process: process: TBP)+≡
    procedure :: get_energy => process_get_energy

(Process: procedures)+≡
    function process_get_energy (process) result (e)
        class(process_t), intent(in) :: process
        real(default), dimension(:), allocatable :: e
        e = process%beam_config%data%get_energy ()
    end function process_get_energy

```

The beam polarization in case of simple degrees.

```

(Process: process: TBP)+≡
    procedure :: get_polarization => process_get_polarization

(Process: procedures)+≡
    function process_get_polarization (process) result (pol)
        class(process_t), intent(in) :: process
        real(default), dimension(2) :: pol
        pol = process%beam_config%data%get_polarization ()
    end function process_get_polarization

```

```

(Process: process: TBP)+≡
    procedure :: get_meta => process_get_meta

(Process: procedures)+≡
    function process_get_meta (process) result (meta)
        type(process_metadata_t) :: meta
        class(process_t), intent(in) :: process
        meta = process%meta
    end function process_get_meta

```

```

(Process: process: TBP)+≡
    procedure :: has_matrix_element => process_has_matrix_element

(Process: procedures)+≡
    function process_has_matrix_element (process, i, is_term_index) result (active)
        logical :: active
        class(process_t), intent(in) :: process
        integer, intent(in), optional :: i
        logical, intent(in), optional :: is_term_index
        integer :: i_component
        logical :: is_term
        is_term = .false.
        if (present (i)) then
            if (present (is_term_index)) is_term = is_term_index
            if (is_term) then
                i_component = process%term(i)%i_component
            else
                i_component = i
            end if
        end if
    end function process_has_matrix_element

```

```

        end if
        active = process%component(i_component)%active
    else
        active = any (process%component%active)
    end if
end function process_has_matrix_element

```

Pointer to the beam data object.

```

<Process: process: TBP>+≡
    procedure :: get_beam_data_ptr => process_get_beam_data_ptr

<Process: procedures>+≡
    function process_get_beam_data_ptr (process) result (beam_data)
        class(process_t), intent(in), target :: process
        type(beam_data_t), pointer :: beam_data
        beam_data => process%beam_config%data
    end function process_get_beam_data_ptr

```

```

<Process: process: TBP>+≡
    procedure :: get_beam_config => process_get_beam_config

<Process: procedures>+≡
    function process_get_beam_config (process) result (beam_config)
        type(process_beam_config_t) :: beam_config
        class(process_t), intent(in) :: process
        beam_config = process%beam_config
    end function process_get_beam_config

```

```

<Process: process: TBP>+≡
    procedure :: get_beam_config_ptr => process_get_beam_config_ptr

<Process: procedures>+≡
    function process_get_beam_config_ptr (process) result (beam_config)
        type(process_beam_config_t), pointer :: beam_config
        class(process_t), intent(in), target :: process
        beam_config => process%beam_config
    end function process_get_beam_config_ptr

```

Get the PDF set currently in use, if any.

```

<Process: process: TBP>+≡
    procedure :: get_pdf_set => process_get_pdf_set

<Process: procedures>+≡
    function process_get_pdf_set (process) result (pdf_set)
        class(process_t), intent(in) :: process
        integer :: pdf_set
        pdf_set = process%beam_config%get_pdf_set ()
    end function process_get_pdf_set

<Process: process: TBP>+≡
    procedure :: pcm_contains_pdfs => process_pcm_contains_pdfs

```

```

(Process: procedures)+≡
function process_pcm_contains_pdfs (process) result (has_pdfs)
  logical :: has_pdfs
  class(process_t), intent(in) :: process
  has_pdfs = process%pcm%has_pdfs
end function process_pcm_contains_pdfs

```

Get the beam spectrum file currently in use, if any.

```

(Process: process: TBP)+≡
procedure :: get_beam_file => process_get_beam_file

(Process: procedures)+≡
function process_get_beam_file (process) result (file)
  class(process_t), intent(in) :: process
  type(string_t) :: file
  file = process%beam_config%get_beam_file ()
end function process_get_beam_file

```

Pointer to the process variable list.

```

(Process: process: TBP)+≡
procedure :: get_var_list_ptr => process_get_var_list_ptr

(Process: procedures)+≡
function process_get_var_list_ptr (process) result (ptr)
  class(process_t), intent(in), target :: process
  type(var_list_t), pointer :: ptr
  ptr => process%env%get_var_list_ptr ()
end function process_get_var_list_ptr

```

Pointer to the common model.

```

(Process: process: TBP)+≡
procedure :: get_model_ptr => process_get_model_ptr

(Process: procedures)+≡
function process_get_model_ptr (process) result (ptr)
  class(process_t), intent(in) :: process
  class(model_data_t), pointer :: ptr
  ptr => process%config%model
end function process_get_model_ptr

```

Use the embedded RNG factory to spawn a new random-number generator instance. (This modifies the state of the factory.)

```

(Process: process: TBP)+≡
procedure :: make_rng => process_make_rng

(Process: procedures)+≡
subroutine process_make_rng (process, rng)
  class(process_t), intent(inout) :: process
  class(rng_t), intent(out), allocatable :: rng
  if (allocated (process%rng_factory)) then
    call process%rng_factory%make (rng)
  else
    call msg_bug ("Process: make rng: factory not allocated")
  end if
end subroutine process_make_rng

```

```

end if
end subroutine process_make_rng

```

30.4.10 Compute an amplitude

Each process variant should allow for computing an amplitude value directly, without generating a process instance.

The process component is selected by the index *i*. The term within the process component is selected by *j*. The momentum combination is transferred as the array *p*. The function sets the specific quantum state via the indices of a flavor *f*, helicity *h*, and color *c* combination. Each index refers to the list of flavor, helicity, and color states, respectively, as stored in the process data.

Optionally, we may set factorization and renormalization scale. If unset, the partonic c.m. energy is inserted.

The function checks arguments for validity. For invalid arguments (quantum states), we return zero.

```

(Process: process: TBP)+≡
  procedure :: compute_amplitude => process_compute_amplitude

(Process: procedures)+≡
  function process_compute_amplitude &
    (process, i_core, i, j, p, f, h, c, fac_scale, ren_scale, alpha_qcd_forced) &
    result (amp)
    class(process_t), intent(in), target :: process
    integer, intent(in) :: i_core
    integer, intent(in) :: i, j
    type(vector4_t), dimension(:), intent(in) :: p
    integer, intent(in) :: f, h, c
    real(default), intent(in), optional :: fac_scale, ren_scale
    real(default), intent(in), allocatable, optional :: alpha_qcd_forced
    real(default) :: fscale, rscale
    real(default), allocatable :: aqcd_forced
    complex(default) :: amp
    class(prc_core_t), pointer :: core
    amp = 0
    if (0 < i .and. i <= process%meta%n_components) then
      if (process%component(i)%active) then
        associate (core => process%core_entry(i_core)%core)
          associate (data => core%data)
            if (size (p) == data%n_in + data%n_out &
              .and. 0 < f .and. f <= data%n_flv &
              .and. 0 < h .and. h <= data%n_hel &
              .and. 0 < c .and. c <= data%n_col) then
              if (present (fac_scale)) then
                fscale = fac_scale
              else
                fscale = sum (p(data%n_in+1:)) ** 1
              end if
              if (present (ren_scale)) then
                rscale = ren_scale
              else
                rscale = fscale
              end if
            end if
          end associate
        end associate
      end if
    end if
  end function

```

```

        end if
        if (present (alpha_qcd_forced)) then
            if (allocated (alpha_qcd_forced)) &
                allocate (aqcd_forced, source = alpha_qcd_forced)
            end if
            amp = core%compute_amplitude (j, p, f, h, c, &
                fscale, rscale, aqcd_forced)
        end if
    end associate
end associate
else
    amp = 0
end if
end if
end function process_compute_amplitude

```

Sanity check for the process library. We abort the program if it has changed after process initialization.

```

(Process: process: TBP)+≡
    procedure :: check_library_sanity => process_check_library_sanity

(Process: procedures)+≡
    subroutine process_check_library_sanity (process)
        class(process_t), intent(in) :: process
        call process%env%check_lib_sanity (process%meta)
    end subroutine process_check_library_sanity

```

Reset the association to a process library.

```

(Process: process: TBP)+≡
    procedure :: reset_library_ptr => process_reset_library_ptr

(Process: procedures)+≡
    subroutine process_reset_library_ptr (process)
        class(process_t), intent(inout) :: process
        call process%env%reset_lib_ptr ()
    end subroutine process_reset_library_ptr

```

```

(Process: process: TBP)+≡
    procedure :: set_component_type => process_set_component_type

(Process: procedures)+≡
    subroutine process_set_component_type (process, i_component, i_type)
        class(process_t), intent(inout) :: process
        integer, intent(in) :: i_component, i_type
        process%component(i_component)%component_type = i_type
    end subroutine process_set_component_type

```

```

(Process: process: TBP)+≡
    procedure :: set_counter_mci_entry => process_set_counter_mci_entry

```



```

<Process: procedures>+≡
  subroutine process_set_counter_mci_entry (process, i_mci, counter)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: i_mci
    type(process_counter_t), intent(in) :: counter
    process%mci_entry(i_mci)%counter = counter
  end subroutine process_set_counter_mci_entry

```

This is for suppression of numerical noise in the integration results stored in the `process_mci_entry` type. As the error and efficiency enter the MD5 sum, we recompute it.

```

<Process: process: TBP>+≡
  procedure :: pacify => process_pacify

<Process: procedures>+≡
  subroutine process_pacify (process, efficiency_reset, error_reset)
    class(process_t), intent(inout) :: process
    logical, intent(in), optional :: efficiency_reset, error_reset
    logical :: eff_reset, err_reset
    integer :: i
    eff_reset = .false.
    err_reset = .false.
    if (present (efficiency_reset)) eff_reset = efficiency_reset
    if (present (error_reset)) err_reset = error_reset
    if (allocated (process%mci_entry)) then
      do i = 1, size (process%mci_entry)
        call process%mci_entry(i)%results%pacify (efficiency_reset)
        if (allocated (process%mci_entry(i)%mci)) then
          associate (mci => process%mci_entry(i)%mci)
            if (process%mci_entry(i)%mci%error_known &
                .and. err_reset) &
              mci%error = 0
            if (process%mci_entry(i)%mci%efficiency_known &
                .and. eff_reset) &
              mci%efficiency = 1
            call mci%pacify (efficiency_reset, error_reset)
            call mci%compute_md5sum ()
          end associate
        end if
      end do
    end if
  end subroutine process_pacify

```

The following methods are used only in the unit tests; the access process internals directly that would otherwise be hidden.

```

<Process: process: TBP>+≡
  procedure :: test_allocate_sf_channels
  procedure :: test_set_component_sf_channel
  procedure :: test_get_mci_ptr

<Process: procedures>+≡
  subroutine test_allocate_sf_channels (process, n)
    class(process_t), intent(inout) :: process
    integer, intent(in) :: n

```

```

        call process%beam_config%allocate_sf_channels (n)
    end subroutine test_allocate_sf_channels

    subroutine test_set_component_sf_channel (process, c)
        class(process_t), intent(inout) :: process
        integer, dimension(:), intent(in) :: c
        call process%component(1)%phs_config%set_sf_channel (c)
    end subroutine test_set_component_sf_channel

    subroutine test_get_mci_ptr (process, mci)
        class(process_t), intent(in), target :: process
        class(mci_t), intent(out), pointer :: mci
        mci => process%mci_entry(1)%mci
    end subroutine test_get_mci_ptr

```

```

<Process: process: TBP>+≡
    procedure :: init_mci_work => process_init_mci_work

<Process: procedures>+≡
    subroutine process_init_mci_work (process, mci_work, i)
        class(process_t), intent(in), target :: process
        type(mci_work_t), intent(out) :: mci_work
        integer, intent(in) :: i
        call mci_work%init (process%mci_entry(i))
    end subroutine process_init_mci_work

```

Prepare the process core with type `test_me`, or otherwise the externally provided `type_string` version. The toy dispatchers as a procedure argument come handy, knowing that we need to support only the `test_me` and `template` matrix-element types.

```

<Process: process: TBP>+≡
    procedure :: setup_test_cores => process_setup_test_cores

<Process: procedures>+≡
    subroutine process_setup_test_cores (process, type_string)
        class(process_t), intent(inout) :: process
        class(prc_core_t), allocatable :: core
        type(string_t), intent(in), optional :: type_string
        if (present (type_string)) then
            select case (char (type_string))
            case ("template")
                call process%setup_cores (dispatch_template_core)
            case ("test_me")
                call process%setup_cores (dispatch_test_me_core)
            case default
                call msg_bug ("process setup test cores: unsupported type string")
            end select
        else
            call process%setup_cores (dispatch_test_me_core)
        end if
    end subroutine process_setup_test_cores

    subroutine dispatch_test_me_core (core, core_def, model, &
        helicity_selection, qcd, use_color_factors, has_beam_pol)

```

```

use prc_test_core, only: test_t
class(prc_core_t), allocatable, intent(inout) :: core
class(prc_core_def_t), intent(in) :: core_def
class(model_data_t), intent(in), target, optional :: model
type(helicity_selection_t), intent(in), optional :: helicity_selection
type(qcd_t), intent(in), optional :: qcd
logical, intent(in), optional :: use_color_factors
logical, intent(in), optional :: has_beam_pol
allocate (test_t :: core)
end subroutine dispatch_test_me_core

subroutine dispatch_template_core (core, core_def, model, &
    helicity_selection, qcd, use_color_factors, has_beam_pol)
use prc_template_me, only: prc_template_me_t
class(prc_core_t), allocatable, intent(inout) :: core
class(prc_core_def_t), intent(in) :: core_def
class(model_data_t), intent(in), target, optional :: model
type(helicity_selection_t), intent(in), optional :: helicity_selection
type(qcd_t), intent(in), optional :: qcd
logical, intent(in), optional :: use_color_factors
logical, intent(in), optional :: has_beam_pol
allocate (prc_template_me_t :: core)
select type (core)
type is (prc_template_me_t)
    call core%set_parameters (model)
end select
end subroutine dispatch_template_core

```

```

(Process: process: TBP)+≡
procedure :: get_connected_states => process_get_connected_states

(Process: procedures)+≡
function process_get_connected_states (process, i_component, &
    connected_terms) result (connected)
type(connected_state_t), dimension(:), allocatable :: connected
class(process_t), intent(in) :: process
integer, intent(in) :: i_component
type(connected_state_t), dimension(:), intent(in) :: connected_terms
integer :: i, i_conn
integer :: n_conn
n_conn = 0
do i = 1, process%get_n_terms ()
    if (process%term(i)%i_component == i_component) then
        n_conn = n_conn + 1
    end if
end do
allocate (connected (n_conn))
i_conn = 1
do i = 1, process%get_n_terms ()
    if (process%term(i)%i_component == i_component) then
        connected (i_conn) = connected_terms(i)
        i_conn = i_conn + 1
    end if
end do
end do

```

```
end function process_get_connected_states
```

30.4.11 NLO specifics

These subroutines (and the NLO specific properties they work on) could potentially be moved to `pcm_nlo_t` and used more generically in `process_t` with an appropriate interface in `pcm_t`

TODO wk 2018: This is used only by event initialization, which deals with an incomplete process object.

```
(Process: process: TBP)+≡
  procedure :: init_nlo_settings => process_init_nlo_settings

(Process: procedures)+≡
  subroutine process_init_nlo_settings (process, var_list)
    class(process_t), intent(inout) :: process
    type(var_list_t), intent(in), target :: var_list
    select type (pcm => process%pcm)
    type is (pcm_nlo_t)
      call pcm%init_nlo_settings (var_list)
      if (debug_active (D_SUBTRACTION) .or. debug_active (D_VIRTUAL)) &
        call pcm%settings%write ()
    class default
      call msg_fatal ("Attempt to set nlo_settings with a non-NLO pcm!")
    end select
  end subroutine process_init_nlo_settings

(Process: process: TBP)+≡
  generic :: get_nlo_type_component => get_nlo_type_component_single
  procedure :: get_nlo_type_component_single => process_get_nlo_type_component_single

(Process: procedures)+≡
  elemental function process_get_nlo_type_component_single (process, i_component) result (val)
    integer :: val
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    val = process%component(i_component)%get_nlo_type ()
  end function process_get_nlo_type_component_single

(Process: process: TBP)+≡
  generic :: get_nlo_type_component => get_nlo_type_component_all
  procedure :: get_nlo_type_component_all => process_get_nlo_type_component_all

(Process: procedures)+≡
  pure function process_get_nlo_type_component_all (process) result (val)
    integer, dimension(:), allocatable :: val
    class(process_t), intent(in) :: process
    allocate (val (size (process%component)))
    val = process%component%get_nlo_type ()
  end function process_get_nlo_type_component_all

(Process: process: TBP)+≡
  procedure :: is_nlo_calculation => process_is_nlo_calculation
```

```

(Process: procedures)+≡
function process_is_nlo_calculation (process) result (nlo)
    logical :: nlo
    class(process_t), intent(in) :: process
    select type (pcm => process%pcm)
    type is (pcm_nlo_t)
        nlo = .true.
    class default
        nlo = .false.
    end select
end function process_is_nlo_calculation

(Process: process: TBP)+≡
procedure :: get_negative_sf => process_get_negative_sf

(Process: procedures)+≡
function process_get_negative_sf (process) result (neg_sf)
    logical :: neg_sf
    class(process_t), intent(in) :: process
    neg_sf = process%config%process_def%get_negative_sf ()
end function process_get_negative_sf

(Process: process: TBP)+≡
procedure :: is_combined_nlo_integration &
    => process_is_combined_nlo_integration

(Process: procedures)+≡
function process_is_combined_nlo_integration (process) result (combined)
    logical :: combined
    class(process_t), intent(in) :: process
    select type (pcm => process%pcm)
    type is (pcm_nlo_t)
        combined = pcm%settings%combined_integration
    class default
        combined = .false.
    end select
end function process_is_combined_nlo_integration

(Process: process: TBP)+≡
procedure :: component_is_real_finite => process_component_is_real_finite

(Process: procedures)+≡
pure function process_component_is_real_finite (process, i_component) &
    result (val)
    logical :: val
    class(process_t), intent(in) :: process
    integer, intent(in) :: i_component
    val = process%component(i_component)%component_type == COMP_REAL_FIN
end function process_component_is_real_finite

```

Return nlo data of a process component

```

(Process: process: TBP)+≡
procedure :: get_component_nlo_type => process_get_component_nlo_type

```

```

(Process: procedures)+≡
    elemental function process_get_component_nlo_type (process, i_component) &
        result (nlo_type)
        integer :: nlo_type
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        nlo_type = process%component(i_component)%config%get_nlo_type ()
    end function process_get_component_nlo_type

```

Return a pointer to the core that belongs to a component.

```

(Process: process: TBP)+≡
    procedure :: get_component_core_ptr => process_get_component_core_ptr

(Process: procedures)+≡
    function process_get_component_core_ptr (process, i_component) result (core)
        class(process_t), intent(in), target :: process
        integer, intent(in) :: i_component
        class(prc_core_t), pointer :: core
        integer :: i_core
        i_core = process%pcm%get_i_core(i_component)
        core => process%core_entry(i_core)%core
    end function process_get_component_core_ptr

```

```

(Process: process: TBP)+≡
    procedure :: get_component_associated_born &
        => process_get_component_associated_born

```

```

(Process: procedures)+≡
    function process_get_component_associated_born (process, i_component) &
        result (i_born)
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        integer :: i_born
        i_born = process%component(i_component)%config%get_associated_born ()
    end function process_get_component_associated_born

```

```

(Process: process: TBP)+≡
    procedure :: get_first_real_component => process_get_first_real_component

```

```

(Process: procedures)+≡
    function process_get_first_real_component (process) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        i_real = process%component(1)%config%get_associated_real ()
    end function process_get_first_real_component

```

```

(Process: process: TBP)+≡
    procedure :: get_first_real_term => process_get_first_real_term

```

```

(Process: procedures)+≡
    function process_get_first_real_term (process) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        integer :: i_component, i_term

```

```

    i_component = process%component(1)%config%get_associated_real ()
    i_real = 0
    do i_term = 1, size (process%term)
        if (process%term(i_term)%i_component == i_component) then
            i_real = i_term
            exit
        end if
    end do
    if (i_real == 0) call msg_fatal ("Did not find associated real term!")
end function process_get_first_real_term

```

<Process: process: TBP>+≡

```

    procedure :: get_associated_real_fin => process_get_associated_real_fin

```

<Process: procedures>+≡

```

    elemental function process_get_associated_real_fin (process, i_component) result (i_real)
        integer :: i_real
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_component
        i_real = process%component(i_component)%config%get_associated_real_fin ()
    end function process_get_associated_real_fin

```

<Process: process: TBP>+≡

```

    procedure :: select_i_term => process_select_i_term

```

<Process: procedures>+≡

```

    pure function process_select_i_term (process, i_mci) result (i_term)
        integer :: i_term
        class(process_t), intent(in) :: process
        integer, intent(in) :: i_mci
        integer :: i_component, i_sub
        i_component = process%mci_entry(i_mci)%i_component(1)
        i_term = process%component(i_component)%i_term(1)
        i_sub = process%term(i_term)%i_sub
        if (i_sub > 0) &
            i_term = process%term(i_sub)%i_term_global
    end function process_select_i_term

```

Would be better to do this at the level of the writer of the core but one has to bring NLO information there.

<Process: process: TBP>+≡

```

    procedure :: prepare_any_external_code &
        => process_prepare_any_external_code

```

<Process: procedures>+≡

```

    subroutine process_prepare_any_external_code (process)
        class(process_t), intent(inout), target :: process
        integer :: i
        if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
            "process_prepare_external_code")
        associate (pcm => process%pcm)
            do i = 1, pcm%n_cores
                call pcm%prepare_any_external_code ( &
                    process%core_entry(i), i, &

```

```

        process%get_library_name (), &
        process%config%model, &
        process%env%get_var_list_ptr ())
    end do
end associate
end subroutine process_prepare_any_external_code

```

30.5 Process config

(process_config.f90)≡
⟨File header⟩

```

module process_config

⟨Use kinds⟩
⟨Use strings⟩
    use format_utils, only: write_separator
    use io_units
    use md5
    use os_interface
    use diagnostics
    use sf_base
    use sf_mappings
    use mappings, only: mapping_defaults_t
    use phs_forests, only: phs_parameters_t
    use sm_qcd
    use physics_defs
    use integration_results
    use model_data
    use models
    use interactions
    use quantum_numbers
    use flavors
    use helicities
    use colors
    use rng_base
    use state_matrices
    use process_libraries
    use process_constants
    use prc_core
    use prc_external
    use prc_openloops, only: prc_openloops_t
    use prc_threshold, only: prc_threshold_t
    use beams
    use dispatch_beams, only: dispatch_qcd
    use mci_base
    use beam_structures
    use phs_base
    use variables
    use expr_base
    use blha_olp_interfaces, only: prc_blha_t

```



```

    <Standard module head>

    <Process config: public>

    <Process config: parameters>

    <Process config: types>

contains

    <Process config: procedures>

```

```
end module process_config
```

Identifiers for the NLO setup.

```

<Process config: parameters>≡
    integer, parameter, public :: COMP_DEFAULT = 0
    integer, parameter, public :: COMP_REAL_FIN = 1
    integer, parameter, public :: COMP_MASTER = 2
    integer, parameter, public :: COMP_VIRT = 3
    integer, parameter, public :: COMP_REAL = 4
    integer, parameter, public :: COMP_REAL_SING = 5
    integer, parameter, public :: COMP_MISMATCH = 6
    integer, parameter, public :: COMP_PDF = 7
    integer, parameter, public :: COMP_SUB = 8
    integer, parameter, public :: COMP_RESUM = 9

```

30.5.1 Output selection flags

We declare a number of identifiers for write methods, so they only displays selected parts. The identifiers can be supplied to the `vlist` array argument of the standard F2008 derived-type writer call.

```

<Process config: parameters>+≡
    integer, parameter, public :: F_PACIFY = 1
    integer, parameter, public :: F_SHOW_VAR_LIST = 11
    integer, parameter, public :: F_SHOW_EXPRESSIONS = 12
    integer, parameter, public :: F_SHOW_LIB = 13
    integer, parameter, public :: F_SHOW_MODEL = 14
    integer, parameter, public :: F_SHOW_QCD = 15
    integer, parameter, public :: F_SHOW_OS_DATA = 16
    integer, parameter, public :: F_SHOW_RNG = 17
    integer, parameter, public :: F_SHOW_BEAMS = 18

```

This is a simple function that returns true if a flag value is present in `v_list`, but not its negative. If neither is present, it returns `default`.

```

<Process config: public>≡
    public :: flagged

<Process config: procedures>≡
    function flagged(v_list, id, def) result(flag)
        logical :: flag
        integer, dimension(:), intent(in) :: v_list
        integer, intent(in) :: id

```

```

logical, intent(in), optional :: def
logical :: default_result
default_result = .false.; if (present (def)) default_result = def
if (default_result) then
    flag = all (v_list /= -id)
else
    flag = all (v_list /= -id) .and. any (v_list == id)
end if
end function flagged

```

Related: if flag is set (unset), append **value** (its negative) to the **v_list**, respectively. **v_list** must be allocated.

```

<Process config: public>+≡
    public :: set_flag

<Process config: procedures>+≡
    subroutine set_flag (v_list, value, flag)
        integer, dimension(:), intent(inout), allocatable :: v_list
        integer, intent(in) :: value
        logical, intent(in), optional :: flag
        if (present (flag)) then
            if (flag) then
                v_list = [v_list, value]
            else
                v_list = [v_list, -value]
            end if
        end if
    end subroutine set_flag

```

30.5.2 Generic configuration data

This information concerns physical and technical properties of the process. It is fixed upon initialization, using data from the process specification and the variable list.

The number **n.in** is the number of incoming beam particles, simultaneously the number of incoming partons, 1 for a decay and 2 for a scattering process. (The number of outgoing partons may depend on the process component.)

The number **n.components** is the number of components that constitute the current process.

The number **n.terms** is the number of distinct contributions to the scattering matrix that constitute the current process. Each component may generate several terms.

The number **n.mci** is the number of independent MC integration configurations that this process uses. Distinct process components that share a MCI configuration may be combined pointwise. (Nevertheless, a given MC variable set may correspond to several “nearby” kinematical configurations.) This is also the number of distinct sampling-function results that this process can generate. Process components that use distinct variable sets are added only once after an integration pass has completed.

The **model** pointer identifies the physics model and its parameters. This is a pointer to an external object.

Various `parse_node_t` objects are taken from the SINDARIN input. They encode expressions for evaluating cuts and scales. The workspaces for evaluating those expressions are set up in the `effective_state` subobjects. Note that these are really pointers, so the actual nodes are not stored inside the process object.

The `md5sum` is taken and used to verify the process configuration when re-reading data from file.

```

(Process config: public)+≡
    public :: process_config_data_t

(Process config: types)≡
    type :: process_config_data_t
        class(process_def_t), pointer :: process_def => null ()
        integer :: n_in = 0
        integer :: n_components = 0
        integer :: n_terms = 0
        integer :: n_mci = 0
        type(string_t) :: model_name
        class(model_data_t), pointer :: model => null ()
        type(qcd_t) :: qcd
        class(expr_factory_t), allocatable :: ef_cuts
        class(expr_factory_t), allocatable :: ef_scale
        class(expr_factory_t), allocatable :: ef_fac_scale
        class(expr_factory_t), allocatable :: ef_ren_scale
        class(expr_factory_t), allocatable :: ef_weight
        character(32) :: md5sum = ""
    contains
        (Process config: process config data: TBP)
    end type process_config_data_t

```

Here, we may compress the expressions for cuts etc.

```

(Process config: process config data: TBP)≡
    procedure :: write => process_config_data_write

(Process config: procedures)+≡
    subroutine process_config_data_write (config, u, counters, model, expressions)
        class(process_config_data_t), intent(in) :: config
        integer, intent(in) :: u
        logical, intent(in) :: counters
        logical, intent(in) :: model
        logical, intent(in) :: expressions
        write (u, "(1x,A)") "Configuration data:"
        if (counters) then
            write (u, "(3x,A,I0)") "Number of incoming particles = ", &
                config%n_in
            write (u, "(3x,A,I0)") "Number of process components = ", &
                config%n_components
            write (u, "(3x,A,I0)") "Number of process terms      = ", &
                config%n_terms
            write (u, "(3x,A,I0)") "Number of MCI configurations = ", &
                config%n_mci
        end if
        if (associated (config%model)) then
            write (u, "(3x,A,A)") "Model = ", char (config%model_name)
            if (model) then

```

```

        call write_separator (u)
        call config%model%write (u)
        call write_separator (u)
    end if
else
    write (u, "(3x,A,A,A)") "Model = ", char (config%model_name), &
        " [not associated]"
end if
call config%qcd%write (u, show_md5sum = .false.)
call write_separator (u)
if (expressions) then
    if (allocated (config%ef_cuts)) then
        call write_separator (u)
        write (u, "(3x,A)") "Cut expression:"
        call config%ef_cuts%write (u)
    end if
    if (allocated (config%ef_scale)) then
        call write_separator (u)
        write (u, "(3x,A)") "Scale expression:"
        call config%ef_scale%write (u)
    end if
    if (allocated (config%ef_fac_scale)) then
        call write_separator (u)
        write (u, "(3x,A)") "Factorization scale expression:"
        call config%ef_fac_scale%write (u)
    end if
    if (allocated (config%ef_ren_scale)) then
        call write_separator (u)
        write (u, "(3x,A)") "Renormalization scale expression:"
        call config%ef_ren_scale%write (u)
    end if
    if (allocated (config%ef_weight)) then
        call write_separator (u)
        write (u, "(3x,A)") "Weight expression:"
        call config%ef_weight%write (u)
    end if
else
    call write_separator (u)
    write (u, "(3x,A)") "Expressions (cut, scales, weight): [not shown]"
end if
if (config%md5sum /= "") then
    call write_separator (u)
    write (u, "(3x,A,A,A)") "MD5 sum (config) = '", config%md5sum, "'"
end if
end subroutine process_config_data_write

```

Initialize. We use information from the process metadata and from the process library, given the process ID. We also store the currently active OS data set.

The model pointer references the model data within the `env` record. That should be an instance of the global model.

We initialize the QCD object, unless the environment information is unavailable (unit tests).

The RNG factory object is imported by moving the allocation.

```

(Process config: process config data: TBP)+≡
  procedure :: init => process_config_data_init

(Process config: procedures)+≡
  subroutine process_config_data_init (config, meta, env)
    class(process_config_data_t), intent(out) :: config
    type(process_metadata_t), intent(in) :: meta
    type(process_environment_t), intent(in) :: env
    config%process_def => env%lib%get_process_def_ptr (meta%id)
    config%n_in = config%process_def%get_n_in ()
    config%n_components = size (meta%component_id)
    config%model => env%get_model_ptr ()
    config%model_name = config%model%get_name ()
    if (env%got_var_list ()) then
      call dispatch_qcd &
        (config%qcd, env%get_var_list_ptr (), env%get_os_data ())
    end if
  end subroutine process_config_data_init

```

Current implementation: nothing to finalize.

```

(Process config: process config data: TBP)+≡
  procedure :: final => process_config_data_final

(Process config: procedures)+≡
  subroutine process_config_data_final (config)
    class(process_config_data_t), intent(inout) :: config
  end subroutine process_config_data_final

```

Return a copy of the QCD data block.

```

(Process config: process config data: TBP)+≡
  procedure :: get_qcd => process_config_data_get_qcd

(Process config: procedures)+≡
  function process_config_data_get_qcd (config) result (qcd)
    class(process_config_data_t), intent(in) :: config
    type(qcd_t) :: qcd
    qcd = config%qcd
  end function process_config_data_get_qcd

```

Compute the MD5 sum of the configuration data. This encodes, in particular, the model and the expressions for cut, scales, weight, etc. It should not contain the IDs and number of components, etc., since the MD5 sum should be useful for integrating individual components.

This is done only once. If the MD5 sum is nonempty, the calculation is skipped.

```

(Process config: process config data: TBP)+≡
  procedure :: compute_md5sum => process_config_data_compute_md5sum

(Process config: procedures)+≡
  subroutine process_config_data_compute_md5sum (config)
    class(process_config_data_t), intent(inout) :: config
    integer :: u
    if (config%md5sum == "") then
      u = free_unit ()

```

```

        open (u, status = "scratch", action = "readwrite")
        call config%write (u, counters = .false., &
            model = .true., expressions = .true.)
        rewind (u)
        config%md5sum = md5sum (u)
        close (u)
    end if
end subroutine process_config_data_compute_md5sum

```

```

<Process config: process config data: TBP>+≡
    procedure :: get_md5sum => process_config_data_get_md5sum

<Process config: procedures>+≡
    pure function process_config_data_get_md5sum (config) result (md5)
        character(32) :: md5
        class(process_config_data_t), intent(in) :: config
        md5 = config%md5sum
    end function process_config_data_get_md5sum

```

30.5.3 Environment

This record stores a snapshot of the process environment at the point where the process object is created.

Model and variable list are implemented as pointer, so they always have the `target` attribute.

For unit-testing purposes, setting the var list is optional. If not set, the pointer is null.

```

<Process config: public>+≡
    public :: process_environment_t

<Process config: types>+≡
    type :: process_environment_t
        private
        type(model_t), pointer :: model => null ()
        type(var_list_t), pointer :: var_list => null ()
        logical :: var_list_is_set = .false.
        type(process_library_t), pointer :: lib => null ()
        type(beam_structure_t) :: beam_structure
        type(os_data_t) :: os_data
    contains
        <Process config: process environment: TBP>
    end type process_environment_t

```

Model and local var list are snapshots and need a finalizer.

```

<Process config: process environment: TBP>≡
    procedure :: final => process_environment_final

<Process config: procedures>+≡
    subroutine process_environment_final (env)
        class(process_environment_t), intent(inout) :: env
        if (associated (env%model)) then
            call env%model%final ()
        end if
    end subroutine process_environment_final

```

```

        deallocate (env%model)
    end if
    if (associated (env%var_list)) then
        call env%var_list%final (follow_link=.true.)
        deallocate (env%var_list)
    end if
end subroutine process_environment_final

```

Output, DTIO compatible.

```

<Process config: process environment: TBP>+≡
    procedure :: write => process_environment_write
    procedure :: write_formatted => process_environment_write_formatted
    ! generic :: write (formatted) => write_formatted

<Process config: procedures>+≡
    subroutine process_environment_write (env, unit, &
        show_var_list, show_model, show_lib, show_beams, show_os_data)
        class(process_environment_t), intent(in) :: env
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_var_list
        logical, intent(in), optional :: show_model
        logical, intent(in), optional :: show_lib
        logical, intent(in), optional :: show_beams
        logical, intent(in), optional :: show_os_data
        integer :: u, iostat
        integer, dimension(:), allocatable :: v_list
        character(0) :: iomsg
        u = given_output_unit (unit)
        allocate (v_list (0))
        call set_flag (v_list, F_SHOW_VAR_LIST, show_var_list)
        call set_flag (v_list, F_SHOW_MODEL, show_model)
        call set_flag (v_list, F_SHOW_LIB, show_lib)
        call set_flag (v_list, F_SHOW_BEAMS, show_beams)
        call set_flag (v_list, F_SHOW_OS_DATA, show_os_data)
        call env%write_formatted (u, "LISTDIRECTED", v_list, iostat, iomsg)
    end subroutine process_environment_write

```

DTIO standard write.

```

<Process config: procedures>+≡
    subroutine process_environment_write_formatted &
        (dtv, unit, iotype, v_list, iostat, iomsg)
        class(process_environment_t), intent(in) :: dtv
        integer, intent(in) :: unit
        character(*), intent(in) :: iotype
        integer, dimension(:), intent(in) :: v_list
        integer, intent(out) :: iostat
        character(*), intent(inout) :: iomsg
        associate (env => dtv)
            if (flagged (v_list, F_SHOW_VAR_LIST, .true.)) then
                write (unit, "(1x,A)") "Variable list:"
                if (associated (env%var_list)) then
                    call write_separator (unit)
                    call env%var_list%write (unit)
                end if
            end if
        end associate
    end subroutine process_environment_write_formatted

```

```

        else
            write (unit, "(3x,A)") "[not allocated]"
        end if
        call write_separator (unit)
    end if
    if (flagged (v_list, F_SHOW_MODEL, .true.)) then
        write (unit, "(1x,A)") "Model:"
        if (associated (env%model)) then
            call write_separator (unit)
            call env%model%write (unit)
        else
            write (unit, "(3x,A)") "[not allocated]"
        end if
        call write_separator (unit)
    end if
    if (flagged (v_list, F_SHOW_LIB, .true.)) then
        write (unit, "(1x,A)") "Process library:"
        if (associated (env%lib)) then
            call write_separator (unit)
            call env%lib%write (unit)
        else
            write (unit, "(3x,A)") "[not allocated]"
        end if
    end if
    if (flagged (v_list, F_SHOW_BEAMS, .true.)) then
        call write_separator (unit)
        call env%beam_structure%write (unit)
    end if
    if (flagged (v_list, F_SHOW_OS_DATA, .true.)) then
        write (unit, "(1x,A)") "Operating-system data:"
        call write_separator (unit)
        call env%os_data%write (unit)
    end if
end associate
iostat = 0
end subroutine process_environment_write_formatted

```

Initialize: Make a snapshot of the provided model. Make a link to the current process library.

Also make a snapshot of the variable list, if provided. If none is provided, there is an empty variable list nevertheless, so a pointer lookup does not return null.

If no beam structure is provided, the beam-structure member is empty and will yield a number of zero beams when queried.

(Process config: process environment: TBP)+≡

```

    procedure :: init => process_environment_init

```

(Process config: procedures)+≡

```

    subroutine process_environment_init &
        (env, model, lib, os_data, var_list, beam_structure)
    class(process_environment_t), intent(out) :: env
    type(model_t), intent(in), target :: model
    type(process_library_t), intent(in), target :: lib
    type(os_data_t), intent(in) :: os_data

```



```

type(var_list_t), intent(in), target, optional :: var_list
type(beam_structure_t), intent(in), optional :: beam_structure
allocate (env%model)
call env%model%init_instance (model)
env%lib => lib
env%os_data = os_data
allocate (env%var_list)
if (present (var_list)) then
    call env%var_list%init_snapshot (var_list, follow_link=.true.)
    env%var_list_is_set = .true.
end if
if (present (beam_structure)) then
    env%beam_structure = beam_structure
end if
end subroutine process_environment_init

```

Indicate whether a variable list has been provided upon initialization.

```

(Process config: process environment: TBP)+≡
    procedure :: got_var_list => process_environment_get_var_list

(Process config: procedures)+≡
    function process_environment_get_var_list (env) result (flag)
        class(process_environment_t), intent(in) :: env
        logical :: flag
        flag = env%var_list_is_set
    end function process_environment_get_var_list

```

Return a pointer to the variable list.

```

(Process config: process environment: TBP)+≡
    procedure :: get_var_list_ptr => process_environment_get_var_list_ptr

(Process config: procedures)+≡
    function process_environment_get_var_list_ptr (env) result (var_list)
        class(process_environment_t), intent(in) :: env
        type(var_list_t), pointer :: var_list
        var_list => env%var_list
    end function process_environment_get_var_list_ptr

```

Return a pointer to the model, if it exists.

```

(Process config: process environment: TBP)+≡
    procedure :: get_model_ptr => process_environment_get_model_ptr

(Process config: procedures)+≡
    function process_environment_get_model_ptr (env) result (model)
        class(process_environment_t), intent(in) :: env
        type(model_t), pointer :: model
        model => env%model
    end function process_environment_get_model_ptr

```

Return the process library pointer.

```

(Process config: process environment: TBP)+≡
    procedure :: get_lib_ptr => process_environment_get_lib_ptr

```

```

(Process config: procedures)+≡
function process_environment_get_lib_ptr (env) result (lib)
  class(process_environment_t), intent(inout) :: env
  type(process_library_t), pointer :: lib
  lib => env%lib
end function process_environment_get_lib_ptr

```

Clear the process library pointer, in case the library is deleted.

```

(Process config: process environment: TBP)+≡
procedure :: reset_lib_ptr => process_environment_reset_lib_ptr

(Process config: procedures)+≡
subroutine process_environment_reset_lib_ptr (env)
  class(process_environment_t), intent(inout) :: env
  env%lib => null ()
end subroutine process_environment_reset_lib_ptr

```

Check whether the process library has changed, in case the library is recompiled, etc.

```

(Process config: process environment: TBP)+≡
procedure :: check_lib_sanity => process_environment_check_lib_sanity

(Process config: procedures)+≡
subroutine process_environment_check_lib_sanity (env, meta)
  class(process_environment_t), intent(in) :: env
  type(process_metadata_t), intent(in) :: meta
  if (associated (env%lib)) then
    if (env%lib%get_update_counter () /= meta%lib_update_counter) then
      call msg_fatal ("Process '" // char (meta%id) &
        // "' : library has been recompiled after integration")
    end if
  end if
end subroutine process_environment_check_lib_sanity

```

Fill the data block using the appropriate process-library access entry.

```

(Process config: process environment: TBP)+≡
procedure :: fill_process_constants => &
  process_environment_fill_process_constants

(Process config: procedures)+≡
subroutine process_environment_fill_process_constants &
  (env, id, i_component, data)
  class(process_environment_t), intent(in) :: env
  type(string_t), intent(in) :: id
  integer, intent(in) :: i_component
  type(process_constants_t), intent(out) :: data
  call env%lib%fill_constants (id, i_component, data)
end subroutine process_environment_fill_process_constants

```

Return the entire beam structure.

```

(Process config: process environment: TBP)+≡
procedure :: get_beam_structure => process_environment_get_beam_structure

```

```

(Process config: procedures)+≡
  function process_environment_get_beam_structure (env) result (beam_structure)
    class(process_environment_t), intent(in) :: env
    type(beam_structure_t) :: beam_structure
    beam_structure = env%beam_structure
  end function process_environment_get_beam_structure

```

Check the beam structure for PDFs.

```

(Process config: process environment: TBP)+≡
  procedure :: has_pdfs => process_environment_has_pdfs

(Process config: procedures)+≡
  function process_environment_has_pdfs (env) result (flag)
    class(process_environment_t), intent(in) :: env
    logical :: flag
    flag = env%beam_structure%has_pdf ()
  end function process_environment_has_pdfs

```

Check the beam structure for polarized beams.

```

(Process config: process environment: TBP)+≡
  procedure :: has_polarized_beams => process_environment_has_polarized_beams

(Process config: procedures)+≡
  function process_environment_has_polarized_beams (env) result (flag)
    class(process_environment_t), intent(in) :: env
    logical :: flag
    flag = env%beam_structure%has_polarized_beams ()
  end function process_environment_has_polarized_beams

```

Return a copy of the OS data block.

```

(Process config: process environment: TBP)+≡
  procedure :: get_os_data => process_environment_get_os_data

(Process config: procedures)+≡
  function process_environment_get_os_data (env) result (os_data)
    class(process_environment_t), intent(in) :: env
    type(os_data_t) :: os_data
    os_data = env%os_data
  end function process_environment_get_os_data

```

30.5.4 Metadata

This information describes the process. It is fixed upon initialization.

The `id` string is the name of the process object, as given by the user. The matrix element generator will use this string for naming Fortran procedures and types, so it should qualify as a Fortran name.

The `num_id` is meaningful if nonzero. It is used for communication with external programs or file standards which do not support string IDs.

The `run_id` string distinguishes among several runs for the same process. It identifies process instances with respect to adapted integration grids and

similar run-specific data. The run ID is kept when copying processes for creating instances, however, so it does not distinguish event samples.

The `lib_name` identifies the process library where the process definition and the process driver are located.

The `lib_index` is the index of entry in the process library that corresponds to the current process.

The `component_id` array identifies the individual process components.

The `component_description` is an array of human-readable strings that characterize the process components, for instance `a, b => c, d`.

The `active` mask array marks those components which are active. The others are skipped.

```

(Process config: public)+≡
    public :: process_metadata_t

(Process config: types)+≡
    type :: process_metadata_t
        integer :: type = PRC_UNKNOWN
        type(string_t) :: id
        integer :: num_id = 0
        type(string_t) :: run_id
        type(string_t), allocatable :: lib_name
        integer :: lib_update_counter = 0
        integer :: lib_index = 0
        integer :: n_components = 0
        type(string_t), dimension(:), allocatable :: component_id
        type(string_t), dimension(:), allocatable :: component_description
        logical, dimension(:), allocatable :: active
    contains
        (Process config: process metadata: TBP)
    end type process_metadata_t

```

Output: ID and run ID. We write the variable list only upon request.

```

(Process config: process metadata: TBP)≡
    procedure :: write => process_metadata_write

(Process config: procedures)+≡
    subroutine process_metadata_write (meta, u, screen)
        class(process_metadata_t), intent(in) :: meta
        integer, intent(in) :: u
        logical, intent(in) :: screen
        integer :: i
        select case (meta%type)
        case (PRC_UNKNOWN)
            if (screen) then
                write (msg_buffer, "(A)") "Process [undefined]"
            else
                write (u, "(1x,A)") "Process [undefined]"
            end if
            return
        case (PRC_DECAY)
            if (screen) then
                write (msg_buffer, "(A,1x,A,A,A)") "Process [decay]:", &
                    "", char (meta%id), ""
            end if
        end select
    end subroutine process_metadata_write

```

```

else
    write (u, "(1x,A)", advance="no") "Process [decay]:"
end if
case (PRC_SCATTERING)
    if (screen) then
        write (msg_buffer, "(A,1x,A,A,A)") "Process [scattering]:", &
            "'", char (meta%id), "'"
    else
        write (u, "(1x,A)", advance="no") "Process [scattering]:"
    end if
case default
    call msg_bug ("process_write: undefined process type")
end select
if (screen) then
    call msg_message ()
else
    write (u, "(1x,A,A,A)") "'", char (meta%id), "'"
end if
if (meta%num_id /= 0) then
    if (screen) then
        write (msg_buffer, "(2x,A,I0)") "ID (num)      = ", meta%num_id
        call msg_message ()
    else
        write (u, "(3x,A,I0)") "ID (num)      = ", meta%num_id
    end if
end if
if (screen) then
    if (meta%run_id /= "") then
        write (msg_buffer, "(2x,A,A,A)") "Run ID      = '", &
            char (meta%run_id), "'"
        call msg_message ()
    end if
else
    write (u, "(3x,A,A,A)") "Run ID      = '", char (meta%run_id), "'"
end if
if (allocated (meta%lib_name)) then
    if (screen) then
        write (msg_buffer, "(2x,A,A,A)") "Library name = '", &
            char (meta%lib_name), "'"
        call msg_message ()
    else
        write (u, "(3x,A,A,A)") "Library name = '", &
            char (meta%lib_name), "'"
    end if
else
    if (screen) then
        write (msg_buffer, "(2x,A)") "Library name = [not associated]"
        call msg_message ()
    else
        write (u, "(3x,A)") "Library name = [not associated]"
    end if
end if
if (screen) then
    write (msg_buffer, "(2x,A,I0)") "Process index = ", meta%lib_index

```

```

        call msg_message ()
    else
        write (u, "(3x,A,I0)") "Process index = ", meta%lib_index
    end if
    if (allocated (meta%component_id)) then
        if (screen) then
            if (any (meta%active)) then
                write (msg_buffer, "(2x,A)") "Process components:"
            else
                write (msg_buffer, "(2x,A)") "Process components: [none]"
            end if
            call msg_message ()
        else
            write (u, "(3x,A)") "Process components:"
        end if
        do i = 1, size (meta%component_id)
            if (.not. meta%active(i)) cycle
            if (screen) then
                write (msg_buffer, "(4x,I0,9A)") i, ": ", &
                    char (meta%component_id (i)), "' : ", &
                    char (meta%component_description (i))
                call msg_message ()
            else
                write (u, "(5x,I0,9A)") i, ": ", &
                    char (meta%component_id (i)), "' : ", &
                    char (meta%component_description (i))
            end if
        end do
    end if
    if (screen) then
        write (msg_buffer, "(A)") repeat (" ", 72)
        call msg_message ()
    else
        call write_separator (u)
    end if
end subroutine process_metadata_write

```

Short output: list components.

(Process config: process metadata: TBP)+≡

procedure :: show => process_metadata_show

(Process config: procedures)+≡

```

subroutine process_metadata_show (meta, u, model_name)
    class(process_metadata_t), intent(in) :: meta
    integer, intent(in) :: u
    type(string_t), intent(in) :: model_name
    integer :: i
    select case (meta%type)
    case (PRC_UNKNOWN)
        write (u, "(A)") "Process: [undefined]"
        return
    case default
        write (u, "(A)", advance="no") "Process:"
    end select

```

```

write (u, "(1x,A)", advance="no") char (meta%id)
select case (meta%num_id)
case (0)
case default
    write (u, "(1x,'( ',I0,')')", advance="no") meta%num_id
end select
select case (char (model_name))
case ("")
case default
    write (u, "(1x,[' ',A,']')", advance="no") char (model_name)
end select
write (u, *)
if (allocated (meta%component_id)) then
    do i = 1, size (meta%component_id)
        if (meta%active(i)) then
            write (u, "(2x,I0,':',1x,A)" i, &
                char (meta%component_description (i))
            end if
        end do
    end if
end if
end subroutine process_metadata_show

```

Initialize. Find process ID and run ID.

Also find the process ID in the process library and retrieve some metadata from there.

```

(Process config: process metadata: TBP)+≡
    procedure :: init => process_metadata_init

(Process config: procedures)+≡
    subroutine process_metadata_init (meta, id, lib, var_list)
        class(process_metadata_t), intent(out) :: meta
        type(string_t), intent(in) :: id
        type(process_library_t), intent(in), target :: lib
        type(var_list_t), intent(in) :: var_list
        select case (lib%get_n_in (id))
        case (1); meta%type = PRC_DECAY
        case (2); meta%type = PRC_SCATTERING
        case default
            call msg_bug ("Process ' ' // char (id) // '': impossible n_in")
        end select
        meta%id = id
        meta%run_id = var_list%get_sval (var_str ("$_run_id"))
        allocate (meta%lib_name)
        meta%lib_name = lib%get_name ()
        meta%lib_update_counter = lib%get_update_counter ()
        if (lib%contains (id)) then
            meta%lib_index = lib%get_entry_index (id)
            meta%num_id = lib%get_num_id (id)
            call lib%get_component_list (id, meta%component_id)
            meta%n_components = size (meta%component_id)
            call lib%get_component_description_list &
                (id, meta%component_description)
            allocate (meta%active (meta%n_components), source = .true.)
        else

```

```

        call msg_fatal ("Process library does not contain process '" &
            // char (id) // "'")
    end if
    if (.not. lib%is_active ()) then
        call msg_bug ("Process init: inactive library not handled yet")
    end if
end subroutine process_metadata_init

```

Mark a component as inactive.

```

<Process config: process metadata: TBP>+≡
    procedure :: deactivate_component => process_metadata_deactivate_component

<Process config: procedures>+≡
    subroutine process_metadata_deactivate_component (meta, i)
        class(process_metadata_t), intent(inout) :: meta
        integer, intent(in) :: i
        call msg_message ("Process component '" &
            // char (meta%component_id(i)) // "': matrix element vanishes")
        meta%active(i) = .false.
    end subroutine process_metadata_deactivate_component

```

30.5.5 Phase-space configuration

A process can have a number of independent phase-space configuration entries, depending on the process definition and evaluation algorithm. Each entry holds various configuration-parameter data and the actual `phs_config_t` record, which can vary in concrete type.

```

<Process config: public>+≡
    public :: process_phs_config_t

<Process config: types>+≡
    type :: process_phs_config_t
        type(phs_parameters_t) :: phs_par
        type(mapping_defaults_t) :: mapping_defs
        class(phs_config_t), allocatable :: phs_config
    contains
        <Process config: process phs config: TBP>
    end type process_phs_config_t

```

Output, DTIO compatible.

```

<Process config: process phs config: TBP>≡
    procedure :: write => process_phs_config_write
    procedure :: write_formatted => process_phs_config_write_formatted
    ! generic :: write (formatted) => write_formatted

<Process config: procedures>+≡
    subroutine process_phs_config_write (phs_config, unit)
        class(process_phs_config_t), intent(in) :: phs_config
        integer, intent(in), optional :: unit
        integer :: u, iostat
        integer, dimension(:), allocatable :: v_list
        character(0) :: iomsg
    end subroutine process_phs_config_write

```



```

    u = given_output_unit (unit)
    allocate (v_list (0))
    call phs_config%write_formatted (u, "LISTDIRECTED", v_list, iostat, iomsg)
end subroutine process_phs_config_write

```

DTIO standard write.

```

<Process config: procedures>+≡
subroutine process_phs_config_write_formatted &
    (dtv, unit, iotype, v_list, iostat, iomsg)
class(process_phs_config_t), intent(in) :: dtv
integer, intent(in) :: unit
character(*), intent(in) :: iotype
integer, dimension(:), intent(in) :: v_list
integer, intent(out) :: iostat
character(*), intent(inout) :: iomsg
associate (phs_config => dtv)
    write (unit, "(1x, A)") "Phase-space configuration entry:"
    call phs_config%phs_par%write (unit)
    call phs_config%mapping_defs%write (unit)
end associate
iostat = 0
end subroutine process_phs_config_write_formatted

```

30.5.6 Beam configuration

The object `data` holds all details about the initial beam configuration. The allocatable array `sf` holds the structure-function configuration blocks. There are `n_strfun` entries in the structure-function chain (not counting the initial beam object). We maintain `n_channel` independent parameterizations of this chain. If this is greater than zero, we need a multi-channel sampling algorithm, where for each point one channel is selected to generate kinematics.

The number of parameters that are required for generating a structure-function chain is `n_sfpar`.

The flag `azimuthal_dependence` tells whether the process setup is symmetric about the beam axis in the c.m. system. This implies that there is no transversal beam polarization. The flag `lab_is_cm` is obvious.

```

<Process config: public>+≡
public :: process_beam_config_t

<Process config: types>+≡
type :: process_beam_config_t
type(beam_data_t) :: data
integer :: n_strfun = 0
integer :: n_channel = 1
integer :: n_sfpar = 0
type(sf_config_t), dimension(:), allocatable :: sf
type(sf_channel_t), dimension(:), allocatable :: sf_channel
logical :: azimuthal_dependence = .false.
logical :: lab_is_cm = .true.
character(32) :: md5sum = ""
logical :: sf_trace = .false.

```

```

    type(string_t) :: sf_trace_file
contains
  <Process config: process beam config: TBP>≡
end type process_beam_config_t

```

Here we write beam data only if they are actually used.

The `verbose` flag is passed to the beam-data writer.

```

<Process config: process beam config: TBP>≡
  procedure :: write => process_beam_config_write

<Process config: procedures>+≡
  subroutine process_beam_config_write (object, unit, verbose)
    class(process_beam_config_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer :: u, i, c
    u = given_output_unit (unit)
    call object%data%write (u, verbose = verbose)
    if (object%data%initialized) then
      write (u, "(3x,A,L1)") "Azimuthal dependence      = ", &
        object%azimuthal_dependence
      write (u, "(3x,A,L1)") "Lab frame is c.m. frame = ", &
        object%lab_is_cm
      if (object%md5sum /= "") then
        write (u, "(3x,A,A,A)") "MD5 sum (beams/strf) = ', &
          object%md5sum, "'"
      end if
      if (allocated (object%sf)) then
        do i = 1, size (object%sf)
          call object%sf(i)%write (u)
        end do
        if (any_sf_channel_has_mapping (object%sf_channel)) then
          write (u, "(1x,A,L1)") "Structure-function mappings per channel:"
          do c = 1, object%n_channel
            write (u, "(3x,I0,':')", advance="no") c
            call object%sf_channel(c)%write (u)
          end do
        end if
      end if
    end if
  end subroutine process_beam_config_write

```

The beam data have a finalizer. We assume that there is none for the structure-function data.

```

<Process config: process beam config: TBP>+≡
  procedure :: final => process_beam_config_final

<Process config: procedures>+≡
  subroutine process_beam_config_final (object)
    class(process_beam_config_t), intent(inout) :: object
    call object%data%final ()
  end subroutine process_beam_config_final

```

Initialize the beam setup with a given beam structure object.

```

(Process config: process beam config: TBP)+≡
  procedure :: init_beam_structure => process_beam_config_init_beam_structure

(Process config: procedures)+≡
  subroutine process_beam_config_init_beam_structure &
    (beam_config, beam_structure, sqrts, model, decay_rest_frame)
    class(process_beam_config_t), intent(out) :: beam_config
    type(beam_structure_t), intent(in) :: beam_structure
    logical, intent(in), optional :: decay_rest_frame
    real(default), intent(in) :: sqrts
    class(model_data_t), intent(in), target :: model
    call beam_config%data%init_structure (beam_structure, &
      sqrts, model, decay_rest_frame)
    beam_config%lab_is_cm = beam_config%data%lab_is_cm
  end subroutine process_beam_config_init_beam_structure

```

Initialize the beam setup for a scattering process with specified flavor combination, other properties taken from the beam structure object (if any).

```

(Process config: process beam config: TBP)+≡
  procedure :: init_scattering => process_beam_config_init_scattering

(Process config: procedures)+≡
  subroutine process_beam_config_init_scattering &
    (beam_config, flv_in, sqrts, beam_structure)
    class(process_beam_config_t), intent(out) :: beam_config
    type(flavor_t), dimension(2), intent(in) :: flv_in
    real(default), intent(in) :: sqrts
    type(beam_structure_t), intent(in), optional :: beam_structure
    if (present (beam_structure)) then
      if (beam_structure%polarized ()) then
        call beam_config%data%init_sqrts (sqrts, flv_in, &
          beam_structure%get_smatrix (), beam_structure%get_pol_f ())
      else
        call beam_config%data%init_sqrts (sqrts, flv_in)
      end if
    else
      call beam_config%data%init_sqrts (sqrts, flv_in)
    end if
  end subroutine process_beam_config_init_scattering

```

Initialize the beam setup for a decay process with specified flavor, other properties taken from the beam structure object (if present).

For a cascade decay, we set `rest_frame` to false, indicating a event-wise varying momentum. The beam data itself are initialized for the particle at rest.

```

(Process config: process beam config: TBP)+≡
  procedure :: init_decay => process_beam_config_init_decay

(Process config: procedures)+≡
  subroutine process_beam_config_init_decay &
    (beam_config, flv_in, rest_frame, beam_structure)
    class(process_beam_config_t), intent(out) :: beam_config
    type(flavor_t), dimension(1), intent(in) :: flv_in
    logical, intent(in), optional :: rest_frame

```

```

type(beam_structure_t), intent(in), optional :: beam_structure
if (present (beam_structure)) then
  if (beam_structure%polarized ()) then
    call beam_config%data%init_decay (flv_in, &
      beam_structure%get_smatrix (), beam_structure%get_pol_f (), &
      rest_frame = rest_frame)
  else
    call beam_config%data%init_decay (flv_in, rest_frame = rest_frame)
  end if
else
  call beam_config%data%init_decay (flv_in, &
    rest_frame = rest_frame)
end if
beam_config%lab_is_cm = beam_config%data%lab_is_cm
end subroutine process_beam_config_init_decay

```

Print an informative message.

```

<Process config: process beam config: TBP>+≡
  procedure :: startup_message => process_beam_config_startup_message

<Process config: procedures>+≡
  subroutine process_beam_config_startup_message &
    (beam_config, unit, beam_structure)
    class(process_beam_config_t), intent(in) :: beam_config
    integer, intent(in), optional :: unit
    type(beam_structure_t), intent(in), optional :: beam_structure
    integer :: u
    u = free_unit ()
    open (u, status="scratch", action="readwrite")
    if (present (beam_structure)) then
      call beam_structure%write (u)
    end if
    call beam_config%data%write (u)
    rewind (u)
    do
      read (u, "(1x,A)", end=1) msg_buffer
      call msg_message ()
    end do
1  continue
  close (u)
end subroutine process_beam_config_startup_message

```

Allocate the structure-function array.

```

<Process config: process beam config: TBP>+≡
  procedure :: init_sf_chain => process_beam_config_init_sf_chain

<Process config: procedures>+≡
  subroutine process_beam_config_init_sf_chain &
    (beam_config, sf_config, sf_trace_file)
    class(process_beam_config_t), intent(inout) :: beam_config
    type(sf_config_t), dimension(:), intent(in) :: sf_config
    type(string_t), intent(in), optional :: sf_trace_file
    integer :: i
    beam_config%n_strfun = size (sf_config)

```

```

allocate (beam_config%sf (beam_config%n_strfun))
do i = 1, beam_config%n_strfun
  associate (sf => sf_config(i))
    call beam_config%sf(i)%init (sf%i, sf%data)
    if (.not. sf%data%is_generator ()) then
      beam_config%n_sfpar = beam_config%n_sfpar + sf%data%get_n_par ()
    end if
  end associate
end do
if (present (sf_trace_file)) then
  beam_config%sf_trace = .true.
  beam_config%sf_trace_file = sf_trace_file
end if
end subroutine process_beam_config_init_sf_chain

```

Allocate the structure-function mapping channel array, given the requested number of channels.

```

(Process config: process beam config: TBP)+≡
  procedure :: allocate_sf_channels => process_beam_config_allocate_sf_channels

(Process config: procedures)+≡
  subroutine process_beam_config_allocate_sf_channels (beam_config, n_channel)
    class(process_beam_config_t), intent(inout) :: beam_config
    integer, intent(in) :: n_channel
    beam_config%n_channel = n_channel
    call allocate_sf_channels (beam_config%sf_channel, &
      n_channel = n_channel, &
      n_strfun = beam_config%n_strfun)
  end subroutine process_beam_config_allocate_sf_channels

```

Set a structure-function mapping channel for an array of structure-function entries, for a single channel. (The default is no mapping.)

```

(Process config: process beam config: TBP)+≡
  procedure :: set_sf_channel => process_beam_config_set_sf_channel

(Process config: procedures)+≡
  subroutine process_beam_config_set_sf_channel (beam_config, c, sf_channel)
    class(process_beam_config_t), intent(inout) :: beam_config
    integer, intent(in) :: c
    type(sf_channel_t), intent(in) :: sf_channel
    beam_config%sf_channel(c) = sf_channel
  end subroutine process_beam_config_set_sf_channel

```

Print an informative startup message.

```

(Process config: process beam config: TBP)+≡
  procedure :: sf_startup_message => process_beam_config_sf_startup_message

(Process config: procedures)+≡
  subroutine process_beam_config_sf_startup_message &
    (beam_config, sf_string, unit)
    class(process_beam_config_t), intent(in) :: beam_config
    type(string_t), intent(in) :: sf_string
    integer, intent(in), optional :: unit

```

```

if (beam_config%n_strfun > 0) then
  call msg_message ("Beam structure: " // char (sf_string), unit = unit)
  write (msg_buffer, "(A,3(1x,I0,1x,A))" &
    "Beam structure:", &
    beam_config%n_channel, "channels,", &
    beam_config%n_sfpar, "dimensions"
  call msg_message (unit = unit)
  if (beam_config%sf_trace) then
    call msg_message ("Beam structure: tracing &
      &values in '" // char (beam_config%sf_trace_file) // "'")
  end if
end if
end subroutine process_beam_config_sf_startup_message

```

Return the PDF set currently in use, if any. This should be unique, so we scan the structure functions until we get a nonzero number.

(This implies that if the PDF set is not unique (e.g., proton and photon structure used together), this does not work correctly.)

```

(Process config: process beam config: TBP)+≡
  procedure :: get_pdf_set => process_beam_config_get_pdf_set
(Process config: procedures)+≡
  function process_beam_config_get_pdf_set (beam_config) result (pdf_set)
    class(process_beam_config_t), intent(in) :: beam_config
    integer :: pdf_set
    integer :: i
    pdf_set = 0
    if (allocated (beam_config%sf)) then
      do i = 1, size (beam_config%sf)
        pdf_set = beam_config%sf(i)%get_pdf_set ()
        if (pdf_set /= 0) return
      end do
    end if
  end function process_beam_config_get_pdf_set

```

Return the beam file.

```

(Process config: process beam config: TBP)+≡
  procedure :: get_beam_file => process_beam_config_get_beam_file
(Process config: procedures)+≡
  function process_beam_config_get_beam_file (beam_config) result (file)
    class(process_beam_config_t), intent(in) :: beam_config
    type(string_t) :: file
    integer :: i
    file = ""
    if (allocated (beam_config%sf)) then
      do i = 1, size (beam_config%sf)
        file = beam_config%sf(i)%get_beam_file ()
        if (file /= "") return
      end do
    end if
  end function process_beam_config_get_beam_file

```

Compute the MD5 sum for the complete beam setup. We rely on the default output of `write` to contain all relevant data.

This is done only once, when the MD5 sum is still empty.

```

<Process config: process beam config: TBP>+≡
  procedure :: compute_md5sum => process_beam_config_compute_md5sum

<Process config: procedures>+≡
  subroutine process_beam_config_compute_md5sum (beam_config)
    class(process_beam_config_t), intent(inout) :: beam_config
    integer :: u
    if (beam_config%md5sum == "") then
      u = free_unit ()
      open (u, status = "scratch", action = "readwrite")
      call beam_config%write (u, verbose=.true.)
      rewind (u)
      beam_config%md5sum = md5sum (u)
      close (u)
    end if
  end subroutine process_beam_config_compute_md5sum

<Process config: process beam config: TBP>+≡
  procedure :: get_md5sum => process_beam_config_get_md5sum

<Process config: procedures>+≡
  pure function process_beam_config_get_md5sum (beam_config) result (md5)
    character(32) :: md5
    class(process_beam_config_t), intent(in) :: beam_config
    md5 = beam_config%md5sum
  end function process_beam_config_get_md5sum

<Process config: process beam config: TBP>+≡
  procedure :: has_structure_function => process_beam_config_has_structure_function

<Process config: procedures>+≡
  pure function process_beam_config_has_structure_function (beam_config) result (has_sf)
    logical :: has_sf
    class(process_beam_config_t), intent(in) :: beam_config
    has_sf = beam_config%n_strfun > 0
  end function process_beam_config_has_structure_function

```

30.5.7 Process components

A process component is an individual contribution to a process (scattering or decay) which needs not be physical. The sum over all components should be physical.

The `index` identifies this component within its parent process.

The actual process component is stored in the `core` subobject. We use a polymorphic subobject instead of an extension of `process_component_t`, because the individual entries in the array of process components can have different types. In short, `process_component_t` is a wrapper for the actual process variants.

If the `active` flag is false, we should skip this component. This happens if the associated process has vanishing matrix element.

The index array `i_term` points to the individual terms generated by this component. The indices refer to the parent process.

The index `i_mci` is the index of the MC integrator and parameter set which are associated to this process component.

```

(Process config: public)+≡
    public :: process_component_t

(Process config: types)+≡
    type :: process_component_t
        type(process_component_def_t), pointer :: config => null ()
        integer :: index = 0
        logical :: active = .false.
        integer, dimension(:), allocatable :: i_term
        integer :: i_mci = 0
        class(phs_config_t), allocatable :: phs_config
        character(32) :: md5sum_phs = ""
        integer :: component_type = COMP_DEFAULT
    contains
        (Process config: process component: TBP)
    end type process_component_t

```

Finalizer. The MCI template may (potentially) need a finalizer. The process configuration finalizer may include closing an open scratch file.

```

(Process config: process component: TBP)≡
    procedure :: final => process_component_final

(Process config: procedures)+≡
    subroutine process_component_final (object)
        class(process_component_t), intent(inout) :: object
        if (allocated (object%phs_config)) then
            call object%phs_config%final ()
        end if
    end subroutine process_component_final

```

The meaning of `verbose` depends on the process variant.

```

(Process config: process component: TBP)+≡
    procedure :: write => process_component_write

(Process config: procedures)+≡
    subroutine process_component_write (object, unit)
        class(process_component_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        if (associated (object%config)) then
            write (u, "(1x,A,I0)") "Component #", object%index
            call object%config%write (u)
            if (object%md5sum_phs /= "") then
                write (u, "(3x,A,A,A)") "MD5 sum (phs)      = '", &
                    object%md5sum_phs, "'"
            end if
        end if
    end subroutine process_component_write

```



```

else
    write (u, "(1x,A)") "Process component: [not allocated]"
end if
if (.not. object%active) then
    write (u, "(1x,A)") "[Inactive]"
    return
end if
write (u, "(1x,A)") "Referenced data:"
if (allocated (object%i_term)) then
    write (u, "(3x,A,999(1x,I0))") "Terms", &
        object%i_term
else
    write (u, "(3x,A)") "Terms" = [undefined]"
end if
if (object%i_mci /= 0) then
    write (u, "(3x,A,I0)") "MC dataset" = ", object%i_mci"
else
    write (u, "(3x,A)") "MC dataset" = [undefined]"
end if
if (allocated (object%phs_config)) then
    call object%phs_config%write (u)
end if
end subroutine process_component_write

```

Initialize the component.

```

<Process config: process component: TBP>+≡
    procedure :: init => process_component_init

<Process config: procedures>+≡
    subroutine process_component_init (component, &
        i_component, env, meta, config, &
        active, &
        phs_config_template)
        class(process_component_t), intent(out) :: component
        integer, intent(in) :: i_component
        type(process_environment_t), intent(in) :: env
        type(process_metadata_t), intent(in) :: meta
        type(process_config_data_t), intent(in) :: config
        logical, intent(in) :: active
        class(phs_config_t), intent(in), allocatable :: phs_config_template

        type(process_constants_t) :: data

        component%index = i_component
        component%config => &
            config%process_def%get_component_def_ptr (i_component)

        component%active = active
        if (component%active) then
            allocate (component%phs_config, source = phs_config_template)
            call env%fill_process_constants (meta%id, i_component, data)
            call component%phs_config%init (data, config%model)
        end if
    end subroutine process_component_init

```

```

(Process config: process component: TBP)+≡
  procedure :: is_active => process_component_is_active

(Process config: procedures)+≡
  elemental function process_component_is_active (component) result (active)
    logical :: active
    class(process_component_t), intent(in) :: component
    active = component%active
  end function process_component_is_active

```

Finalize the phase-space configuration.

```

(Process config: process component: TBP)+≡
  procedure :: configure_phs => process_component_configure_phs

(Process config: procedures)+≡
  subroutine process_component_configure_phs &
    (component, sqrts, beam_config, rebuild, &
     ignore_mismatch, subdir)
    class(process_component_t), intent(inout) :: component
    real(default), intent(in) :: sqrts
    type(process_beam_config_t), intent(in) :: beam_config
    logical, intent(in), optional :: rebuild
    logical, intent(in), optional :: ignore_mismatch
    type(string_t), intent(in), optional :: subdir
    logical :: no_strfun
    integer :: nlo_type
    no_strfun = beam_config%n_strfun == 0
    nlo_type = component%config%get_nlo_type ()
    call component%phs_config%configure (sqrts, &
      azimuthal_dependence = beam_config%azimuthal_dependence, &
      sqrts_fixed = no_strfun, &
      lab_is_cm = beam_config%lab_is_cm .and. no_strfun, &
      rebuild = rebuild, ignore_mismatch = ignore_mismatch, &
      nlo_type = nlo_type, &
      subdir = subdir)
  end subroutine process_component_configure_phs

```

The process component possesses two MD5 sums: the checksum of the component definition, which should be available when the component is initialized, and the phase-space MD5 sum, which is available after configuration.

```

(Process config: process component: TBP)+≡
  procedure :: compute_md5sum => process_component_compute_md5sum

(Process config: procedures)+≡
  subroutine process_component_compute_md5sum (component)
    class(process_component_t), intent(inout) :: component
    component%md5sum_phs = component%phs_config%get_md5sum ()
  end subroutine process_component_compute_md5sum

```

Match phase-space channels with structure-function channels, where applicable.

This calls a method of the `phs_config` phase-space implementation.

```

(Process config: process component: TBP)+≡
  procedure :: collect_channels => process_component_collect_channels

```

```

(Process config: procedures)+≡
  subroutine process_component_collect_channels (component, coll)
    class(process_component_t), intent(inout) :: component
    type(phs_channel_collection_t), intent(inout) :: coll
    call component%phs_config%collect_channels (coll)
  end subroutine process_component_collect_channels

(Process config: process component: TBP)+≡
  procedure :: get_config => process_component_get_config

(Process config: procedures)+≡
  function process_component_get_config (component) &
    result (config)
    type(process_component_def_t) :: config
    class(process_component_t), intent(in) :: component
    config = component%config
  end function process_component_get_config

(Process config: process component: TBP)+≡
  procedure :: get_md5sum => process_component_get_md5sum

(Process config: procedures)+≡
  pure function process_component_get_md5sum (component) result (md5)
    type(string_t) :: md5
    class(process_component_t), intent(in) :: component
    md5 = component%config%get_md5sum () // component%md5sum_phs
  end function process_component_get_md5sum

Return the number of phase-space parameters.

(Process config: process component: TBP)+≡
  procedure :: get_n_phs_par => process_component_get_n_phs_par

(Process config: procedures)+≡
  function process_component_get_n_phs_par (component) result (n_par)
    class(process_component_t), intent(in) :: component
    integer :: n_par
    n_par = component%phs_config%get_n_par ()
  end function process_component_get_n_phs_par

(Process config: process component: TBP)+≡
  procedure :: get_phs_config => process_component_get_phs_config

(Process config: procedures)+≡
  subroutine process_component_get_phs_config (component, phs_config)
    class(process_component_t), intent(in), target :: component
    class(phs_config_t), intent(out), pointer :: phs_config
    phs_config => component%phs_config
  end subroutine process_component_get_phs_config

(Process config: process component: TBP)+≡
  procedure :: get_nlo_type => process_component_get_nlo_type

```

```

<Process config: procedures>+≡
  elemental function process_component_get_nlo_type (component) result (nlo_type)
    integer :: nlo_type
    class(process_component_t), intent(in) :: component
    nlo_type = component%config%get_nlo_type ()
  end function process_component_get_nlo_type

<Process config: process component: TBP>+≡
  procedure :: needs_mci_entry => process_component_needs_mci_entry

<Process config: procedures>+≡
  function process_component_needs_mci_entry (component, combined_integration) result (value)
    logical :: value
    class(process_component_t), intent(in) :: component
    logical, intent(in), optional :: combined_integration
    value = component%active
    if (present (combined_integration)) then
      if (combined_integration) &
        value = value .and. component%component_type <= COMP_MASTER
    end if
  end function process_component_needs_mci_entry

<Process config: process component: TBP>+≡
  procedure :: can_be_integrated => process_component_can_be_integrated

<Process config: procedures>+≡
  elemental function process_component_can_be_integrated (component) result (active)
    logical :: active
    class(process_component_t), intent(in) :: component
    active = component%config%can_be_integrated ()
  end function process_component_can_be_integrated

```

30.5.8 Process terms

For straightforward tree-level calculations, each process component corresponds to a unique elementary interaction. However, in the case of NLO calculations with subtraction terms, a process component may split into several separate contributions to the scattering, which are qualified by interactions with distinct kinematics and particle content. We represent their configuration as `process_term_t` objects, the actual instances will be introduced below as `term_instance_t`. In any case, the process term contains an elementary interaction with a definite quantum-number and momentum content.

The index `i_term_global` identifies the term relative to the process.

The index `i_component` identifies the process component which generates this term, relative to the parent process.

The index `i_term` identifies the term relative to the process component (not the process).

The `data` subobject holds all process constants.

The number of allowed flavor/helicity/color combinations is stored as `n_allowed`. This is the total number of independent entries in the density matrix. For each

combination, the index of the flavor, helicity, and color state is stored in the arrays `flv`, `hel`, and `col`, respectively.

The flag `rearrange` is true if we need to rearrange the particles of the hard interaction, to obtain the effective parton state.

The interaction `int` holds the quantum state for the (resolved) hard interaction, the parent-child relations of the particles, and their momenta. The momenta are not filled yet; this is postponed to copies of `int` which go into the process instances.

If recombination is in effect, we should allocate `int_eff` to describe the rearranged partonic state.

This type is public only for use in a unit test.

```

<Process config: public>+≡
  public :: process_term_t
<Process config: types>+≡
  type :: process_term_t
    integer :: i_term_global = 0
    integer :: i_component = 0
    integer :: i_term = 0
    integer :: i_sub = 0
    integer :: i_core = 0
    integer :: n_allowed = 0
    type(process_constants_t) :: data
    real(default) :: alpha_s = 0
    integer, dimension(:), allocatable :: flv, hel, col
    integer :: n_sub, n_sub_color, n_sub_spin
    type(interaction_t) :: int
    type(interaction_t), pointer :: int_eff => null ()
  contains
    <Process config: process term: TBP>
  end type process_term_t

```

For the output, we skip the process constants and the tables of allowed quantum numbers. Those can also be read off from the interaction object.

```

<Process config: process term: TBP>≡
  procedure :: write => process_term_write
<Process config: procedures>+≡
  subroutine process_term_write (term, unit)
    class(process_term_t), intent(in) :: term
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A,I0)") "Term #", term%i_term_global
    write (u, "(3x,A,I0)") "Process component index      = ", &
      term%i_component
    write (u, "(3x,A,I0)") "Term index w.r.t. component = ", &
      term%i_term
    call write_separator (u)
    write (u, "(1x,A)") "Hard interaction:"
    call write_separator (u)
    call term%int%basic_write (u)
  end subroutine process_term_write

```

Write an account of all quantum number states and their current status.

```

(Process config: process term: TBP)+≡
  procedure :: write_state_summary => process_term_write_state_summary

(Process config: procedures)+≡
  subroutine process_term_write_state_summary (term, core, unit)
    class(process_term_t), intent(in) :: term
    class(prc_core_t), intent(in) :: core
    integer, intent(in), optional :: unit
    integer :: u, i, f, h, c
    type(state_iterator_t) :: it
    character :: sgn
    u = given_output_unit (unit)
    write (u, "(1x,A,I0)") "Term #", term%i_term_global
    call it%init (term%int%get_state_matrix_ptr ())
    do while (it%is_valid ())
      i = it%get_me_index ()
      f = term%flv(i)
      h = term%hel(i)
      if (allocated (term%col)) then
        c = term%col(i)
      else
        c = 1
      end if
      if (core%is_allowed (term%i_term, f, h, c)) then
        sgn = "+"
      else
        sgn = " "
      end if
      write (u, "(1x,A1,1x,I0,2x)", advance="no") sgn, i
      call quantum_numbers_write (it%get_quantum_numbers (), u)
      write (u, *)
      call it%advance ()
    end do
  end subroutine process_term_write_state_summary

```

Finalizer: the `int` and potentially `int_eff` components have a finalizer that we must call.

```

(Process config: process term: TBP)+≡
  procedure :: final => process_term_final

(Process config: procedures)+≡
  subroutine process_term_final (term)
    class(process_term_t), intent(inout) :: term
    call term%int%final ()
  end subroutine process_term_final

```

Initialize the term. We copy the process constants from the `core` object and set up the `int` hard interaction accordingly.

The `alpha_s` value is useful for writing external event records. This is the constant value which may be overridden by a event-specific running value. If the model does not contain the strong coupling, the value is zero.

The `rearrange` part is commented out; this or something equivalent could become relevant for NLO algorithms.

```

(Process config: process term: TBP)+≡
  procedure :: init => process_term_init

(Process config: procedures)+≡
  subroutine process_term_init &
    (term, i_term_global, i_component, i_term, core, model, &
     nlo_type, use_beam_pol, subtraction_method, &
     has_pdfs, n_emitters)
    class(process_term_t), intent(inout), target :: term
    integer, intent(in) :: i_term_global
    integer, intent(in) :: i_component
    integer, intent(in) :: i_term
    class(prc_core_t), intent(inout) :: core
    class(model_data_t), intent(in), target :: model
    integer, intent(in), optional :: nlo_type
    logical, intent(in), optional :: use_beam_pol
    type(string_t), intent(in), optional :: subtraction_method
    logical, intent(in), optional :: has_pdfs
    integer, intent(in), optional :: n_emitters
    class(modelpar_data_t), pointer :: alpha_s_ptr
    logical :: use_internal_color
    term%i_term_global = i_term_global
    term%i_component = i_component
    term%i_term = i_term
    call core%get_constants (term%data, i_term)
    alpha_s_ptr => model%get_par_data_ptr (var_str ("alphas"))
    if (associated (alpha_s_ptr)) then
      term%alpha_s = alpha_s_ptr%get_real ()
    else
      term%alpha_s = -1
    end if
    use_internal_color = .false.
    if (present (subtraction_method)) &
      use_internal_color = (char (subtraction_method) == 'omega') &
        .or. (char (subtraction_method) == 'threshold')
    call term%setup_interaction (core, model, nlo_type = nlo_type, &
      pol_beams = use_beam_pol, use_internal_color = use_internal_color, &
      has_pdfs = has_pdfs, n_emitters = n_emitters)
  end subroutine process_term_init

```

We fetch the process constants which determine the quantum numbers and use those to create the interaction. The interaction contains incoming and outgoing particles, no virtuals. The incoming particles are parents of the outgoing ones.

Keeping previous WHIZARD conventions, we invert the color assignment (but not flavor or helicity) for the incoming particles. When the color-flow square matrix is evaluated, this inversion is done again, so in the color-flow sequence we get the color assignments of the matrix element.

Why are these four subtraction entries for structure-function aware interactions? Taking the soft or collinear limit of the real-emission matrix element, the behavior of the parton energy fractions has to be taken into account.

In the pure real case, x_{\oplus} and x_{\ominus} are given by

$$x_{\oplus} = \frac{\bar{x}_{\oplus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1-y)}{2-\xi(1+y)}}, \quad x_{\ominus} = \frac{\bar{x}_{\ominus}}{\sqrt{1-\xi}} \sqrt{\frac{2-\xi(1+y)}{2-\xi(1-y)}}.$$

In the soft limit, $\xi \rightarrow 0$, this yields $x_{\oplus} = \bar{x}_{\oplus}$ and $x_{\ominus} = \bar{x}_{\ominus}$. In the collinear limit, $y \rightarrow 1$, it is $x_{\oplus} = \bar{x}_{\oplus}/(1-\xi)$ and $x_{\ominus} = \bar{x}_{\ominus}$. Likewise, in the anti-collinear limit $y \rightarrow -1$, the inverse relation holds. We therefore have to distinguish four cases with the PDF assignments $f(x_{\oplus}) \cdot f(x_{\ominus})$, $f(\bar{x}_{\oplus}) \cdot f(\bar{x}_{\ominus})$, $f(\bar{x}_{\oplus}/(1-\xi)) \cdot f(\bar{x}_{\ominus})$ and $f(\bar{x}_{\oplus}) \cdot f(\bar{x}_{\ominus}/(1-\xi))$.

The `n_emitters` optional argument is provided by the caller if this term requires spin-correlated matrix elements, and thus involves additional subtractions.

```

(Process config: process term: TBP)+≡
  procedure :: setup_interaction => process_term_setup_interaction

(Process config: procedures)+≡
  subroutine process_term_setup_interaction (term, core, model, &
    nlo_type, pol_beams, has_pdfs, use_internal_color, n_emitters)
    class(process_term_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
    class(model_data_t), intent(in), target :: model
    logical, intent(in), optional :: pol_beams
    logical, intent(in), optional :: has_pdfs
    integer, intent(in), optional :: nlo_type
    logical, intent(in), optional :: use_internal_color
    integer, intent(in), optional :: n_emitters
    integer :: n, n_tot
    type(flavor_t), dimension(:), allocatable :: flv
    type(color_t), dimension(:), allocatable :: col
    type(helicity_t), dimension(:), allocatable :: hel
    type(quantum_numbers_t), dimension(:), allocatable :: qn
    logical :: is_pol, use_color
    integer :: nlo_t, n_sub
    is_pol = .false.; if (present (pol_beams)) is_pol = pol_beams
    nlo_t = BORN; if (present (nlo_type)) nlo_t = nlo_type
    n_tot = term%data%n_in + term%data%n_out
    call count_number_of_states ()
    term%n_allowed = n
    call compute_n_sub (n_emitters, has_pdfs)
    call fill_quantum_numbers ()
    call term%int%basic_init &
      (term%data%n_in, 0, term%data%n_out, set_relations = .true.)
    select type (core)
    class is (prc_blha_t)
      call setup_states_blha_olp ()
    type is (prc_threshold_t)
      call setup_states_threshold ()
    class is (prc_external_t)
      call setup_states_other_prc_external ()
    class default
      call setup_states_omega ()
    end select
    call term%int%freeze ()

```



```

contains
subroutine count_number_of_states ()
  integer :: f, h, c
  n = 0
  select type (core)
  class is (prc_external_t)
    do f = 1, term%data%n_flv
      do h = 1, term%data%n_hel
        do c = 1, term%data%n_col
          n = n + 1
        end do
      end do
    end do
  class default !!! Omega and all test cores
    do f = 1, term%data%n_flv
      do h = 1, term%data%n_hel
        do c = 1, term%data%n_col
          if (core%is_allowed (term%i_term, f, h, c)) n = n + 1
        end do
      end do
    end do
  end select
end subroutine count_number_of_states

subroutine compute_n_sub (n_emitters, has_pdfs)
  integer, intent(in), optional :: n_emitters
  logical, intent(in), optional :: has_pdfs
  logical :: can_have_sub
  integer :: n_sub_color, n_sub_spin
  use_color = .false.; if (present (use_internal_color)) &
    use_color = use_internal_color
  can_have_sub = nlo_t == NLO_VIRTUAL .or. &
    (nlo_t == NLO_REAL .and. term%i_term_global == term%i_sub) .or. &
    nlo_t == NLO_MISMATCH .or. nlo_t == NLO_DGLAP
  n_sub_color = 0; n_sub_spin = 0
  if (can_have_sub) then
    if (.not. use_color) n_sub_color = n_tot * (n_tot - 1) / 2
    if (nlo_t == NLO_REAL) then
      if (present (n_emitters)) then
        n_sub_spin = 6 * n_emitters
      end if
    end if
  end if
  n_sub = n_sub_color + n_sub_spin
  !!! For the virtual subtraction we also need the finite virtual contribution
  !!! corresponding to the  $\epsilon^0$ -pole
  if (nlo_t == NLO_VIRTUAL) n_sub = n_sub + 1
  if (present (has_pdfs)) then
    if (has_pdfs &
      .and. ((nlo_t == NLO_REAL .and. can_have_sub) &
        .or. nlo_t == NLO_DGLAP)) then
      !!! necessary dummy, needs refactoring,
      !!! c.f. [[term_instance_evaluate_interaction_userdef_tree]]
      n_sub = n_sub + n_beams_rescaled
    end if
  end if
end subroutine compute_n_sub

```

```

        end if
    end if
    term%n_sub = n_sub
    term%n_sub_color = n_sub_color
    term%n_sub_spin = n_sub_spin
end subroutine compute_n_sub

subroutine fill_quantum_numbers ()
    integer :: nn
    logical :: can_have_sub
    select type (core)
    class is (prc_external_t)
        can_have_sub = nlo_t == NLO_VIRTUAL .or. &
            (nlo_t == NLO_REAL .and. term%i_term_global == term%i_sub) .or. &
            nlo_t == NLO_MISMATCH .or. nlo_t == NLO_DGLAP
        if (can_have_sub) then
            nn = (n_sub + 1) * n
        else
            nn = n
        end if
    class default
        nn = n
    end select
    allocate (term%flv (nn), term%col (nn), term%hel (nn))
    allocate (flv (n_tot), col (n_tot), hel (n_tot))
    allocate (qn (n_tot))
end subroutine fill_quantum_numbers

subroutine setup_states_blha_olp ()
    integer :: s, f, c, h, i
    i = 0
    associate (data => term%data)
        do s = 0, n_sub
            do f = 1, data%n_flv
                do h = 1, data%n_hel
                    do c = 1, data%n_col
                        i = i + 1
                        term%flv(i) = f
                        term%hel(i) = h
                        !!! Dummy-initialization of color
                        term%col(i) = c
                        call flv%init (data%flv_state (:,f), model)
                        call color_init_from_array (col, &
                            data%col_state(:, :, c), data%ghost_flag(:, c))
                        call col(1:data%n_in)%invert ()
                        if (is_pol) then
                            select type (core)
                            type is (prc_openloops_t)
                                call hel%init (data%hel_state (:,h))
                                call qn%init (flv, hel, col, s)
                            class default
                                call msg_fatal ("Polarized beams only supported by OpenLoops")
                            end select
                        else

```

```

        call qn%init (flv, col, s)
    end if
    call qn%tag_hard_process ()
    call term%int%add_state (qn)
end do
end do
end do
end do
end associate
end subroutine setup_states_blha_olp

subroutine setup_states_threshold ()
    integer :: s, f, c, h, i
    i = 0
    n_sub = 0; if (nlo_t == NLO_VIRTUAL) n_sub = 1
    associate (data => term%data)
        do s = 0, n_sub
            do f = 1, term%data%n_flv
                do h = 1, data%n_hel
                    do c = 1, data%n_col
                        i = i + 1
                        term%flv(i) = f
                        term%hel(i) = h
                        !!! Dummy-initialization of color
                        term%col(i) = 1
                        call flv%init (term%data%flv_state (:,f), model)
                        if (is_pol) then
                            call hel%init (data%hel_state (:,h))
                            call qn%init (flv, hel, s)
                        else
                            call qn%init (flv, s)
                        end if
                        call qn%tag_hard_process ()
                        call term%int%add_state (qn)
                    end do
                end do
            end do
        end do
    end associate
end subroutine setup_states_threshold

subroutine setup_states_other_prc_external ()
    integer :: s, f, i, c, h
    if (is_pol) &
        call msg_fatal ("Polarized beams only supported by OpenLoops")
    i = 0
    !!! n_sub = 0; if (nlo_t == NLO_VIRTUAL) n_sub = 1
    associate (data => term%data)
        do s = 0, n_sub
            do f = 1, data%n_flv
                do h = 1, data%n_hel
                    do c = 1, data%n_col
                        i = i + 1
                        term%flv(i) = f

```

```

        term%hel(i) = h
        !!! Dummy-initialization of color
        term%col(i) = c
        call flv%init (data%flv_state (:,f), model)
        call color_init_from_array (col, &
            data%col_state(:, :,c), data%ghost_flag(:,c))
        call col(1:data%n_in)%invert ()
        call qn%init (flv, col, s)
        call qn%tag_hard_process ()
        call term%int%add_state (qn)
    end do
end do
end do
end do
end associate
end subroutine setup_states_other_prc_external

subroutine setup_states_omega ()
    integer :: f, h, c, i
    i = 0
    associate (data => term%data)
        do f = 1, data%n_flv
            do h = 1, data%n_hel
                do c = 1, data%n_col
                    if (core%is_allowed (term%i_term, f, h, c)) then
                        i = i + 1
                        term%flv(i) = f
                        term%hel(i) = h
                        term%col(i) = c
                        call flv%init (data%flv_state(:,f), model)
                        call color_init_from_array (col, &
                            data%col_state(:, :,c), &
                            data%ghost_flag(:,c))
                        call col(:data%n_in)%invert ()
                        call hel%init (data%hel_state(:,h))
                        call qn%init (flv, col, hel)
                        call qn%tag_hard_process ()
                        call term%int%add_state (qn)
                    end if
                end do
            end do
        end do
    end associate
end subroutine setup_states_omega

end subroutine process_term_setup_interaction

<Process config: process term: TBP>+≡
    procedure :: get_process_constants => process_term_get_process_constants

<Process config: procedures>+≡
    subroutine process_term_get_process_constants &
        (term, prc_constants)
    class(process_term_t), intent(inout) :: term

```

```

    type(process_constants_t), intent(out) :: prc_constants
    prc_constants = term%data
end subroutine process_term_get_process_constants

```

30.6 Process call statistics

Very simple object for statistics. Could be moved to a more basic chapter.

```

<process_counter.f90>≡
  <File header>

  module process_counter

    use io_units

    <Standard module head>

    <Process counter: public>

    <Process counter: parameters>

    <Process counter: types>

    contains

    <Process counter: procedures>

  end module process_counter

```

This object can record process calls, categorized by evaluation status. It is a part of the `mci_entry` component below.

```

<Process counter: public>≡
  public :: process_counter_t

<Process counter: types>≡
  type :: process_counter_t
    integer :: total = 0
    integer :: failed_kinematics = 0
    integer :: failed_cuts = 0
    integer :: has_passed = 0
    integer :: evaluated = 0
    integer :: complete = 0
    contains
    <Process counter: process counter: TBP>
  end type process_counter_t

```

Here are the corresponding numeric codes:

```

<Process counter: parameters>≡
  integer, parameter, public :: STAT_UNDEFINED = 0
  integer, parameter, public :: STAT_INITIAL = 1
  integer, parameter, public :: STAT_ACTIVATED = 2
  integer, parameter, public :: STAT_BEAM_MOMENTA = 3
  integer, parameter, public :: STAT_FAILED_KINEMATICS = 4

```

```

integer, parameter, public :: STAT_SEED_KINEMATICS = 5
integer, parameter, public :: STAT_HARD_KINEMATICS = 6
integer, parameter, public :: STAT_EFF_KINEMATICS = 7
integer, parameter, public :: STAT_FAILED_CUTS = 8
integer, parameter, public :: STAT_PASSED_CUTS = 9
integer, parameter, public :: STAT_EVALUATED_TRACE = 10
integer, parameter, public :: STAT_EVENT_COMPLETE = 11

```

Output.

```

(Process counter: process counter: TBP)≡
  procedure :: write => process_counter_write

(Process counter: procedures)≡
  subroutine process_counter_write (object, unit)
    class(process_counter_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    if (object%total > 0) then
      write (u, "(1x,A)") "Call statistics (current run):"
      write (u, "(3x,A,I0)") "total          = ", object%total
      write (u, "(3x,A,I0)") "failed kin. = ", object%failed_kinematics
      write (u, "(3x,A,I0)") "failed cuts = ", object%failed_cuts
      write (u, "(3x,A,I0)") "passed cuts = ", object%has_passed
      write (u, "(3x,A,I0)") "evaluated   = ", object%evaluated
    else
      write (u, "(1x,A)") "Call statistics (current run): [no calls]"
    end if
  end subroutine process_counter_write

```

Reset. Just enforce default initialization.

```

(Process counter: process counter: TBP)+≡
  procedure :: reset => process_counter_reset

(Process counter: procedures)+≡
  subroutine process_counter_reset (counter)
    class(process_counter_t), intent(out) :: counter
    counter%total = 0
    counter%failed_kinematics = 0
    counter%failed_cuts = 0
    counter%has_passed = 0
    counter%evaluated = 0
    counter%complete = 0
  end subroutine process_counter_reset

```

We record an event according to the lowest status code greater or equal to the actual status. This is actually done by the process instance; the process object just copies the instance counter.

```

(Process counter: process counter: TBP)+≡
  procedure :: record => process_counter_record

(Process counter: procedures)+≡
  subroutine process_counter_record (counter, status)
    class(process_counter_t), intent(inout) :: counter

```

```

integer, intent(in) :: status
if (status <= STAT_FAILED_KINEMATICS) then
    counter%failed_kinematics = counter%failed_kinematics + 1
else if (status <= STAT_FAILED_CUTS) then
    counter%failed_cuts = counter%failed_cuts + 1
else if (status <= STAT_PASSED_CUTS) then
    counter%has_passed = counter%has_passed + 1
else
    counter%evaluated = counter%evaluated + 1
end if
counter%total = counter%total + 1
end subroutine process_counter_record

```

30.7 Multi-channel integration

```

<process_mci.f90>≡
  <File header>

  module process_mci

    <Use kinds>
    <Use strings>
    <Use debug>
    use io_units
    use diagnostics
    use physics_defs
    use md5
    use cputime
    use rng_base
    use mci_base
    use variables
    use integration_results
    use process_libraries
    use phs_base
    use process_counter
    use process_config

    <Standard module head>

    <Process mci: public>

    <Process mci: parameters>

    <Process mci: types>

    contains

    <Process mci: procedures>

  end module process_mci

```

30.7.1 Process MCI entry

The `process_mci_entry_t` block contains, for each process component that is integrated independently, the configuration data for its MC input parameters. Each input parameter set is handled by a `mci_t` integrator.

The MC input parameter set is broken down into the parameters required by the structure-function chain and the parameters required by the phase space of the elementary process.

The MD5 sum collects all information about the associated processes that may affect the integration. It does not contain the MCI object itself or integration results.

MC integration is organized in passes. Each pass may consist of several iterations, and for each iteration there is a number of calls. We store explicitly the values that apply to the current pass. Previous values are archived in the `results` object.

The `counter` receives the counter statistics from the associated process instance, for diagnostics.

The `results` object records results, broken down in passes and iterations.

```

(Process mci: public)≡
    public :: process_mci_entry_t

(Process mci: types)≡
    type :: process_mci_entry_t
        integer :: i_mci = 0
        integer, dimension(:), allocatable :: i_component
        integer :: process_type = PRC_UNKNOWN
        integer :: n_par = 0
        integer :: n_par_sf = 0
        integer :: n_par_phs = 0
        character(32) :: md5sum = ""
        integer :: pass = 0
        integer :: n_it = 0
        integer :: n_calls = 0
        logical :: activate_timer = .false.
        real(default) :: error_threshold = 0
        class(mci_t), allocatable :: mci
        type(process_counter_t) :: counter
        type(integration_results_t) :: results
        logical :: negative_weights = .false.
        logical :: combined_integration = .false.
        integer :: real_partition_type = REAL_FULL
    contains
        (Process mci: process mci entry: TBP)
    end type process_mci_entry_t

```

Finalizer for the `mci` component.

```

(Process mci: process mci entry: TBP)≡
    procedure :: final => process_mci_entry_final

(Process mci: procedures)≡
    subroutine process_mci_entry_final (object)
        class(process_mci_entry_t), intent(inout) :: object
        if (allocated (object%mci)) call object%mci%final ()
    end subroutine

```



```
end subroutine process_mci_entry_final
```

Output. Write pass/iteration information only if set (the pass index is nonzero). Write the MCI block only if it exists (for some self-tests it does not). Write results only if there are any.

```
<Process mci: process mci entry: TBP>+≡
  procedure :: write => process_mci_entry_write

<Process mci: procedures>+≡
  subroutine process_mci_entry_write (object, unit, pacify)
    class(process_mci_entry_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacify
    integer :: u
    u = given_output_unit (unit)
    write (u, "(3x,A,I0)") "Associated components = ", object%i_component
    write (u, "(3x,A,I0)") "MC input parameters   = ", object%n_par
    write (u, "(3x,A,I0)") "MC parameters (SF)   = ", object%n_par_sf
    write (u, "(3x,A,I0)") "MC parameters (PHS)  = ", object%n_par_phs
    if (object%pass > 0) then
      write (u, "(3x,A,I0)") "Current pass           = ", object%pass
      write (u, "(3x,A,I0)") "Number of iterations  = ", object%n_it
      write (u, "(3x,A,I0)") "Number of calls       = ", object%n_calls
    end if
    if (object%md5sum /= "") then
      write (u, "(3x,A,A,A)") "MD5 sum (components) = '", object%md5sum, "'"
    end if
    if (allocated (object%mci)) then
      call object%mci%write (u)
    end if
    call object%counter%write (u)
    if (object%results%exist ()) then
      call object%results%write (u, suppress = pacify)
      call object%results%write_chain_weights (u)
    end if
  end subroutine process_mci_entry_write
```

Configure the MCI entry. This is intent(inout) since some specific settings may be done before this. The actual `mci_t` object is an instance of the `mci_template` argument, which determines the concrete types.

In a unit-test context, the `mci_template` argument may be unallocated.

We obtain the number of channels and the number of parameters, separately for the structure-function chain and for the associated process component. We assume that the phase-space object has already been configured.

We assume that there is only one process component directly associated with a MCI entry.

```
<Process mci: process mci entry: TBP>+≡
  procedure :: configure => process_mci_entry_configure

<Process mci: procedures>+≡
  subroutine process_mci_entry_configure (mci_entry, mci_template, &
    process_type, i_mci, i_component, component, &
    n_sfpar, rng_factory)
```

```

class(process_mci_entry_t), intent(inout) :: mci_entry
class(mci_t), intent(in), allocatable :: mci_template
integer, intent(in) :: process_type
integer, intent(in) :: i_mci
integer, intent(in) :: i_component
type(process_component_t), intent(in), target :: component
integer, intent(in) :: n_sfpar
class(rng_factory_t), intent(inout) :: rng_factory
class(rng_t), allocatable :: rng
associate (phs_config => component%phs_config)
    mci_entry%i_mci = i_mci
    call mci_entry%create_component_list (i_component, component%get_config ())
    mci_entry%n_par_sf = n_sfpar
    mci_entry%n_par_phs = phs_config%get_n_par ()
    mci_entry%n_par = mci_entry%n_par_sf + mci_entry%n_par_phs
    mci_entry%process_type = process_type
    if (allocated (mci_template)) then
        allocate (mci_entry%mci, source = mci_template)
        call mci_entry%mci%record_index (mci_entry%i_mci)
        call mci_entry%mci%set_dimensions &
            (mci_entry%n_par, phs_config%get_n_channel ())
        call mci_entry%mci%declare_flat_dimensions &
            (phs_config%get_flat_dimensions ())
        if (phs_config%provides_equivalences) then
            call mci_entry%mci%declare_equivalences &
                (phs_config%channel, mci_entry%n_par_sf)
        end if
        if (phs_config%provides_chains) then
            call mci_entry%mci%declare_chains (phs_config%chain)
        end if
        call rng_factory%make (rng)
        call mci_entry%mci%import_rng (rng)
    end if
    call mci_entry%results%init (process_type)
end associate
end subroutine process_mci_entry_configure

```

(Process mci: parameters)≡

```

integer, parameter, public :: REAL_FULL = 0
integer, parameter, public :: REAL_SINGULAR = 1
integer, parameter, public :: REAL_FINITE = 2

```

(Process mci: process mci entry: TBP)+≡

```

procedure :: create_component_list => &
    process_mci_entry_create_component_list

```

(Process mci: procedures)+≡

```

subroutine process_mci_entry_create_component_list (mci_entry, &
    i_component, component_config)
class (process_mci_entry_t), intent(inout) :: mci_entry
integer, intent(in) :: i_component
type(process_component_def_t), intent(in) :: component_config
integer, dimension(:), allocatable :: i_list
integer :: n
integer, save :: i_rfin_offset = 0

```

```

if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, "process_mci_entry_create_component_list"
if (mci_entry%combined_integration) then
  if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, &
    "mci_entry%real_partition_type", mci_entry%real_partition_type)
  n = get_n_components (mci_entry%real_partition_type)
  allocate (i_list (n))
  select case (mci_entry%real_partition_type)
  case (REAL_FULL)
    i_list = component_config%get_association_list ()
    allocate (mci_entry%i_component (size (i_list)))
    mci_entry%i_component = i_list
  case (REAL_SINGULAR)
    i_list = component_config%get_association_list (ASSOCIATED_REAL_FIN)
    allocate (mci_entry%i_component (size(i_list)))
    mci_entry%i_component = i_list
  case (REAL_FINITE)
    allocate (mci_entry%i_component (1))
    mci_entry%i_component(1) = &
      component_config%get_associated_real_fin () + i_rfin_offset
    i_rfin_offset = i_rfin_offset + 1
  end select
else
  allocate (mci_entry%i_component (1))
  mci_entry%i_component(1) = i_component
end if
contains
function get_n_components (real_partition_type) result (n_components)
  integer :: n_components
  integer, intent(in) :: real_partition_type
  select case (real_partition_type)
  case (REAL_FULL)
    n_components = size (component_config%get_association_list ())
  case (REAL_SINGULAR)
    n_components = size (component_config%get_association_list &
      (ASSOCIATED_REAL_FIN))
  end select
  if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, "n_components", n_components)
end function get_n_components
end subroutine process_mci_entry_create_component_list

```

Set some additional parameters.

```

(Process mci: process mci entry: TBP)+≡
  procedure :: set_parameters => process_mci_entry_set_parameters

(Process mci: procedures)+≡
  subroutine process_mci_entry_set_parameters (mci_entry, var_list)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    type(var_list_t), intent(in) :: var_list
    integer :: integration_results_verbosity
    real(default) :: error_threshold
    integration_results_verbosity = &
      var_list%get_ival (var_str ("integration_results_verbosity"))
    error_threshold = &
      var_list%get_rval (var_str ("error_threshold"))
  end subroutine

```

```

mci_entry%activate_timer = &
    var_list%get_lval (var_str ("?integration_timer"))
call mci_entry%results%set_verbosity (integration_results_verbosity)
call mci_entry%results%set_error_threshold (error_threshold)
end subroutine process_mci_entry_set_parameters

```

Compute an MD5 sum that summarizes all information that could influence integration results, for the associated process components. We take the process-configuration MD5 sum which represents parameters, cuts, etc., the MD5 sums for the process component definitions and their phase space objects (which should be configured), and the beam configuration MD5 sum. (The QCD setup is included in the process configuration data MD5 sum.)

Done only once, when the MD5 sum is still empty.

```

(Process mci: process mci entry: TBP)+≡
    procedure :: compute_md5sum => process_mci_entry_compute_md5sum
(Process mci: procedures)+≡
    subroutine process_mci_entry_compute_md5sum (mci_entry, &
        config, component, beam_config)
        class(process_mci_entry_t), intent(inout) :: mci_entry
        type(process_config_data_t), intent(in) :: config
        type(process_component_t), dimension(:), intent(in) :: component
        type(process_beam_config_t), intent(in) :: beam_config
        type(string_t) :: buffer
        integer :: i
        if (mci_entry%md5sum == "") then
            buffer = config%get_md5sum () // beam_config%get_md5sum ()
            do i = 1, size (component)
                if (component(i)%is_active ()) then
                    buffer = buffer // component(i)%get_md5sum ()
                end if
            end do
            mci_entry%md5sum = md5sum (char (buffer))
        end if
        if (allocated (mci_entry%pci)) then
            call mci_entry%pci%set_md5sum (mci_entry%md5sum)
        end if
    end subroutine process_mci_entry_compute_md5sum

```

Test the MCI sampler by calling it a given number of time, discarding the results. The instance should be initialized.

The `mci_entry` is `intent(inout)` because the integrator contains the random-number state.

```

(Process mci: process mci entry: TBP)+≡
    procedure :: sampler_test => process_mci_entry_sampler_test
(Process mci: procedures)+≡
    subroutine process_mci_entry_sampler_test (mci_entry, mci_sampler, n_calls)
        class(process_mci_entry_t), intent(inout) :: mci_entry
        class(mci_sampler_t), intent(inout), target :: mci_sampler
        integer, intent(in) :: n_calls
        call mci_entry%pci%sampler_test (mci_sampler, n_calls)
    end subroutine process_mci_entry_sampler_test

```

Integrate.

The `integrate` method counts as an integration pass; the pass count is increased by one. We transfer the pass parameters (number of iterations and number of calls) to the actual integration routine.

The `mci_entry` is `intent(inout)` because the integrator contains the random-number state.

Note: The results are written to screen and to logfile. This behavior is hardcoded.

```

(Process mci: process mci entry: TBP)+≡
  procedure :: integrate => process_mci_entry_integrate
  procedure :: final_integration => process_mci_entry_final_integration

(Process mci: procedures)+≡
  subroutine process_mci_entry_integrate (mci_entry, mci_instance, &
    mci_sampler, n_it, n_calls, &
    adapt_grids, adapt_weights, final, pacify, &
    nlo_type)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_instance_t), intent(inout) :: mci_instance
    class(mci_sampler_t), intent(inout) :: mci_sampler
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: adapt_grids
    logical, intent(in), optional :: adapt_weights
    logical, intent(in), optional :: final, pacify
    integer, intent(in), optional :: nlo_type
    integer :: u_log
    u_log = logfile_unit ()
    mci_entry%pass = mci_entry%pass + 1
    mci_entry%n_it = n_it
    mci_entry%n_calls = n_calls
    if (mci_entry%pass == 1) &
      call mci_entry%mc%startup_message (n_calls = n_calls)
    call mci_entry%mc%set_timer (active = mci_entry%activate_timer)
    call mci_entry%results%display_init (screen = .true., unit = u_log)
    call mci_entry%results%new_pass ()
    if (present (nlo_type)) then
      select case (nlo_type)
      case (NLO_VIRTUAL, NLO_REAL, NLO_MISMATCH, NLO_DGLAP)
        mci_instance%negative_weights = .true.
      end select
    end if
    call mci_entry%mc%add_pass (adapt_grids, adapt_weights, final)
    call mci_entry%mc%start_timer ()
    call mci_entry%mc%integrate (mci_instance, mci_sampler, n_it, &
      n_calls, mci_entry%results, pacify = pacify)
    call mci_entry%mc%stop_timer ()
    if (signal_is_pending ()) return
  end subroutine process_mci_entry_integrate

  subroutine process_mci_entry_final_integration (mci_entry)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    call mci_entry%results%display_final ()
    call mci_entry%time_message ()
  end subroutine process_mci_entry_final_integration

```

```
end subroutine process_mci_entry_final_integration
```

If appropriate, issue an informative message about the expected time for an event sample.

```
(Process mci: process mci entry: TBP)+≡
  procedure :: get_time => process_mci_entry_get_time
  procedure :: time_message => process_mci_entry_time_message

(Process mci: procedures)+≡
  subroutine process_mci_entry_get_time (mci_entry, time, sample)
    class(process_mci_entry_t), intent(in) :: mci_entry
    type(time_t), intent(out) :: time
    integer, intent(in) :: sample
    real(default) :: time_last_pass, efficiency, calls
    time_last_pass = mci_entry%mci%get_time ()
    calls = mci_entry%results%get_n_calls ()
    efficiency = mci_entry%mci%get_efficiency ()
    if (time_last_pass > 0 .and. calls > 0 .and. efficiency > 0) then
      time = nint (time_last_pass / calls / efficiency * sample)
    end if
  end subroutine process_mci_entry_get_time

  subroutine process_mci_entry_time_message (mci_entry)
    class(process_mci_entry_t), intent(in) :: mci_entry
    type(time_t) :: time
    integer :: sample
    sample = 10000
    call mci_entry%get_time (time, sample)
    if (time%is_known ()) then
      call msg_message ("Time estimate for generating 10000 events: " &
        // char (time%to_string_dhms ()))
    end if
  end subroutine process_mci_entry_time_message
```

Prepare event generation. (For the test integrator, this does nothing. It is relevant for the VAMP integrator.)

```
(Process mci: process mci entry: TBP)+≡
  procedure :: prepare_simulation => process_mci_entry_prepare_simulation

(Process mci: procedures)+≡
  subroutine process_mci_entry_prepare_simulation (mci_entry)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    call mci_entry%mci%prepare_simulation ()
  end subroutine process_mci_entry_prepare_simulation
```

Generate an event. The instance should be initialized, otherwise event generation is directed by the mci integrator subobject. The integrator instance is contained in a *mci_work* subobject of the process instance, which simultaneously serves as the sampler object. (We avoid the anti-aliasing rules if we assume that the sampling itself does not involve the integrator instance contained in the process instance.)

Regarding weighted events, we only take events which are valid, which means that they have valid kinematics and have passed cuts. Therefore, we have a

rejection loop. For unweighted events, the unweighting routine should already take care of this.

The `keep_failed` flag determines whether events which failed cuts are nevertheless produced, to be recorded with zero weight. Alternatively, failed events are dropped, and this fact is recorded by the counter `n_dropped`.

```

(Process mci: process mci entry: TBP)+≡
  procedure :: generate_weighted_event => &
    process_mci_entry_generate_weighted_event
  procedure :: generate_unweighted_event => &
    process_mci_entry_generate_unweighted_event

(Process mci: procedures)+≡
  subroutine process_mci_entry_generate_weighted_event (mci_entry, &
    mci_instance, mci_sampler, keep_failed)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_instance_t), intent(inout) :: mci_instance
    class(mci_sampler_t), intent(inout) :: mci_sampler
    logical, intent(in) :: keep_failed
    logical :: generate_new
    generate_new = .true.
    call mci_instance%reset_n_event_dropped ()
    REJECTION: do while (generate_new)
      call mci_entry%mci%generate_weighted_event (mci_instance, mci_sampler)
      if (signal_is_pending ()) return
      if (.not. mci_sampler%is_valid()) then
        if (keep_failed) then
          generate_new = .false.
        else
          call mci_instance%record_event_dropped ()
          generate_new = .true.
        end if
      else
        generate_new = .false.
      end if
    end do REJECTION
  end subroutine process_mci_entry_generate_weighted_event

  subroutine process_mci_entry_generate_unweighted_event (mci_entry, mci_instance, mci_sampler)
    class(process_mci_entry_t), intent(inout) :: mci_entry
    class(mci_instance_t), intent(inout) :: mci_instance
    class(mci_sampler_t), intent(inout) :: mci_sampler
    call mci_entry%mci%generate_unweighted_event (mci_instance, mci_sampler)
  end subroutine process_mci_entry_generate_unweighted_event

```

Extract results.

```

(Process mci: process mci entry: TBP)+≡
  procedure :: has_integral => process_mci_entry_has_integral
  procedure :: get_integral => process_mci_entry_get_integral
  procedure :: get_error => process_mci_entry_get_error
  procedure :: get_accuracy => process_mci_entry_get_accuracy
  procedure :: get_chi2 => process_mci_entry_get_chi2
  procedure :: get_efficiency => process_mci_entry_get_efficiency

```

```

(Process mci: procedures)+≡
function process_mci_entry_has_integral (mci_entry) result (flag)
  class(process_mci_entry_t), intent(in) :: mci_entry
  logical :: flag
  flag = mci_entry%results%exist ()
end function process_mci_entry_has_integral

function process_mci_entry_get_integral (mci_entry) result (integral)
  class(process_mci_entry_t), intent(in) :: mci_entry
  real(default) :: integral
  integral = mci_entry%results%get_integral ()
end function process_mci_entry_get_integral

function process_mci_entry_get_error (mci_entry) result (error)
  class(process_mci_entry_t), intent(in) :: mci_entry
  real(default) :: error
  error = mci_entry%results%get_error ()
end function process_mci_entry_get_error

function process_mci_entry_get_accuracy (mci_entry) result (accuracy)
  class(process_mci_entry_t), intent(in) :: mci_entry
  real(default) :: accuracy
  accuracy = mci_entry%results%get_accuracy ()
end function process_mci_entry_get_accuracy

function process_mci_entry_get_chi2 (mci_entry) result (chi2)
  class(process_mci_entry_t), intent(in) :: mci_entry
  real(default) :: chi2
  chi2 = mci_entry%results%get_chi2 ()
end function process_mci_entry_get_chi2

function process_mci_entry_get_efficiency (mci_entry) result (efficiency)
  class(process_mci_entry_t), intent(in) :: mci_entry
  real(default) :: efficiency
  efficiency = mci_entry%results%get_efficiency ()
end function process_mci_entry_get_efficiency

```

Return the MCI checksum. This may be the one used for configuration, but may also incorporate results, if they change the state of the integrator (adaptation).

```

(Process mci: process mci entry: TBP)+≡
procedure :: get_md5sum => process_mci_entry_get_md5sum

(Process mci: procedures)+≡
pure function process_mci_entry_get_md5sum (entry) result (md5sum)
  class(process_mci_entry_t), intent(in) :: entry
  character(32) :: md5sum
  md5sum = entry%mci%get_md5sum ()
end function process_mci_entry_get_md5sum

```

30.7.2 MC parameter set and MCI instance

For each process component that is associated with a multi-channel integration (MCI) object, the `mci.work.t` object contains the currently active parameter

set. It also holds the implementation of the `mci_instance_t` that the integrator needs for doing its work.

```

(Process mci: public)+≡
    public :: mci_work_t

(Process mci: types)+≡
    type :: mci_work_t
        type(process_mci_entry_t), pointer :: config => null ()
        real(default), dimension(:), allocatable :: x
        class(mci_instance_t), pointer :: mci => null ()
        type(process_counter_t) :: counter
        logical :: keep_failed_events = .false.
        integer :: n_event_dropped = 0
    contains
        (Process mci: mci work: TBP)
    end type mci_work_t

```

First write configuration data, then the current values.

```

(Process mci: mci work: TBP)≡
    procedure :: write => mci_work_write

(Process mci: procedures)+≡
    subroutine mci_work_write (mci_work, unit, testflag)
        class(mci_work_t), intent(in) :: mci_work
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1x,A,I0,A)") "Active MCI instance #", &
            mci_work%config%i_mci, " ="
        write (u, "(2x)", advance="no")
        do i = 1, mci_work%config%n_par
            write (u, "(1x,F7.5)", advance="no") mci_work%x(i)
            if (i == mci_work%config%n_par_sf) &
                write (u, "(1x,'|')", advance="no")
        end do
        write (u, *)
        if (associated (mci_work%mci)) then
            call mci_work%mci%write (u, pacify = testflag)
            call mci_work%counter%write (u)
        end if
    end subroutine mci_work_write

```

The `mci` component may require finalization.

```

(Process mci: mci work: TBP)+≡
    procedure :: final => mci_work_final

(Process mci: procedures)+≡
    subroutine mci_work_final (mci_work)
        class(mci_work_t), intent(inout) :: mci_work
        if (associated (mci_work%mci)) then
            call mci_work%mci%final ()
            deallocate (mci_work%mci)
        end if
    end subroutine mci_work_final

```

```
end subroutine mci_work_final
```

Initialize with the maximum length that we will need. Contents are not initialized.

The integrator inside the `mci_entry` object is responsible for allocating and initializing its own instance, which is referred to by a pointer in the `mci_work` object.

```
<Process mci: mci work: TBP>+≡
  procedure :: init => mci_work_init

<Process mci: procedures>+≡
  subroutine mci_work_init (mci_work, mci_entry)
    class(mci_work_t), intent(out) :: mci_work
    type(process_mci_entry_t), intent(in), target :: mci_entry
    mci_work%config => mci_entry
    allocate (mci_work%x (mci_entry%n_par))
    if (allocated (mci_entry%mci)) then
      call mci_entry%mci%allocate_instance (mci_work%mci)
      call mci_work%mci%init (mci_entry%mci)
    end if
  end subroutine mci_work_init
```

Set parameters explicitly, either all at once, or separately for the structure-function and process parts.

```
<Process mci: mci work: TBP>+≡
  procedure :: set => mci_work_set
  procedure :: set_x_strfun => mci_work_set_x_strfun
  procedure :: set_x_process => mci_work_set_x_process

<Process mci: procedures>+≡
  subroutine mci_work_set (mci_work, x)
    class(mci_work_t), intent(inout) :: mci_work
    real(default), dimension(:), intent(in) :: x
    mci_work%x = x
  end subroutine mci_work_set

  subroutine mci_work_set_x_strfun (mci_work, x)
    class(mci_work_t), intent(inout) :: mci_work
    real(default), dimension(:), intent(in) :: x
    mci_work%x(1 : mci_work%config%n_par_sf) = x
  end subroutine mci_work_set_x_strfun

  subroutine mci_work_set_x_process (mci_work, x)
    class(mci_work_t), intent(inout) :: mci_work
    real(default), dimension(:), intent(in) :: x
    mci_work%x(mci_work%config%n_par_sf + 1 : mci_work%config%n_par) = x
  end subroutine mci_work_set_x_process
```

Return the array of active components, i.e., those that correspond to the currently selected MC parameter set.

```
<Process mci: mci work: TBP>+≡
  procedure :: get_active_components => mci_work_get_active_components
```

```

(Process mci: procedures)+≡
function mci_work_get_active_components (mci_work) result (i_component)
  class(mci_work_t), intent(in) :: mci_work
  integer, dimension(:), allocatable :: i_component
  allocate (i_component (size (mci_work%config%i_component)))
  i_component = mci_work%config%i_component
end function mci_work_get_active_components

```

Return the active parameters as a simple array with correct length. Do this separately for the structure-function parameters and the process parameters.

```

(Process mci: mci work: TBP)+≡
  procedure :: get_x_strfun => mci_work_get_x_strfun
  procedure :: get_x_process => mci_work_get_x_process

(Process mci: procedures)+≡
  pure function mci_work_get_x_strfun (mci_work) result (x)
    class(mci_work_t), intent(in) :: mci_work
    real(default), dimension(mci_work%config%n_par_sf) :: x
    x = mci_work%x(1 : mci_work%config%n_par_sf)
  end function mci_work_get_x_strfun

  pure function mci_work_get_x_process (mci_work) result (x)
    class(mci_work_t), intent(in) :: mci_work
    real(default), dimension(mci_work%config%n_par_phs) :: x
    x = mci_work%x(mci_work%config%n_par_sf + 1 : mci_work%config%n_par)
  end function mci_work_get_x_process

```

Initialize and finalize event generation for the specified MCI entry. This also resets the counter.

```

(Process mci: mci work: TBP)+≡
  procedure :: init_simulation => mci_work_init_simulation
  procedure :: final_simulation => mci_work_final_simulation

(Process mci: procedures)+≡
  subroutine mci_work_init_simulation (mci_work, safety_factor, keep_failed_events)
    class(mci_work_t), intent(inout) :: mci_work
    real(default), intent(in), optional :: safety_factor
    logical, intent(in), optional :: keep_failed_events
    call mci_work%mci%init_simulation (safety_factor)
    call mci_work%counter%reset ()
    if (present (keep_failed_events)) &
      mci_work%keep_failed_events = keep_failed_events
  end subroutine mci_work_init_simulation

  subroutine mci_work_final_simulation (mci_work)
    class(mci_work_t), intent(inout) :: mci_work
    call mci_work%mci%final_simulation ()
  end subroutine mci_work_final_simulation

```

Counter.

```

(Process mci: mci work: TBP)+≡
  procedure :: reset_counter => mci_work_reset_counter
  procedure :: record_call => mci_work_record_call
  procedure :: get_counter => mci_work_get_counter

```

```

<Process mci: procedures>+=
  subroutine mci_work_reset_counter (mci_work)
    class(mci_work_t), intent(inout) :: mci_work
    call mci_work%counter%reset ()
  end subroutine mci_work_reset_counter

  subroutine mci_work_record_call (mci_work, status)
    class(mci_work_t), intent(inout) :: mci_work
    integer, intent(in) :: status
    call mci_work%counter%record (status)
  end subroutine mci_work_record_call

  pure function mci_work_get_counter (mci_work) result (counter)
    class(mci_work_t), intent(in) :: mci_work
    type(process_counter_t) :: counter
    counter = mci_work%counter
  end function mci_work_get_counter

```

30.8 Process component manager

```

<pcm.f90>=
  <File header>

  module pcm

    <Use kinds>
    <Use strings>
    <Use debug>

    use constants, only: zero, two
    use diagnostics
    use lorentz
    use phs_points, only: assignment(=)
    use io_units, only: free_unit
    use os_interface
    use process_constants, only: process_constants_t
    use physics_defs
    use model_data, only: model_data_t
    use models, only: model_t
    use interactions, only: interaction_t
    use quantum_numbers, only: quantum_numbers_t, quantum_numbers_mask_t
    use flavors, only: flavor_t
    use variables, only: var_list_t
    use nlo_data, only: nlo_settings_t
    use mci_base, only: mci_t
    use phs_base, only: phs_config_t
    use mappings, only: mapping_defaults_t
    use phs_forests, only: phs_parameters_t
    use phs_fks, only: isr_kinematics_t, real_kinematics_t
    use phs_fks, only: phs_identifier_t
    use dispatch_fks, only: dispatch_fks_s
    use fks_regions, only: region_data_t
    use nlo_data, only: fks_template_t

```

```

use phs_fks, only: phs_fks_generator_t
use phs_fks, only: dalitz_plot_t
use phs_fks, only: phs_fks_config_t, get_filtered_resonance_histories
use dispatch_phase_space, only: dispatch_phs
use process_libraries, only: process_component_def_t
use real_subtraction, only: real_subtraction_t, soft_mismatch_t
use real_subtraction, only: FIXED_ORDER_EVENTS, POWHEG
use real_subtraction, only: real_partition_t, powheg_damping_simple_t
use real_subtraction, only: real_partition_fixed_order_t
use virtual, only: virtual_t
use dglap_remnant, only: dglap_remnant_t
use prc_threshold, only: threshold_def_t
use resonances, only: resonance_history_t, resonance_history_set_t
use nlo_data, only: FKS_DEFAULT, FKS_RESONANCES
use blha_config, only: blha_master_t
use blha_olp_interfaces, only: prc_blha_t

use pcm_base
use process_config
use process_mci, only: process_mci_entry_t
use process_mci, only: REAL_SINGULAR, REAL_FINITE

<Standard module head>

<Pcm: public>

<Pcm: types>

contains

<Pcm: procedures>

end module pcm

```

30.8.1 Default process component manager

This is the configuration object which has the duty of allocating the corresponding instance. The default version is trivial.

```

<Pcm: public>≡
    public :: pcm_default_t

<Pcm: types>≡
    type, extends (pcm_t) :: pcm_default_t
    contains
    <Pcm: pcm default: TBP>
    end type pcm_default_t

<Pcm: pcm default: TBP>≡
    procedure :: allocate_workspace => pcm_default_allocate_workspace

<Pcm: procedures>≡
    subroutine pcm_default_allocate_workspace (pcm, work)
    class(pcm_default_t), intent(in) :: pcm
    class(pcm_workspace_t), intent(inout), allocatable :: work

```

```

        allocate (pcm_default_workspace_t :: work)
    end subroutine pcm_default_allocate_workspace

```

Finalizer: apply to core manager.

```

<Pcm: pcm default: TBP>+≡
    procedure :: final => pcm_default_final

<Pcm: procedures>+≡
    subroutine pcm_default_final (pcm)
        class(pcm_default_t), intent(inout) :: pcm
    end subroutine pcm_default_final

```

```

<Pcm: pcm default: TBP>+≡
    procedure :: is_nlo => pcm_default_is_nlo

<Pcm: procedures>+≡
    function pcm_default_is_nlo (pcm) result (is_nlo)
        logical :: is_nlo
        class(pcm_default_t), intent(in) :: pcm
        is_nlo = .false.
    end function pcm_default_is_nlo

```

Initialize configuration data, using environment variables.

```

<Pcm: pcm default: TBP>+≡
    procedure :: init => pcm_default_init

<Pcm: procedures>+≡
    subroutine pcm_default_init (pcm, env, meta)
        class(pcm_default_t), intent(out) :: pcm
        type(process_environment_t), intent(in) :: env
        type(process_metadata_t), intent(in) :: meta
        pcm%has_pdfs = env%has_pdfs ()
        call pcm%set_blha_defaults &
            (env%has_polarized_beams (), env%get_var_list_ptr ())
        pcm%os_data = env%get_os_data ()
    end subroutine pcm_default_init

```

```

<Pcm: types>+≡
    type, extends (pcm_workspace_t) :: pcm_default_workspace_t
    contains
    <Pcm: pcm instance default: TBP>
    end type pcm_default_workspace_t

```

```

<Pcm: pcm instance default: TBP>≡
    procedure :: final => pcm_default_workspace_final

<Pcm: procedures>+≡
    subroutine pcm_default_workspace_final (pcm_work)
        class(pcm_default_workspace_t), intent(inout) :: pcm_work
    end subroutine pcm_default_workspace_final

```

```

<Pcm: pcm instance default: TBP>+≡
    procedure :: is_nlo => pcm_default_workspace_is_nlo

```

```

(Pcm: procedures)+≡
  function pcm_default_workspace_is_nlo (pcm_work) result (is_nlo)
    logical :: is_nlo
    class(pcm_default_workspace_t), intent(inout) :: pcm_work
    is_nlo = .false.
  end function pcm_default_workspace_is_nlo

```

30.8.2 Implementations for the default manager

Categorize components. Nothing to do here, all components are of Born type.

```

(Pcm: pcm default: TBP)+≡
  procedure :: categorize_components => pcm_default_categorize_components

(Pcm: procedures)+≡
  subroutine pcm_default_categorize_components (pcm, config)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_config_data_t), intent(in) :: config
  end subroutine pcm_default_categorize_components

```

Phase-space configuration

Default setup for tree processes: a single phase-space configuration that is valid for all components.

```

(Pcm: pcm default: TBP)+≡
  procedure :: init_phs_config => pcm_default_init_phs_config

(Pcm: procedures)+≡
  subroutine pcm_default_init_phs_config &
    (pcm, phs_entry, meta, env, phs_par, mapping_defs)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_phs_config_t), &
      dimension(:), allocatable, intent(out) :: phs_entry
    type(process_metadata_t), intent(in) :: meta
    type(process_environment_t), intent(in) :: env
    type(mapping_defaults_t), intent(in) :: mapping_defs
    type(phs_parameters_t), intent(in) :: phs_par
    allocate (phs_entry (1))
    allocate (pcm%i_phs_config (pcm%n_components), source=1)
    call dispatch_phs (phs_entry(1)%phs_config, &
      env%get_var_list_ptr (), &
      env%get_os_data (), &
      meta%id, &
      mapping_defs, phs_par)
  end subroutine pcm_default_init_phs_config

```

Core management

The default component manager assigns one core per component. We allocate and configure the core objects, using the process-component configuration data.

```

(Pcm: pcm default: TBP)+≡
  procedure :: allocate_cores => pcm_default_allocate_cores

```

```

(Pcm: procedures)+≡
subroutine pcm_default_allocate_cores (pcm, config, core_entry)
  class(pcm_default_t), intent(inout) :: pcm
  type(process_config_data_t), intent(in) :: config
  type(core_entry_t), dimension(:), allocatable, intent(out) :: core_entry
  type(process_component_def_t), pointer :: component_def
  integer :: i
  allocate (pcm%i_core (pcm%n_components), source = 0)
  pcm%n_cores = pcm%n_components
  allocate (core_entry (pcm%n_cores))
  do i = 1, pcm%n_cores
    pcm%i_core(i) = i
    core_entry(i)%i_component = i
    component_def => config%process_def%get_component_def_ptr (i)
    core_entry(i)%core_def => component_def%get_core_def_ptr ()
    core_entry(i)%active = component_def%can_be_integrated ()
  end do
end subroutine pcm_default_allocate_cores

```

Extra code is required for certain core types (threshold) or if BLHA uses an external OLP (Born only, this case) for getting its matrix elements.

```

(Pcm: pcm default: TBP)+≡
  procedure :: prepare_any_external_code => &
    pcm_default_prepare_any_external_code

(Pcm: procedures)+≡
subroutine pcm_default_prepare_any_external_code &
  (pcm, core_entry, i_core, libname, model, var_list)
  class(pcm_default_t), intent(in) :: pcm
  type(core_entry_t), intent(inout) :: core_entry
  integer, intent(in) :: i_core
  type(string_t), intent(in) :: libname
  type(model_data_t), intent(in), target :: model
  type(var_list_t), intent(in) :: var_list
  if (core_entry%active) then
    associate (core => core_entry%core)
      if (core%needs_external_code ()) then
        call core%prepare_external_code &
          (core%data%flv_state, &
           var_list, pcm%os_data, libname, model, i_core, .false.)
      end if
      call core%set_equivalent_flv_hel_indices ()
    end associate
  end if
end subroutine pcm_default_prepare_any_external_code

```

Allocate and configure the BLHA record for a specific core, assuming that the core type requires it. In the default case, this is a Born configuration.

```

(Pcm: pcm default: TBP)+≡
  procedure :: setup_blha => pcm_default_setup_blha

(Pcm: procedures)+≡
subroutine pcm_default_setup_blha (pcm, core_entry)
  class(pcm_default_t), intent(in) :: pcm

```



```

    type(core_entry_t), intent(inout) :: core_entry
    allocate (core_entry%blha_config, source = pcm%blha_defaults)
    call core_entry%blha_config%set_born ()
end subroutine pcm_default_setup_blha

```

Apply the configuration, using pcm data.

```

(Pcm: pcm default: TBP)+≡
    procedure :: prepare_blha_core => pcm_default_prepare_blha_core

(Pcm: procedures)+≡
    subroutine pcm_default_prepare_blha_core (pcm, core_entry, model)
        class(pcm_default_t), intent(in) :: pcm
        type(core_entry_t), intent(inout) :: core_entry
        class(model_data_t), intent(in), target :: model
        integer :: n_in
        integer :: n_legs
        integer :: n_flv
        integer :: n_hel
        select type (core => core_entry%core)
        class is (prc_blha_t)
            associate (blha_config => core_entry%blha_config)
                n_in = core%data%n_in
                n_legs = core%data%get_n_tot ()
                n_flv = core%data%n_flv
                n_hel = blha_config%get_n_hel (core%data%flv_state (1:n_in,1), model)
                call core%init_blha (blha_config, n_in, n_legs, n_flv, n_hel)
                call core%init_driver (pcm%os_data)
            end associate
        end select
    end subroutine pcm_default_prepare_blha_core

```

Read the method settings from the variable list and store them in the BLHA master. This version: no NLO flag.

```

(Pcm: pcm default: TBP)+≡
    procedure :: set_blha_methods => pcm_default_set_blha_methods

(Pcm: procedures)+≡
    subroutine pcm_default_set_blha_methods (pcm, blha_master, var_list)
        class(pcm_default_t), intent(inout) :: pcm
        type(blha_master_t), intent(inout) :: blha_master
        type(var_list_t), intent(in) :: var_list
        call blha_master%set_methods (.false., var_list)
    end subroutine pcm_default_set_blha_methods

```

Produce the LO and NLO flavor-state tables (as far as available), as appropriate for BLHA configuration.

The default version looks at the first process core only, to get the Born data. (Multiple cores are thus unsupported.) The NLO flavor table is left unallocated.

```

(Pcm: pcm default: TBP)+≡
    procedure :: get_blha_flv_states => pcm_default_get_blha_flv_states

```

```

(Pcm: procedures)+≡
  subroutine pcm_default_get_blha_flv_states &
    (pcm, core_entry, flv_born, flv_real)
    class(pcm_default_t), intent(in) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    integer, dimension(:,:), allocatable, intent(out) :: flv_born
    integer, dimension(:,:), allocatable, intent(out) :: flv_real
    flv_born = core_entry(1)%core%data%flv_state
  end subroutine pcm_default_get_blha_flv_states

```

Allocate and configure the MCI (multi-channel integrator) records. There is one record per active process component. Second procedure: call the MCI dispatcher with default-setup arguments.

```

(Pcm: pcm default: TBP)+≡
  procedure :: setup_mci => pcm_default_setup_mci
  procedure :: call_dispatch_mci => pcm_default_call_dispatch_mci

(Pcm: procedures)+≡
  subroutine pcm_default_setup_mci (pcm, mci_entry)
    class(pcm_default_t), intent(inout) :: pcm
    type(process_mci_entry_t), &
      dimension(:), allocatable, intent(out) :: mci_entry
    class(mci_t), allocatable :: mci_template
    integer :: i, i_mci
    pcm%n_mci = count (pcm%component_active)
    allocate (pcm%i_mci (pcm%n_components), source = 0)
    i_mci = 0
    do i = 1, pcm%n_components
      if (pcm%component_active(i)) then
        i_mci = i_mci + 1
        pcm%i_mci(i) = i_mci
      end if
    end do
    allocate (mci_entry (pcm%n_mci))
  end subroutine pcm_default_setup_mci

  subroutine pcm_default_call_dispatch_mci (pcm, &
    dispatch_mci, var_list, process_id, mci_template)
    class(pcm_default_t), intent(inout) :: pcm
    procedure(dispatch_mci_proc) :: dispatch_mci
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_id
    class(mci_t), allocatable, intent(out) :: mci_template
    call dispatch_mci (mci_template, var_list, process_id)
  end subroutine pcm_default_call_dispatch_mci

```

Nothing left to do for the default algorithm.

```

(Pcm: pcm default: TBP)+≡
  procedure :: complete_setup => pcm_default_complete_setup

(Pcm: procedures)+≡
  subroutine pcm_default_complete_setup (pcm, core_entry, component, model)
    class(pcm_default_t), intent(inout) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry

```

```

        type(process_component_t), dimension(:), intent(inout) :: component
        type(model_t), intent(in), target :: model
    end subroutine pcm_default_complete_setup

```

Component management

Initialize a single component. We require all process-configuration blocks, and specific templates for the phase-space and integrator configuration.

We also provide the current component index `i` and the `active` flag.

In the default mode, all components are marked as master components.

```

<Pcm: pcm default: TBP>+≡
    procedure :: init_component => pcm_default_init_component

<Pcm: procedures>+≡
    subroutine pcm_default_init_component &
        (pcm, component, i, active, &
         phs_config, env, meta, config)
        class(pcm_default_t), intent(in) :: pcm
        type(process_component_t), intent(out) :: component
        integer, intent(in) :: i
        logical, intent(in) :: active
        class(phs_config_t), allocatable, intent(in) :: phs_config
        type(process_environment_t), intent(in) :: env
        type(process_metadata_t), intent(in) :: meta
        type(process_config_data_t), intent(in) :: config
        call component%init (i, &
                             env, meta, config, &
                             active, &
                             phs_config)
        component%component_type = COMP_MASTER
    end subroutine pcm_default_init_component

```

30.8.3 NLO process component manager

The NLO-aware version of the process-component manager.

This is the configuration object, which has the duty of allocating the corresponding instance. This is the nontrivial NLO version.

```

<Pcm: public>+≡
    public :: pcm_nlo_t

<Pcm: types>+≡
    type, extends (pcm_t) :: pcm_nlo_t
        type(string_t) :: id
        logical :: combined_integration = .false.
        logical :: vis_fks_regions = .false.
        integer, dimension(:), allocatable :: nlo_type
        integer, dimension(:), allocatable :: nlo_type_core
        integer, dimension(:), allocatable :: component_type
        integer :: i_born = 0
        integer :: i_real = 0
        integer :: i_sub = 0

```

```

    type(nlo_settings_t) :: settings
    type(region_data_t) :: region_data
    logical :: use_real_partition = .false.
    logical :: use_real_singular = .false.
    real(default) :: real_partition_scale = 0
    class(real_partition_t), allocatable :: real_partition
    type(dalitz_plot_t) :: dalitz_plot
    type(quantum_numbers_t), dimension(:,,:), allocatable :: qn_real, qn_born
contains
  <Pcm: pcm nlo: TBP>
end type pcm_nlo_t

```

Initialize configuration data, using environment variables.

```

  <Pcm: pcm nlo: TBP>≡
    procedure :: init => pcm_nlo_init

  <Pcm: procedures>+≡
    subroutine pcm_nlo_init (pcm, env, meta)
      class(pcm_nlo_t), intent(out) :: pcm
      type(process_metadata_t), intent(in) :: meta
      type(process_environment_t), intent(in) :: env
      type(var_list_t), pointer :: var_list
      type(fks_template_t) :: fks_template
      pcm%id = meta%id
      pcm%has_pdfs = env%has_pdfs ()
      var_list => env%get_var_list_ptr ()
      call dispatch_fks_s (fks_template, var_list)
      call pcm%settings%init (var_list, fks_template)
      pcm%combined_integration = &
        var_list%get_lval (var_str ('?combined_nlo_integration'))
      select case (char (var_list%get_sval (var_str ("real_partition_mode"))))
      case ("default", "off")
        pcm%use_real_partition = .false.
        pcm%use_real_singular = .false.
      case ("all", "on", "singular")
        pcm%use_real_partition = .true.
        pcm%use_real_singular = .true.
      case ("finite")
        pcm%use_real_partition = .true.
        pcm%use_real_singular = .false.
      case default
        call msg_fatal ("The real partition mode can only be " // &
          "default, off, all, on, singular or finite.")
      end select
      pcm%real_partition_scale = &
        var_list%get_rval (var_str ("real_partition_scale"))
      pcm%vis_fks_regions = &
        var_list%get_lval (var_str ("?vis_fks_regions"))
      call pcm%set_blha_defaults &
        (env%has_polarized_beams (), env%get_var_list_ptr ())
      pcm%os_data = env%get_os_data ()
    end subroutine pcm_nlo_init

```

Init/rewrite NLO settings without the FKS template.

```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: init_nlo_settings => pcm_nlo_init_nlo_settings

(Pcm: procedures)+≡
  subroutine pcm_nlo_init_nlo_settings (pcm, var_list)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(var_list_t), intent(in), target :: var_list
    call pcm%settings%init (var_list)
  end subroutine pcm_nlo_init_nlo_settings

```

As appropriate for the NLO/FKS algorithm, the category defined by the process, is called `nlo_type`. We refine this by setting the component category `component_type` separately.

The component types `COMP_MISMATCH`, `COMP_PDF`, `COMP_SUB` are set only if the algorithm uses combined integration. Otherwise, they are set to `COMP_DEFAULT`.

The component type `COMP_REAL` is further distinguished between `COMP_REAL_SING` or `COMP_REAL_FIN`, if the algorithm uses real partitions. The former acts as a reference component for the latter, and we always assume that it is the first real component.

Each component is assigned its own core. Exceptions: the finite-real component gets the same core as the singular-real component. The mismatch component gets the same core as the subtraction component.

TODO wk 2018: this convention for real components can be improved. Check whether all component types should be assigned, not just for combined integration.

```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: categorize_components => pcm_nlo_categorize_components

(Pcm: procedures)+≡
  subroutine pcm_nlo_categorize_components (pcm, config)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(process_config_data_t), intent(in) :: config
    type(process_component_def_t), pointer :: component_def
    integer :: i
    allocate (pcm%nlo_type (pcm%n_components), source = COMPONENT_UNDEFINED)
    allocate (pcm%component_type (pcm%n_components), source = COMP_DEFAULT)
    do i = 1, pcm%n_components
      component_def => config%process_def%get_component_def_ptr (i)
      pcm%nlo_type(i) = component_def%get_nlo_type ()
      if (pcm%combined_integration) then
        select case (pcm%nlo_type(i))
          case (BORN)
            pcm%i_born = i
            pcm%component_type(i) = COMP_MASTER
          case (NLO_REAL)
            pcm%component_type(i) = COMP_REAL
          case (NLO_VIRTUAL)
            pcm%component_type(i) = COMP_VIRT
          case (NLO_MISMATCH)
            pcm%component_type(i) = COMP_MISMATCH
          case (NLO_DGLAP)
            pcm%component_type(i) = COMP_PDF
        end select
      end if
    end do
  end subroutine pcm_nlo_categorize_components

```

```

        case (NLO_SUBTRACTION)
            pcm%component_type(i) = COMP_SUB
            pcm%i_sub = i
        end select
    else
        select case (pcm%nlo_type(i))
        case (BORN)
            pcm%i_born = i
            pcm%component_type(i) = COMP_MASTER
        case (NLO_REAL)
            pcm%component_type(i) = COMP_REAL
        case (NLO_VIRTUAL)
            pcm%component_type(i) = COMP_VIRT
        case (NLO_MISMATCH)
            pcm%component_type(i) = COMP_MISMATCH
        case (NLO_SUBTRACTION)
            pcm%i_sub = i
        end select
    end if
end do
call refine_real_type ( &
    pack ([i, i=1, pcm%n_components]), &
    pcm%component_type==COMP_REAL))
contains
subroutine refine_real_type (i_real)
    integer, dimension(:), intent(in) :: i_real
    pcm%i_real = i_real(1)
    if (pcm%use_real_partition) then
        pcm%component_type (i_real(1)) = COMP_REAL_SING
        pcm%component_type (i_real(2:)) = COMP_REAL_FIN
    end if
end subroutine refine_real_type
end subroutine pcm_nlo_categorize_components

```

Phase-space initial configuration

Setup for the NLO/PHS processes: two phase-space configurations, (1) Born/wood, (2) real correction/FKS. All components use either one of these two configurations.

TODO wk 2018: The `first_real_component` identifier is really ugly. Nothing should rely on the ordering.

```

(Pcm: pcm nlo: TBP)+≡
    procedure :: init_phs_config => pcm_nlo_init_phs_config
(Pcm: procedures)+≡
    subroutine pcm_nlo_init_phs_config &
        (pcm, phs_entry, meta, env, phs_par, mapping_defs)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(process_phs_config_t), &
            dimension(:), allocatable, intent(out) :: phs_entry
        type(process_metadata_t), intent(in) :: meta
        type(process_environment_t), intent(in) :: env
        type(mapping_defaults_t), intent(in) :: mapping_defs
    end subroutine

```

```

type(phs_parameters_t), intent(in) :: phs_par
integer :: i
logical :: first_real_component
allocate (phs_entry (2))
call dispatch_phs (phs_entry(1)%phs_config, &
    env%get_var_list_ptr (), &
    env%get_os_data (), &
    meta%id, &
    mapping_defs, phs_par, &
    var_str ("wood"))
call dispatch_phs (phs_entry(2)%phs_config, &
    env%get_var_list_ptr (), &
    env%get_os_data (), &
    meta%id, &
    mapping_defs, phs_par, &
    var_str ("fks"))
allocate (pcm%i_phs_config (pcm%n_components), source=0)
first_real_component = .true.
do i = 1, pcm%n_components
    select case (pcm%nlo_type(i))
    case (BORN, NLO_VIRTUAL, NLO_SUBTRACTION)
        pcm%i_phs_config(i) = 1
    case (NLO_REAL)
        if (pcm%use_real_partition) then
            if (pcm%use_real_singular) then
                if (first_real_component) then
                    pcm%i_phs_config(i) = 2
                    first_real_component = .false.
                else
                    pcm%i_phs_config(i) = 1
                end if
            else
                pcm%i_phs_config(i) = 1
            end if
        else
            pcm%i_phs_config(i) = 1
        end if
    case (NLO_MISMATCH, NLO_DGLAP, GKS)
        pcm%i_phs_config(i) = 2
    end select
end do
end subroutine pcm_nlo_init_phs_config

```

Core management

Allocate the core (matrix-element interface) objects that we will need for evaluation. Every component gets an associated core, except for the real-finite and mismatch components (if any). Those components are associated with their previous corresponding real-singular and subtraction cores, respectively.

After cores are allocated, configure the region-data block that is maintained by the NLO process-component manager.

$\langle Pcm: pcm\ nlo: TBP \rangle + \equiv$

```

procedure :: allocate_cores => pcm_nlo_allocate_cores
<Pcm: procedures>+≡
subroutine pcm_nlo_allocate_cores (pcm, config, core_entry)
  class(pcm_nlo_t), intent(inout) :: pcm
  type(process_config_data_t), intent(in) :: config
  type(core_entry_t), dimension(:), allocatable, intent(out) :: core_entry
  type(process_component_def_t), pointer :: component_def
  integer :: i, i_core
  allocate (pcm%i_core (pcm%n_components), source = 0)
  pcm%n_cores = pcm%n_components &
    - count (pcm%component_type(:) == COMP_REAL_FIN) &
    - count (pcm%component_type(:) == COMP_MISMATCH)
  allocate (core_entry (pcm%n_cores))
  allocate (pcm%nlo_type_core (pcm%n_cores), source = BORN)
  i_core = 0
  do i = 1, pcm%n_components
    select case (pcm%component_type(i))
    case default
      i_core = i_core + 1
      pcm%i_core(i) = i_core
      pcm%nlo_type_core(i_core) = pcm%nlo_type(i)
      core_entry(i_core)%i_component = i
      component_def => config%process_def%get_component_def_ptr (i)
      core_entry(i_core)%core_def => component_def%get_core_def_ptr ()
      select case (pcm%nlo_type(i))
      case default
        core_entry(i)%active = component_def%can_be_integrated ()
      case (NLO_REAL, NLO_SUBTRACTION)
        core_entry(i)%active = .true.
      end select
    case (COMP_REAL_FIN)
      pcm%i_core(i) = pcm%i_core(pcm%i_real)
    case (COMP_MISMATCH)
      pcm%i_core(i) = pcm%i_core(pcm%i_sub)
    end select
  end do
end subroutine pcm_nlo_allocate_cores

```

Extra code is required for certain core types (threshold) or if BLHA uses an external OLP for getting its matrix elements. OMega matrix elements, by definition, do not need extra code. NLO-virtual or subtraction matrix elements always need extra code.

More precisely: for the Born and virtual matrix element, the extra code is accessed only if the component is active. The radiation (real) and the subtraction corrections (singular and finite), extra code is accessed in any case.

The flavor state is taken from the `region_data` table in the `pcm` record. We use the Born and real flavor-state tables as appropriate.

```

<Pcm: pcm nlo: TBP>+≡
  procedure :: prepare_any_external_code => &
    pcm_nlo_prepare_any_external_code
<Pcm: procedures>+≡
  subroutine pcm_nlo_prepare_any_external_code &

```



```

      (pcm, core_entry, i_core, libname, model, var_list)
class(pcm_nlo_t), intent(in) :: pcm
type(core_entry_t), intent(inout) :: core_entry
integer, intent(in) :: i_core
type(string_t), intent(in) :: libname
type(model_data_t), intent(in), target :: model
type(var_list_t), intent(in) :: var_list
integer, dimension(:, :), allocatable :: flv_born, flv_real
integer :: i
call pcm%region_data%get_all_flv_states (flv_born, flv_real)
if (core_entry%active) then
  associate (core => core_entry%core)
    if (core%needs_external_code ()) then
      select case (pcm%nlo_type (core_entry%i_component))
      case default
        call core%data%set_flv_state (flv_born)
      case (NLO_REAL)
        call core%data%set_flv_state (flv_real)
      end select
      call core%prepare_external_code &
        (core%data%flv_state, &
          var_list, pcm%os_data, libname, model, i_core, .true.)
    end if
    call core%set_equivalent_flv_hel_indices ()
  end associate
end if
end subroutine pcm_nlo_prepare_any_external_code

```

Allocate and configure the BLHA record for a specific core, assuming that the core type requires it. The configuration depends on the NLO type of the core.

(Pcm: pcm_nlo: TBP)+≡

```

  procedure :: setup_blha => pcm_nlo_setup_blha

```

(Pcm: procedures)+≡

```

subroutine pcm_nlo_setup_blha (pcm, core_entry)
  class(pcm_nlo_t), intent(in) :: pcm
  type(core_entry_t), intent(inout) :: core_entry
  allocate (core_entry%blha_config, source = pcm%blha_defaults)
  select case (pcm%nlo_type(core_entry%i_component))
  case (BORN)
    call core_entry%blha_config%set_born ()
  case (NLO_REAL)
    call core_entry%blha_config%set_real_trees ()
  case (NLO_VIRTUAL)
    call core_entry%blha_config%set_loop ()
  case (NLO_SUBTRACTION)
    call core_entry%blha_config%set_subtraction ()
    call core_entry%blha_config%set_internal_color_correlations ()
  case (NLO_DGLAP)
    call core_entry%blha_config%set_dglap ()
  end select
end subroutine pcm_nlo_setup_blha

```

After phase-space configuration data and core entries are available, we fill tables and compute the remaining NLO data that will steer the integration and subtraction algorithm.

There are three parts: recognize a threshold-type process core (if it exists), prepare the region-data tables (always), and prepare for real partitioning (if requested).

The real-component phase space acts as the source for resonance-history information, required for the region data.

```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: complete_setup => pcm_nlo_complete_setup

(Pcm: procedures)+≡
  subroutine pcm_nlo_complete_setup (pcm, core_entry, component, model)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    type(process_component_t), dimension(:), intent(inout) :: component
    type(model_t), intent(in), target :: model
    integer :: alpha_power, alphas_power
    call pcm%handle_threshold_core (core_entry)
    call component(1)%config%get_coupling_powers (alpha_power, alphas_power)
    call pcm%setup_region_data &
      (core_entry, component(pcm%i_real)%phs_config, model, alpha_power, alphas_power)
    call pcm%setup_real_partition ()
  end subroutine pcm_nlo_complete_setup

```

Apply the BLHA configuration to a core object, using the region data from pcm for determining the particle content.

```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: prepare_blha_core => pcm_nlo_prepare_blha_core

(Pcm: procedures)+≡
  subroutine pcm_nlo_prepare_blha_core (pcm, core_entry, model)
    class(pcm_nlo_t), intent(in) :: pcm
    type(core_entry_t), intent(inout) :: core_entry
    class(model_data_t), intent(in), target :: model
    integer :: n_in
    integer :: n_legs
    integer :: n_flv
    integer :: n_hel
    select type (core => core_entry%core)
    class is (prc_blha_t)
      associate (blha_config => core_entry%blha_config)
        n_in = core%data%n_in
        select case (pcm%nlo_type(core_entry%i_component))
        case (NLO_REAL)
          n_legs = pcm%region_data%get_n_legs_real ()
          n_flv = pcm%region_data%get_n_flv_real ()
        case default
          n_legs = pcm%region_data%get_n_legs_born ()
          n_flv = pcm%region_data%get_n_flv_born ()
        end select
        n_hel = blha_config%get_n_hel (core%data%flv_state (1:n_in,1), model)
        call core%init_blha (blha_config, n_in, n_legs, n_flv, n_hel)
        call core%init_driver (pcm%os_data)
      end associate
    end select
  end subroutine pcm_nlo_prepare_blha_core

```

```

        end associate
    end select
end subroutine pcm_nlo_prepare_blha_core

```

Read the method settings from the variable list and store them in the BLHA master. This version: NLO flag set.

```

<Pcm: pcm_nlo: TBP>+≡
    procedure :: set_blha_methods => pcm_nlo_set_blha_methods

<Pcm: procedures>+≡
    subroutine pcm_nlo_set_blha_methods (pcm, blha_master, var_list)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(blha_master_t), intent(inout) :: blha_master
        type(var_list_t), intent(in) :: var_list
        call blha_master%set_methods (.true., var_list)
        call pcm%blha_defaults%set_loop_method (blha_master)
    end subroutine pcm_nlo_set_blha_methods

```

Produce the LO and NLO flavor-state tables (as far as available), as appropriate for BLHA configuration.

The NLO version copies the tables from the region data inside pcm. The core array is not needed.

```

<Pcm: pcm_nlo: TBP>+≡
    procedure :: get_blha_flv_states => pcm_nlo_get_blha_flv_states

<Pcm: procedures>+≡
    subroutine pcm_nlo_get_blha_flv_states &
        (pcm, core_entry, flv_born, flv_real)
        class(pcm_nlo_t), intent(in) :: pcm
        type(core_entry_t), dimension(:), intent(in) :: core_entry
        integer, dimension(:,:), allocatable, intent(out) :: flv_born
        integer, dimension(:,:), allocatable, intent(out) :: flv_real
        call pcm%region_data%get_all_flv_states (flv_born, flv_real)
    end subroutine pcm_nlo_get_blha_flv_states

```

Allocate and configure the MCI (multi-channel integrator) records. The relation depends on the `combined_integration` setting. If we integrate components separately, each component gets its own record, except for the subtraction component. If we do the combination, there is one record for the master (Born) component and a second one for the real-finite component, if present.

Each entry acquires some NLO-specific initialization. Generic configuration follows later.

Second procedure: call the MCI dispatcher with NLO-setup arguments.

```

<Pcm: pcm_nlo: TBP>+≡
    procedure :: setup_mci => pcm_nlo_setup_mci
    procedure :: call_dispatch_mci => pcm_nlo_call_dispatch_mci

<Pcm: procedures>+≡
    subroutine pcm_nlo_setup_mci (pcm, mci_entry)
        class(pcm_nlo_t), intent(inout) :: pcm
        type(process_mci_entry_t), &
            dimension(:), allocatable, intent(out) :: mci_entry

```

```

class(mci_t), allocatable :: mci_template
integer :: i, i_mci
if (pcm%combined_integration) then
  pcm%n_mci = 1 &
    + count (pcm%component_active(:) &
      & .and. pcm%component_type(:) == COMP_REAL_FIN)
  allocate (pcm%i_mci (pcm%n_components), source = 0)
  do i = 1, pcm%n_components
    if (pcm%component_active(i)) then
      select case (pcm%component_type(i))
      case (COMP_MASTER)
        pcm%i_mci(i) = 1
      case (COMP_REAL_FIN)
        pcm%i_mci(i) = 2
      end select
    end if
  end do
else
  pcm%n_mci = count (pcm%component_active(:) &
    & .and. pcm%nlo_type(:) /= NLO_SUBTRACTION)
  allocate (pcm%i_mci (pcm%n_components), source = 0)
  i_mci = 0
  do i = 1, pcm%n_components
    if (pcm%component_active(i)) then
      select case (pcm%nlo_type(i))
      case default
        i_mci = i_mci + 1
        pcm%i_mci(i) = i_mci
      case (NLO_SUBTRACTION)
      end select
    end if
  end do
end if
allocate (mci_entry (pcm%n_mci))
mci_entry(:)%combined_integration = pcm%combined_integration
if (pcm%use_real_partition) then
  do i = 1, pcm%n_components
    i_mci = pcm%i_mci(i)
    if (i_mci > 0) then
      select case (pcm%component_type(i))
      case (COMP_REAL_FIN)
        mci_entry(i_mci)%real_partition_type = REAL_FINITE
      case default
        mci_entry(i_mci)%real_partition_type = REAL_SINGULAR
      end select
    end if
  end do
end if
end subroutine pcm_nlo_setup_mci

subroutine pcm_nlo_call_dispatch_mci (pcm, &
  dispatch_mci, var_list, process_id, mci_template)
class(pcm_nlo_t), intent(inout) :: pcm
procedure(dispatch_mci_proc) :: dispatch_mci

```

```

type(var_list_t), intent(in) :: var_list
type(string_t), intent(in) :: process_id
class(mci_t), allocatable, intent(out) :: mci_template
call dispatch_mci (mci_template, var_list, process_id, is_nlo = .true.)
end subroutine pcm_nlo_call_dispatch_mci

```

Check for a threshold core and adjust the configuration accordingly, before singular region data are considered.

```

<Pcm: pcm_nlo: TBP>+≡
  procedure :: handle_threshold_core => pcm_nlo_handle_threshold_core

<Pcm: procedures>+≡
  subroutine pcm_nlo_handle_threshold_core (pcm, core_entry)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    integer :: i
    do i = 1, size (core_entry)
      select type (core => core_entry(i)%core_def)
        type is (threshold_def_t)
          pcm%settings%factorization_mode = FACTORIZATION_THRESHOLD
          return
        end select
      end do
    end subroutine pcm_nlo_handle_threshold_core

```

Configure the singular-region tables based on the process data for the Born and Real (singular) cores, using also the appropriate FKS phase-space configuration object.

In passing, we may create a table of resonance histories that are relevant for the singular-region configuration.

TODO wk 2018: check whether `phs_entry` needs to be `intent(inout)`.

```

<Pcm: pcm_nlo: TBP>+≡
  procedure :: setup_region_data => pcm_nlo_setup_region_data

<Pcm: procedures>+≡
  subroutine pcm_nlo_setup_region_data &
    (pcm, core_entry, phs_config, model, alpha_power, alphas_power)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(core_entry_t), dimension(:), intent(in) :: core_entry
    class(phs_config_t), intent(inout) :: phs_config
    type(model_t), intent(in), target :: model
    type(process_constants_t) :: data_born, data_real
    integer, dimension (:,:), allocatable :: flavor_born, flavor_real
    type(resonance_history_t), dimension(:), allocatable :: resonance_histories
    type(var_list_t), pointer :: var_list
    integer, intent(in) :: alpha_power, alphas_power
    logical :: success
    data_born = core_entry(pcm%i_core(pcm%i_born))%core%data
    data_real = core_entry(pcm%i_core(pcm%i_real))%core%data
    call data_born%get_flv_state (flavor_born)
    call data_real%get_flv_state (flavor_real)
    call pcm%region_data%init &
      (data_born%n_in, model, flavor_born, flavor_real, &

```

```

        pcm%settings%nlo_correction_type, alpha_power, alphas_power)
associate (template => pcm%settings%fks_template)
    if (template%mapping_type == FKS_RESONANCES) then
        select type (phs_config)
        type is (phs_fks_config_t)
            call get_filtered_resonance_histories (phs_config, &
                data_born%n_in, flavor_born, model, &
                template%excluded_resonances, &
                resonance_histories, success)
        end select
        if (.not. success) template%mapping_type = FKS_DEFAULT
    end if
    call pcm%region_data%setup_fks_mappings (template, data_born%n_in)
!!! Check again, mapping_type might have changed
    if (template%mapping_type == FKS_RESONANCES) then
        call pcm%region_data%set_resonance_mappings (resonance_histories)
        call pcm%region_data%init_resonance_information ()
        pcm%settings%use_resonance_mappings = .true.
    end if
end associate
if (pcm%settings%factorization_mode == FACTORIZATION_THRESHOLD) then
    call pcm%region_data%set_isr_pseudo_regions ()
    call pcm%region_data%split_up_interference_regions_for_threshold ()
end if
call pcm%region_data%compute_number_of_phase_spaces ()
call pcm%region_data%set_i_phs_to_i_con ()
call pcm%region_data%write_to_file &
    (pcm%id, pcm%vis_fks_regions, pcm%os_data)
if (debug_active (D_SUBTRACTION)) &
    call pcm%region_data%check_consistency (.true.)
end subroutine pcm_nlo_setup_region_data

```

After region data are set up, we allocate and configure the `real_partition` objects, if requested.

```

(Pcm: pcm_nlo: TBP)+≡
    procedure :: setup_real_partition => pcm_nlo_setup_real_partition
(Pcm: procedures)+≡
    subroutine pcm_nlo_setup_real_partition (pcm)
        class(pcm_nlo_t), intent(inout) :: pcm
        if (pcm%use_real_partition) then
            if (.not. allocated (pcm%real_partition)) then
                allocate (real_partition_fixed_order_t :: pcm%real_partition)
                select type (partition => pcm%real_partition)
                type is (real_partition_fixed_order_t)
                    call pcm%region_data%get_all_ftuples (partition%fks_pairs)
                    partition%scale = pcm%real_partition_scale
                end select
            end if
        end if
    end subroutine pcm_nlo_setup_real_partition

```

Initialize a single component. We require all process-configuration blocks, and specific templates for the phase-space and integrator configuration.

We also provide the current component index `i` and the `active` flag. For a subtraction component, the `active` flag is overridden.

In the `nlo` mode, the component types have been determined before.

TODO wk 2018: the component type need not be stored in the component; we may remove this when everything is controlled by `pcm`.

```

(Pcm: pcm nlo: TBP)+≡
  procedure :: init_component => pcm_nlo_init_component

(Pcm: procedures)+≡
  subroutine pcm_nlo_init_component &
    (pcm, component, i, active, &
     phs_config, env, meta, config)
    class(pcm_nlo_t), intent(in) :: pcm
    type(process_component_t), intent(out) :: component
    integer, intent(in) :: i
    logical, intent(in) :: active
    class(phs_config_t), allocatable, intent(in) :: phs_config
    type(process_environment_t), intent(in) :: env
    type(process_metadata_t), intent(in) :: meta
    type(process_config_data_t), intent(in) :: config
    logical :: activate
    select case (pcm%nlo_type(i))
    case default;          activate = active
    case (NLO_SUBTRACTION); activate = .false.
    end select
    call component%init (i, &
                        env, meta, config, &
                        activate, &
                        phs_config)
    component%component_type = pcm%component_type(i)
  end subroutine pcm_nlo_init_component

```

Override the base method: record the active components in the PCM object, and report inactive components (except for the subtraction component).

```

(Pcm: pcm nlo: TBP)+≡
  procedure :: record_inactive_components => pcm_nlo_record_inactive_components

(Pcm: procedures)+≡
  subroutine pcm_nlo_record_inactive_components (pcm, component, meta)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(process_component_t), dimension(:), intent(in) :: component
    type(process_metadata_t), intent(inout) :: meta
    integer :: i
    pcm%component_active = component%active
    do i = 1, pcm%n_components
      select case (pcm%nlo_type(i))
      case (NLO_SUBTRACTION)
      case default
        if (.not. component(i)%active) call meta%deactivate_component (i)
      end select
    end do
  end subroutine pcm_nlo_record_inactive_components

```

```

(Pcm: pcm_nlo: TBP)+≡
    procedure :: core_is_radiation => pcm_nlo_core_is_radiation
(Pcm: procedures)+≡
    function pcm_nlo_core_is_radiation (pcm, i_core) result (is_rad)
        logical :: is_rad
        class(pcm_nlo_t), intent(in) :: pcm
        integer, intent(in) :: i_core
        is_rad = pcm%nlo_type(i_core) == NLO_REAL ! .and. .not. pcm%cm%sub(i_core)
    end function pcm_nlo_core_is_radiation

(Pcm: pcm_nlo: TBP)+≡
    procedure :: get_n_flv_born => pcm_nlo_get_n_flv_born
(Pcm: procedures)+≡
    function pcm_nlo_get_n_flv_born (pcm_nlo) result (n_flv)
        integer :: n_flv
        class(pcm_nlo_t), intent(in) :: pcm_nlo
        n_flv = pcm_nlo%region_data%n_flv_born
    end function pcm_nlo_get_n_flv_born

(Pcm: pcm_nlo: TBP)+≡
    procedure :: get_n_flv_real => pcm_nlo_get_n_flv_real
(Pcm: procedures)+≡
    function pcm_nlo_get_n_flv_real (pcm_nlo) result (n_flv)
        integer :: n_flv
        class(pcm_nlo_t), intent(in) :: pcm_nlo
        n_flv = pcm_nlo%region_data%n_flv_real
    end function pcm_nlo_get_n_flv_real

(Pcm: pcm_nlo: TBP)+≡
    procedure :: get_n_alr => pcm_nlo_get_n_alr
(Pcm: procedures)+≡
    function pcm_nlo_get_n_alr (pcm) result (n_alr)
        integer :: n_alr
        class(pcm_nlo_t), intent(in) :: pcm
        n_alr = pcm%region_data%n_regions
    end function pcm_nlo_get_n_alr

(Pcm: pcm_nlo: TBP)+≡
    procedure :: get_flv_states => pcm_nlo_get_flv_states
(Pcm: procedures)+≡
    function pcm_nlo_get_flv_states (pcm, born) result (flv)
        integer, dimension(:,:), allocatable :: flv
        class(pcm_nlo_t), intent(in) :: pcm
        logical, intent(in) :: born
        if (born) then
            flv = pcm%region_data%get_flv_states_born ()
        else
            flv = pcm%region_data%get_flv_states_real ()
        end if
    end function pcm_nlo_get_flv_states

```



```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: get_qn => pcm_nlo_get_qn

(Pcm: procedures)+≡
  function pcm_nlo_get_qn (pcm, born) result (qn)
    type(quantum_numbers_t), dimension(:,:), allocatable :: qn
    class(pcm_nlo_t), intent(in) :: pcm
    logical, intent(in) :: born
    if (born) then
      qn = pcm%qn_born
    else
      qn = pcm%qn_real
    end if
  end function pcm_nlo_get_qn

```

Check if there are massive emitters. Since the mass-structure of all underlying Born configurations have to be the same (**This does not have to be the case when different components are generated at LO**) , we just use the first one to determine this.

```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: has_massive_emitter => pcm_nlo_has_massive_emitter

(Pcm: procedures)+≡
  function pcm_nlo_has_massive_emitter (pcm) result (val)
    logical :: val
    class(pcm_nlo_t), intent(in) :: pcm
    integer :: i
    val = .false.
    associate (reg_data => pcm%region_data)
      do i = reg_data%n_in + 1, reg_data%n_legs_born
        if (any (i == reg_data%emitters)) &
          val = val .or. reg_data%flv_born(1)%massive(i)
      end do
    end associate
  end function pcm_nlo_has_massive_emitter

```

Returns an array which specifies if the particle at position *i* is massive.

```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: get_mass_info => pcm_nlo_get_mass_info

(Pcm: procedures)+≡
  function pcm_nlo_get_mass_info (pcm, i_flv) result (massive)
    class(pcm_nlo_t), intent(in) :: pcm
    integer, intent(in) :: i_flv
    logical, dimension(:), allocatable :: massive
    allocate (massive (size (pcm%region_data%flv_born(i_flv)%massive)))
    massive = pcm%region_data%flv_born(i_flv)%massive
  end function pcm_nlo_get_mass_info

```

```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: allocate_workspace => pcm_nlo_allocate_workspace

```

```

(Pcm: procedures)+≡
subroutine pcm_nlo_allocate_workspace (pcm, work)
  class(pcm_nlo_t), intent(in) :: pcm
  class(pcm_workspace_t), intent(inout), allocatable :: work
  allocate (pcm_nlo_workspace_t :: work)
end subroutine pcm_nlo_allocate_workspace

(Pcm: pcm nlo: TBP)+≡
procedure :: init_qn => pcm_nlo_init_qn

(Pcm: procedures)+≡
subroutine pcm_nlo_init_qn (pcm, model)
  class(pcm_nlo_t), intent(inout) :: pcm
  class(model_data_t), intent(in) :: model
  integer, dimension(:,:), allocatable :: flv_states
  type(flavor_t), dimension(:), allocatable :: flv
  integer :: i
  type(quantum_numbers_t), dimension(:), allocatable :: qn
  allocate (flv_states (pcm%region_data%n_legs_born, pcm%region_data%n_flv_born))
  flv_states = pcm%get_flv_states (.true.)
  allocate (pcm%qn_born (size (flv_states, dim = 1), size (flv_states, dim = 2)))
  allocate (flv (size (flv_states, dim = 1)))
  allocate (qn (size (flv_states, dim = 1)))
  do i = 1, pcm%get_n_flv_born ()
    call flv%init (flv_states (:,i), model)
    call qn%init (flv)
    pcm%qn_born(:,i) = qn
  end do
  deallocate (flv); deallocate (qn)
  deallocate (flv_states)
  allocate (flv_states (pcm%region_data%n_legs_real, pcm%region_data%n_flv_real))
  flv_states = pcm%get_flv_states (.false.)
  allocate (pcm%qn_real (size (flv_states, dim = 1), size (flv_states, dim = 2)))
  allocate (flv (size (flv_states, dim = 1)))
  allocate (qn (size (flv_states, dim = 1)))
  do i = 1, pcm%get_n_flv_real ()
    call flv%init (flv_states (:,i), model)
    call qn%init (flv)
    pcm%qn_real(:,i) = qn
  end do
end subroutine pcm_nlo_init_qn

(Pcm: pcm nlo: TBP)+≡
procedure :: allocate_ps_matching => pcm_nlo_allocate_ps_matching

(Pcm: procedures)+≡
subroutine pcm_nlo_allocate_ps_matching (pcm)
  class(pcm_nlo_t), intent(inout) :: pcm
  if (.not. allocated (pcm%real_partition)) then
    allocate (powheg_damping_simple_t :: pcm%real_partition)
  end if
end subroutine pcm_nlo_allocate_ps_matching

```

```

(Pcm: pcm_nlo: TBP)+≡
  procedure :: activate_dalitz_plot => pcm_nlo_activate_dalitz_plot

(Pcm: procedures)+≡
  subroutine pcm_nlo_activate_dalitz_plot (pcm, filename)
    class(pcm_nlo_t), intent(inout) :: pcm
    type(string_t), intent(in) :: filename
    call pcm%dalitz_plot%init (free_unit (), filename, .false.)
    call pcm%dalitz_plot%write_header ()
  end subroutine pcm_nlo_activate_dalitz_plot

(Pcm: pcm_nlo: TBP)+≡
  procedure :: register_dalitz_plot => pcm_nlo_register_dalitz_plot

(Pcm: procedures)+≡
  subroutine pcm_nlo_register_dalitz_plot (pcm, emitter, p)
    class(pcm_nlo_t), intent(inout) :: pcm
    integer, intent(in) :: emitter
    type(vector4_t), intent(in), dimension(:) :: p
    real(default) :: k0_n, k0_np1
    k0_n = p(emitter)%p(0)
    k0_np1 = p(size(p))%p(0)
    call pcm%dalitz_plot%register (k0_n, k0_np1)
  end subroutine pcm_nlo_register_dalitz_plot

(Pcm: pcm_nlo: TBP)+≡
  procedure :: setup_phs_generator => pcm_nlo_setup_phs_generator

(Pcm: procedures)+≡
  subroutine pcm_nlo_setup_phs_generator (pcm, pcm_work, generator, &
    sqrts, mode, singular_jacobian)
    class(pcm_nlo_t), intent(in) :: pcm
    type(phs_fks_generator_t), intent(inout) :: generator
    type(pcm_nlo_workspace_t), intent(in), target :: pcm_work
    real(default), intent(in) :: sqrts
    integer, intent(in), optional :: mode
    logical, intent(in), optional :: singular_jacobian
    logical :: yorn
    yorn = .false.; if (present (singular_jacobian)) yorn = singular_jacobian
    call generator%connect_kinematics (pcm_work%isr_kinematics, &
      pcm_work%real_kinematics, pcm%has_massive_emitter ())
    generator%n_in = pcm%region_data%n_in
    call generator%set_sqrts_hat (sqrts)
    call generator%set_emitters (pcm%region_data%emitters)
    call generator%setup_masses (pcm%region_data%n_legs_born)
    generator%is_massive = pcm%get_mass_info (1)
    generator%singular_jacobian = yorn
    if (present (mode)) generator%mode = mode
    call generator%set_xi_and_y_bounds (pcm%settings%fks_template%xi_min, &
      pcm%settings%fks_template%y_max)
  end subroutine pcm_nlo_setup_phs_generator

(Pcm: pcm_nlo: TBP)+≡
  procedure :: final => pcm_nlo_final

```

```

<Pcm: procedures>+≡
  subroutine pcm_nlo_final (pcm)
    class(pcm_nlo_t), intent(inout) :: pcm
    if (allocated (pcm%real_partition)) deallocate (pcm%real_partition)
    call pcm%dalitz_plot%final ()
  end subroutine pcm_nlo_final

```

```

<Pcm: pcm nlo: TBP>+≡
  procedure :: is_nlo => pcm_nlo_is_nlo

```

```

<Pcm: procedures>+≡
  function pcm_nlo_is_nlo (pcm) result (is_nlo)
    logical :: is_nlo
    class(pcm_nlo_t), intent(in) :: pcm
    is_nlo = .true.
  end function pcm_nlo_is_nlo

```

As a first implementation, it acts as a wrapper for the NLO controller object and the squared matrix-element collector.

```

<Pcm: public>+≡
  public :: pcm_nlo_workspace_t

<Pcm: types>+≡
  type, extends (pcm_workspace_t) :: pcm_nlo_workspace_t
    type(real_kinematics_t), pointer :: real_kinematics => null ()
    type(isr_kinematics_t), pointer :: isr_kinematics => null ()
    type(real_subtraction_t) :: real_sub
    type(virtual_t) :: virtual
    type(soft_mismatch_t) :: soft_mismatch
    type(dglap_remnant_t) :: dglap_remnant
    integer, dimension(:), allocatable :: i_mci_to_real_component
  contains
    <Pcm: pcm instance: TBP>
  end type pcm_nlo_workspace_t

```

```

<Pcm: pcm instance: TBP>≡
  procedure :: set_radiation_event => pcm_nlo_workspace_set_radiation_event
  procedure :: set_subtraction_event => pcm_nlo_workspace_set_subtraction_event

```

```

<Pcm: procedures>+≡
  subroutine pcm_nlo_workspace_set_radiation_event (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    pcm_work%real_sub%radiation_event = .true.
    pcm_work%real_sub%subtraction_event = .false.
  end subroutine pcm_nlo_workspace_set_radiation_event

  subroutine pcm_nlo_workspace_set_subtraction_event (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    pcm_work%real_sub%radiation_event = .false.
    pcm_work%real_sub%subtraction_event = .true.
  end subroutine pcm_nlo_workspace_set_subtraction_event

```

```

<Pcm: pcm instance: TBP>+≡
  procedure :: disable_subtraction => pcm_nlo_workspace_disable_subtraction

```

```

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_disable_subtraction (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    pcm_work%real_sub%subtraction_deactivated = .true.
  end subroutine pcm_nlo_workspace_disable_subtraction

(Pcm: pcm instance: TBP)+≡
  procedure :: init_config => pcm_nlo_workspace_init_config

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_init_config (pcm_work, pcm, active_components, &
    nlo_types, energy, i_real_fin, model)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    class(pcm_t), intent(in) :: pcm
    logical, intent(in), dimension(:) :: active_components
    integer, intent(in), dimension(:) :: nlo_types
    real(default), intent(in), dimension(:) :: energy
    integer, intent(in) :: i_real_fin
    class(model_data_t), intent(in) :: model
    integer :: i_component
    if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, "pcm_nlo_workspace_init_config")
    call pcm_work%init_real_and_isr_kinematics (pcm, energy)
    select type (pcm)
    type is (pcm_nlo_t)
      do i_component = 1, size (active_components)
        if (active_components(i_component) .or. pcm%settings%combined_integration) then
          select case (nlo_types(i_component))
          case (NLO_REAL)
            if (i_component /= i_real_fin) then
              call pcm_work%setup_real_component (pcm, &
                pcm%settings%fks_template%subtraction_disabled)
            end if
          case (NLO_VIRTUAL)
            call pcm_work%init_virtual (pcm, model)
          case (NLO_MISMATCH)
            call pcm_work%init_soft_mismatch (pcm)
          case (NLO_DGLAP)
            call pcm_work%init_dglap_remnant (pcm)
          end select
        end if
      end do
    end select
  end subroutine pcm_nlo_workspace_init_config

(Pcm: pcm instance: TBP)+≡
  procedure :: setup_real_component => pcm_nlo_workspace_setup_real_component

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_setup_real_component (pcm_work, pcm, &
    subtraction_disabled)
    class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
    class(pcm_t), intent(in) :: pcm
    logical, intent(in) :: subtraction_disabled
    select type (pcm)

```

```

    type is (pcm_nlo_t)
        call pcm_work%init_real_subtraction (pcm)
        if (subtraction_disabled) call pcm_work%disable_subtraction ()
    end select
end subroutine pcm_nlo_workspace_setup_real_component

(Pcm: pcm instance: TBP)+≡
    procedure :: init_real_and_isr_kinematics => &
        pcm_nlo_workspace_init_real_and_isr_kinematics

(Pcm: procedures)+≡
    subroutine pcm_nlo_workspace_init_real_and_isr_kinematics (pcm_work, pcm, energy)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        real(default), dimension(:), intent(in) :: energy
        integer :: n_contr
        allocate (pcm_work%real_kinematics)
        allocate (pcm_work%isr_kinematics)
        select type (pcm)
        type is (pcm_nlo_t)
            associate (region_data => pcm%region_data)
                if (allocated (region_data%alr_contributors)) then
                    n_contr = size (region_data%alr_contributors)
                else if (pcm%settings%factorization_mode == FACTORIZATION_THRESHOLD) then
                    n_contr = 2
                else
                    n_contr = 1
                end if
                call pcm_work%real_kinematics%init &
                    (region_data%n_legs_real, region_data%n_phs, &
                     region_data%n_regions, n_contr)
                if (pcm%settings%factorization_mode == FACTORIZATION_THRESHOLD) &
                    call pcm_work%real_kinematics%init_onshell &
                        (region_data%n_legs_real, region_data%n_phs)
                pcm_work%isr_kinematics%n_in = region_data%n_in
            end associate
        end select
        pcm_work%isr_kinematics%beam_energy = energy
    end subroutine pcm_nlo_workspace_init_real_and_isr_kinematics

(Pcm: pcm instance: TBP)+≡
    procedure :: set_real_and_isr_kinematics => &
        pcm_nlo_workspace_set_real_and_isr_kinematics

(Pcm: procedures)+≡
    subroutine pcm_nlo_workspace_set_real_and_isr_kinematics (pcm_work, phs_identifiers, sqrts)
        class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
        type(phs_identifer_t), intent(in), dimension(:) :: phs_identifiers
        real(default), intent(in) :: sqrts
        call pcm_work%real_sub%set_real_kinematics &
            (pcm_work%real_kinematics)
        call pcm_work%real_sub%set_isr_kinematics &
            (pcm_work%isr_kinematics)
    end subroutine pcm_nlo_workspace_set_real_and_isr_kinematics

```

```

(Pcm: pcm instance: TBP)+≡
  procedure :: init_real_subtraction => pcm_nlo_workspace_init_real_subtraction

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_init_real_subtraction (pcm_work, pcm)
    class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
    class(pcm_t), intent(in) :: pcm
    select type (pcm)
    type is (pcm_nlo_t)
      associate (region_data => pcm%region_data)
        call pcm_work%real_sub%init (region_data, pcm%settings)
        if (allocated (pcm%settings%selected_alr)) then
          associate (selected_alr => pcm%settings%selected_alr)
            if (any (selected_alr < 0)) then
              call msg_fatal ("Fixed alpha region must be non-negative!")
            else if (any (selected_alr > region_data%n_regions)) then
              call msg_fatal ("Fixed alpha region is larger than the total"&
                &" number of singular regions!")
            else
              allocate (pcm_work%real_sub%selected_alr (size (selected_alr)))
              pcm_work%real_sub%selected_alr = selected_alr
            end if
          end associate
        end associate
      end if
    end select
  end subroutine pcm_nlo_workspace_init_real_subtraction

(Pcm: pcm instance: TBP)+≡
  procedure :: set_momenta_and_scales_virtual => &
    pcm_nlo_workspace_set_momenta_and_scales_virtual

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_set_momenta_and_scales_virtual (pcm_work, p, &
    ren_scale, fac_scale, es_scale)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), intent(in) :: ren_scale, fac_scale, es_scale
    associate (virtual => pcm_work%virtual)
      call virtual%set_ren_scale (p, ren_scale)
      call virtual%set_fac_scale (p, fac_scale)
      call virtual%set_ellis_sexton_scale (es_scale)
    end associate
  end subroutine pcm_nlo_workspace_set_momenta_and_scales_virtual

(Pcm: pcm instance: TBP)+≡
  procedure :: set_fac_scale => pcm_nlo_workspace_set_fac_scale

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_set_fac_scale (pcm_work, fac_scale)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    real(default), intent(in) :: fac_scale
    pcm_work%isr_kinematics%fac_scale = fac_scale
  end subroutine pcm_nlo_workspace_set_fac_scale

```

```

(Pcm: pcm instance: TBP)+≡
  procedure :: set_momenta => pcm_nlo_workspace_set_momenta

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_set_momenta (pcm_work, p_born, p_real, i_phs, cms)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    type(vector4_t), dimension(:), intent(in) :: p_born, p_real
    integer, intent(in) :: i_phs
    logical, intent(in), optional :: cms
    logical :: yorn
    yorn = .false.; if (present (cms)) yorn = cms
    associate (kinematics => pcm_work%real_kinematics)
      if (yorn) then
        if (.not. kinematics%p_born_cms%initialized) &
          call kinematics%p_born_cms%init (size (p_born), 1)
        if (.not. kinematics%p_real_cms%initialized) &
          call kinematics%p_real_cms%init (size (p_real), 1)
        kinematics%p_born_cms%phs_point(1) = p_born
        kinematics%p_real_cms%phs_point(i_phs) = p_real
      else
        if (.not. kinematics%p_born_lab%initialized) &
          call kinematics%p_born_lab%init (size (p_born), 1)
        if (.not. kinematics%p_real_lab%initialized) &
          call kinematics%p_real_lab%init (size (p_real), 1)
        kinematics%p_born_lab%phs_point(1) = p_born
        kinematics%p_real_lab%phs_point(i_phs) = p_real
      end if
    end associate
  end subroutine pcm_nlo_workspace_set_momenta

```

```

(Pcm: pcm instance: TBP)+≡
  procedure :: get_momenta => pcm_nlo_workspace_get_momenta

(Pcm: procedures)+≡
  function pcm_nlo_workspace_get_momenta (pcm_work, pcm, &
    i_phs, born_phsp, cms) result (p)
    type(vector4_t), dimension(:), allocatable :: p
    class(pcm_nlo_workspace_t), intent(in) :: pcm_work
    class(pcm_t), intent(in) :: pcm
    integer, intent(in) :: i_phs
    logical, intent(in) :: born_phsp
    logical, intent(in), optional :: cms
    logical :: yorn
    yorn = .false.; if (present (cms)) yorn = cms
    select type (pcm)
    type is (pcm_nlo_t)
      if (born_phsp) then
        if (yorn) then
          p = pcm_work%real_kinematics%p_born_cms%phs_point(1)
        else
          p = pcm_work%real_kinematics%p_born_lab%phs_point(1)
        end if
      else
        if (yorn) then
          p = pcm_work%real_kinematics%p_real_cms%phs_point(i_phs)

```



```

        else
            p = pcm_work%real_kinematics%p_real_lab%phs_point(i_phs)
        end if
    end if
end select
end function pcm_nlo_workspace_get_momenta

```

<Pcm: pcm instance: TBP>+≡

```

    procedure :: get_xi_max => pcm_nlo_workspace_get_xi_max

```

<Pcm: procedures>+≡

```

    function pcm_nlo_workspace_get_xi_max (pcm_work, alr) result (xi_max)
        real(default) :: xi_max
        class(pcm_nlo_workspace_t), intent(in) :: pcm_work
        integer, intent(in) :: alr
        integer :: i_phs
        i_phs = pcm_work%real_kinematics%alr_to_i_phs (alr)
        xi_max = pcm_work%real_kinematics%xi_max (i_phs)
    end function pcm_nlo_workspace_get_xi_max

```

<Pcm: pcm instance: TBP>+≡

```

    procedure :: set_x_rad => pcm_nlo_workspace_set_x_rad

```

<Pcm: procedures>+≡

```

    subroutine pcm_nlo_workspace_set_x_rad (pcm_work, x_tot)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        real(default), intent(in), dimension(:) :: x_tot
        integer :: n_par
        n_par = size (x_tot)
        if (n_par < 3) then
            pcm_work%real_kinematics%x_rad = zero
        else
            pcm_work%real_kinematics%x_rad = x_tot (n_par - 2 : n_par)
        end if
    end subroutine pcm_nlo_workspace_set_x_rad

```

<Pcm: pcm instance: TBP>+≡

```

    procedure :: init_virtual => pcm_nlo_workspace_init_virtual

```

<Pcm: procedures>+≡

```

    subroutine pcm_nlo_workspace_init_virtual (pcm_work, pcm, model)
        class(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
        class(pcm_t), intent(in) :: pcm
        class(model_data_t), intent(in) :: model
        select type (pcm)
        type is (pcm_nlo_t)
            associate (region_data => pcm%region_data)
                call pcm_work%virtual%init (region_data%get_flv_states_born (), &
                    region_data%n_in, pcm%settings, model, pcm%has_pdfs)
            end associate
        end select
    end subroutine pcm_nlo_workspace_init_virtual

```

```

(Pcm: pcm instance: TBP)+≡
  procedure :: disable_virtual_subtraction => pcm_nlo_workspace_disable_virtual_subtraction

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_disable_virtual_subtraction (pcm_work)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  end subroutine pcm_nlo_workspace_disable_virtual_subtraction

(Pcm: pcm instance: TBP)+≡
  procedure :: compute_sqme_virt => pcm_nlo_workspace_compute_sqme_virt

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_compute_sqme_virt (pcm_work, pcm, p, &
    alpha_coupling, separate_uborns, sqme_virt)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    class(pcm_t), intent(in) :: pcm
    type(vector4_t), intent(in), dimension(:) :: p
    real(default), dimension(2), intent(in) :: alpha_coupling
    logical, intent(in) :: separate_uborns
    real(default), dimension(:), allocatable, intent(inout) :: sqme_virt
    type(vector4_t), dimension(:), allocatable :: pp
    associate (virtual => pcm_work%virtual)
      allocate (pp (size (p)))
      if (virtual%settings%factorization_mode == FACTORIZATION_THRESHOLD) then
        pp = pcm_work%real_kinematics%p_born_onshell%get_momenta (1)
      else
        pp = p
      end if
      select type (pcm)
      type is (pcm_nlo_t)
        if (separate_uborns) then
          allocate (sqme_virt (pcm%get_n_flv_born ()))
        else
          allocate (sqme_virt (1))
        end if
        sqme_virt = zero
        call virtual%evaluate (pcm%region_data, &
          alpha_coupling, pp, separate_uborns, sqme_virt)
      end select
    end associate
  end subroutine pcm_nlo_workspace_compute_sqme_virt

(Pcm: pcm instance: TBP)+≡
  procedure :: compute_sqme_mismatch => pcm_nlo_workspace_compute_sqme_mismatch

(Pcm: procedures)+≡
  subroutine pcm_nlo_workspace_compute_sqme_mismatch (pcm_work, pcm, &
    alpha_s, separate_uborns, sqme_mism)
    class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
    class(pcm_t), intent(in) :: pcm
    real(default), intent(in) :: alpha_s
    logical, intent(in) :: separate_uborns
    real(default), dimension(:), allocatable, intent(inout) :: sqme_mism
    select type (pcm)
    type is (pcm_nlo_t)

```

```

        if (separate_uborns) then
            allocate (sqme_mism (pcm%get_n_flv_born ()))
        else
            allocate (sqme_mism (1))
        end if
        sqme_mism = zero
        sqme_mism = pcm_work%soft_mismatch%evaluate (alpha_s)
    end select
end subroutine pcm_nlo_workspace_compute_sqme_mismatch

```

<Pcm: pcm instance: TBP>+≡

```

    procedure :: compute_sqme_dglap_remnant => pcm_nlo_workspace_compute_sqme_dglap_remnant

```

<Pcm: procedures>+≡

```

    subroutine pcm_nlo_workspace_compute_sqme_dglap_remnant (pcm_work, pcm, &
        alpha_coupling, separate_uborns, sqme_dglap)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        class(pcm_t), intent(in) :: pcm
        real(default), dimension(2), intent(in) :: alpha_coupling
        logical, intent(in) :: separate_uborns
        real(default), dimension(:), allocatable, intent(inout) :: sqme_dglap
        select type (pcm)
        type is (pcm_nlo_t)
            if (separate_uborns) then
                allocate (sqme_dglap (pcm%get_n_flv_born ()))
            else
                allocate (sqme_dglap (1))
            end if
        end select
        sqme_dglap = zero
        call pcm_work%dglap_remnant%evaluate (alpha_coupling, separate_uborns, sqme_dglap)
    end subroutine pcm_nlo_workspace_compute_sqme_dglap_remnant

```

<Pcm: pcm instance: TBP>+≡

```

    procedure :: set_fixed_order_event_mode => pcm_nlo_workspace_set_fixed_order_event_mode

```

<Pcm: procedures>+≡

```

    subroutine pcm_nlo_workspace_set_fixed_order_event_mode (pcm_work)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        pcm_work%real_sub%purpose = FIXED_ORDER_EVENTS
    end subroutine pcm_nlo_workspace_set_fixed_order_event_mode

```

<Pcm: pcm instance: TBP>+≡

```

    procedure :: set_powheg_mode => pcm_nlo_workspace_set_powheg_mode

```

<Pcm: procedures>+≡

```

    subroutine pcm_nlo_workspace_set_powheg_mode (pcm_work)
        class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
        pcm_work%real_sub%purpose = POWHEG
    end subroutine pcm_nlo_workspace_set_powheg_mode

```

<Pcm: pcm instance: TBP>+≡

```

    procedure :: init_soft_mismatch => pcm_nlo_workspace_init_soft_mismatch

```

```

(Pcm: procedures)+≡
subroutine pcm_nlo_workspace_init_soft_mismatch (pcm_work, pcm)
  class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  class(pcm_t), intent(in) :: pcm
  select type (pcm)
  type is (pcm_nlo_t)
    call pcm_work%soft_mismatch%init (pcm%region_data, &
      pcm_work%real_kinematics, pcm%settings%factorization_mode)
  end select
end subroutine pcm_nlo_workspace_init_soft_mismatch

(Pcm: pcm instance: TBP)+≡
procedure :: init_dglap_remnant => pcm_nlo_workspace_init_dglap_remnant

(Pcm: procedures)+≡
subroutine pcm_nlo_workspace_init_dglap_remnant (pcm_work, pcm)
  class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  class(pcm_t), intent(in) :: pcm
  select type (pcm)
  type is (pcm_nlo_t)
    call pcm_work%dglap_remnant%init ( &
      pcm%settings, &
      pcm%region_data, &
      pcm_work%isr_kinematics)
  end select
end subroutine pcm_nlo_workspace_init_dglap_remnant

(Pcm: pcm instance: TBP)+≡
procedure :: is_fixed_order_nlo_events &
  => pcm_nlo_workspace_is_fixed_order_nlo_events

(Pcm: procedures)+≡
function pcm_nlo_workspace_is_fixed_order_nlo_events (pcm_work) result (is_fnlo)
  logical :: is_fnlo
  class(pcm_nlo_workspace_t), intent(in) :: pcm_work
  is_fnlo = pcm_work%real_sub%purpose == FIXED_ORDER_EVENTS
end function pcm_nlo_workspace_is_fixed_order_nlo_events

(Pcm: pcm instance: TBP)+≡
procedure :: final => pcm_nlo_workspace_final

(Pcm: procedures)+≡
subroutine pcm_nlo_workspace_final (pcm_work)
  class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
  call pcm_work%real_sub%final ()
  call pcm_work%virtual%final ()
  call pcm_work%soft_mismatch%final ()
  call pcm_work%dglap_remnant%final ()
  if (associated (pcm_work%real_kinematics)) then
    call pcm_work%real_kinematics%final ()
    nullify (pcm_work%real_kinematics)
  end if
  if (associated (pcm_work%isr_kinematics)) then
    nullify (pcm_work%isr_kinematics)
  end if
end subroutine pcm_nlo_workspace_final

```

```

        end if
    end subroutine pcm_nlo_workspace_final

    <Pcm: pcm instance: TBP>+≡
        procedure :: is_nlo => pcm_nlo_workspace_is_nlo

    <Pcm: procedures>+≡
        function pcm_nlo_workspace_is_nlo (pcm_work) result (is_nlo)
            logical :: is_nlo
            class(pcm_nlo_workspace_t), intent(inout) :: pcm_work
            is_nlo = .true.
        end function pcm_nlo_workspace_is_nlo

```

30.9 Kinematics instance

In this data type we combine all objects (instances) necessary for generating (or recovering) a kinematical configuration. The components work together as an implementation of multi-channel phase space.

sf_chain is an instance of the structure-function chain. It is used both for generating kinematics and, after the proper scale has been determined, evaluating the structure function entries.

phs is an instance of the phase space for the elementary process.

The array **f** contains the products of the Jacobians that originate from parameter mappings in the structure-function chain or in the phase space. We allocate this explicitly if either **sf_chain** or **phs** are explicitly allocated, otherwise we can take over a pointer.

All components are implemented as pointers to (anonymous) targets. For each component, there is a flag that tells whether this component is to be regarded as a proper component ('owned' by the object) or as a pointer.

```

<kinematics.f90>≡
    <File header>

    module kinematics

    <Use kinds>
    <Use debug>
        use format_utils, only: write_separator
        use diagnostics
        use io_units
        use lorentz
        use phs_points, only: assignment(=), size
        use physics_defs
        use sf_base
        use phs_base
        use interactions
        use mci_base
        use phs_fks
        use fks_regions
        use process_config
        use process_mci

```

```

    use pcm_base, only: pcm_t, pcm_workspace_t
    use pcm, only: pcm_nlo_t, pcm_nlo_workspace_t
    use ttv_formfactors, only: mls_to_mpole

    <Standard module head>

    <Kinematics: public>

    <Kinematics: types>

contains

    <Kinematics: procedures>

end module kinematics

<Kinematics: public>≡
    public :: kinematics_t

<Kinematics: types>≡
    type :: kinematics_t
        integer :: n_in = 0
        integer :: n_channel = 0
        integer :: selected_channel = 0
        type(sf_chain_instance_t), pointer :: sf_chain => null ()
        class(phs_t), pointer :: phs => null ()
        real(default), dimension(:), pointer :: f => null ()
        real(default) :: phs_factor
        logical :: sf_chain_allocated = .false.
        logical :: phs_allocated = .false.
        logical :: f_allocated = .false.
        integer :: emitter = -1
        integer :: i_phs = 0
        integer :: i_con = 0
        logical :: only_cm_frame = .false.
        logical :: new_seed = .true.
        logical :: threshold = .false.
    contains
        <Kinematics: kinematics: TBP>
end type kinematics_t

```

Output. Show only those components which are marked as owned.

```

<Kinematics: kinematics: TBP>≡
    procedure :: write => kinematics_write

<Kinematics: procedures>≡
    subroutine kinematics_write (object, unit)
        class(kinematics_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, c
        u = given_output_unit (unit)
        if (object%f_allocated) then
            write (u, "(1x,A)") "Flux * PHS volume:"
            write (u, "(2x,ES19.12)") object%phs_factor
            write (u, "(1x,A)") "Jacobian factors per channel:"

```

```

do c = 1, size (object%f)
  write (u, "(3x,I0,':',1x,ES14.7)", advance="no") c, object%f(c)
  if (c == object%selected_channel) then
    write (u, "(1x,A)") "[selected]"
  else
    write (u, *)
  end if
end do
end if
if (object%sf_chain_allocated) then
  call write_separator (u)
  call object%sf_chain%write (u)
end if
if (object%phs_allocated) then
  call write_separator (u)
  call object%phs%write (u)
end if
end subroutine kinematics_write

```

Finalizer. Delete only those components which are marked as owned.

```

<Kinematics: kinematics: TBP>+≡
  procedure :: final => kinematics_final

<Kinematics: procedures>+≡
  subroutine kinematics_final (object)
    class(kinematics_t), intent(inout) :: object
    if (object%sf_chain_allocated) then
      call object%sf_chain%final ()
      deallocate (object%sf_chain)
      object%sf_chain_allocated = .false.
    end if
    if (object%phs_allocated) then
      call object%phs%final ()
      deallocate (object%phs)
      object%phs_allocated = .false.
    end if
    if (object%f_allocated) then
      deallocate (object%f)
      object%f_allocated = .false.
    end if
  end subroutine kinematics_final

```

Configure the kinematics object. This consists of several configuration steps which correspond to individual procedures. In essence, we configure the structure-function part, the partonic phase-space part, and various NLO items.

TODO wk 19-03-01: This includes some region-data setup within `pcm`, hence `pcm` is `intent(inout)`. This should be moved elsewhere, so `pcm` can become strictly `intent(in)`.

```

<Kinematics: kinematics: TBP>+≡
  procedure :: configure => kinematics_configure

<Kinematics: procedures>+≡
  subroutine kinematics_configure (kin, pcm, pcm_work, &

```

```

        sf_chain, beam_config, phs_config, nlo_type, is_i_sub)
class(kinematics_t), intent(out) :: kin
class(pcm_t), intent(inout) :: pcm
class(pcm_workspace_t), intent(in) :: pcm_work
type(sf_chain_t), intent(in), target :: sf_chain
type(process_beam_config_t), intent(in), target :: beam_config
class(phs_config_t), intent(in), target :: phs_config
integer, intent(in) :: nlo_type
logical, intent(in) :: is_i_sub
logical :: extended_sf
extended_sf = nlo_type == NLO_DGLAP .or. (nlo_type == NLO_REAL .and. is_i_sub)
call kin%init_sf_chain (sf_chain, beam_config, &
    extended_sf = pcm%has_pdfs .and. extended_sf)
!!! Add one for additional Born matrix element
call kin%init_phs (phs_config)
call kin%set_nlo_info (nlo_type)
select type (phs => kin%phs)
type is (phs_fks_t)
    call phs%allocate_momenta (phs_config, .not. (nlo_type == NLO_REAL))
    select type (pcm)
    type is (pcm_nlo_t)
        call pcm%region_data%init_phs_identifiers (phs%phs_identifiers)
        !!! The triple select type pyramid of doom
        select type (pcm_work)
        type is (pcm_nlo_workspace_t)
            if (allocated (pcm_work%real_kinematics%alr_to_i_phs)) &
                call pcm%region_data%set_alr_to_i_phs (phs%phs_identifiers, &
                    pcm_work%real_kinematics%alr_to_i_phs)
        end select
    end select
end select
end subroutine kinematics_configure

```

Set the flags indicating whether the phase space shall be set up for the calculation of the real contribution. For this case, also set the emitter.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: set_nlo_info => kinematics_set_nlo_info

<Kinematics: procedures>+≡
    subroutine kinematics_set_nlo_info (k, nlo_type)
        class(kinematics_t), intent(inout) :: k
        integer, intent(in) :: nlo_type
        if (nlo_type == NLO_VIRTUAL) k%only_cm_frame = .true.
    end subroutine kinematics_set_nlo_info

```

```

<Kinematics: kinematics: TBP>+≡
    procedure :: set_threshold => kinematics_set_threshold

<Kinematics: procedures>+≡
    subroutine kinematics_set_threshold (kin, factorization_mode)
        class(kinematics_t), intent(inout) :: kin
        integer, intent(in) :: factorization_mode
        kin%threshold = factorization_mode == FACTORIZATION_THRESHOLD
    end subroutine kinematics_set_threshold

```


Allocate the structure-function chain instance, initialize it as a copy of the `sf_chain` template, and prepare it for evaluation.

The `sf_chain` remains a target because the (usually constant) beam momenta are taken from there.

(Kinematics: kinematics: TBP)+≡

```
procedure :: init_sf_chain => kinematics_init_sf_chain
```

(Kinematics: procedures)+≡

```
subroutine kinematics_init_sf_chain (k, sf_chain, config, extended_sf)
  class(kinematics_t), intent(inout) :: k
  type(sf_chain_t), intent(in), target :: sf_chain
  type(process_beam_config_t), intent(in) :: config
  logical, intent(in), optional :: extended_sf
  integer :: n_strfun, n_channel
  integer :: c
  k%n_in = config%data%get_n_in ()
  n_strfun = config%n_strfun
  n_channel = config%n_channel
  allocate (k%sf_chain)
  k%sf_chain_allocated = .true.
  call k%sf_chain%init (sf_chain, n_channel)
  if (n_strfun /= 0) then
    do c = 1, n_channel
      call k%sf_chain%set_channel (c, config%sf_channel(c))
    end do
  end if
  call k%sf_chain%link_interactions ()
  call k%sf_chain%exchange_mask ()
  call k%sf_chain%init_evaluators (extended_sf = extended_sf)
end subroutine kinematics_init_sf_chain
```

Allocate and initialize the phase-space part and the array of Jacobian factors.

(Kinematics: kinematics: TBP)+≡

```
procedure :: init_phs => kinematics_init_phs
```

(Kinematics: procedures)+≡

```
subroutine kinematics_init_phs (k, config)
  class(kinematics_t), intent(inout) :: k
  class(phs_config_t), intent(in), target :: config
  k%n_channel = config%get_n_channel ()
  call config%allocate_instance (k%phs)
  call k%phs%init (config)
  k%phs_allocated = .true.
  allocate (k%f (k%n_channel))
  k%f = 0
  k%f_allocated = .true.
end subroutine kinematics_init_phs
```

(Kinematics: kinematics: TBP)+≡

```
procedure :: evaluate_radiation_kinematics => kinematics_evaluate_radiation_kinematics
```

```

<Kinematics: procedures>+≡
  subroutine kinematics_evaluate_radiation_kinematics (k, r_in)
    class(kinematics_t), intent(inout) :: k
    real(default), intent(in), dimension(:) :: r_in
    select type (phs => k%phs)
    type is (phs_fks_t)
      if (phs%mode == PHS_MODE_ADDITIONAL_PARTICLE) then
        call phs%generate_radiation_variables &
          (r_in(phs%n_r_born + 1 : phs%n_r_born + 3), threshold = k%threshold)
        call phs%compute_cms_energy ()
      end if
    end select
  end subroutine kinematics_evaluate_radiation_kinematics

<Kinematics: kinematics: TBP>+≡
  procedure :: generate_fsr_in => kinematics_generate_fsr_in

<Kinematics: procedures>+≡
  subroutine kinematics_generate_fsr_in (kin)
    class(kinematics_t), intent(inout) :: kin
    select type (phs => kin%phs)
    type is (phs_fks_t)
      call phs%generate_fsr_in ()
    end select
  end subroutine kinematics_generate_fsr_in

<Kinematics: kinematics: TBP>+≡
  procedure :: compute_xi_ref_momenta => kinematics_compute_xi_ref_momenta

<Kinematics: procedures>+≡
  subroutine kinematics_compute_xi_ref_momenta (k, reg_data, nlo_type)
    class(kinematics_t), intent(inout) :: k
    type(region_data_t), intent(in) :: reg_data
    integer, intent(in) :: nlo_type
    logical :: use_contributors
    use_contributors = allocated (reg_data%alr_contributors)
    select type (phs => k%phs)
    type is (phs_fks_t)
      if (use_contributors) then
        call phs%compute_xi_ref_momenta (contributors = reg_data%alr_contributors)
      else if (k%threshold) then
        if (.not. is_subtraction_component (k%emitter, nlo_type)) &
          call phs%compute_xi_ref_momenta_threshold ()
      else
        call phs%compute_xi_ref_momenta ()
      end if
    end select
  end subroutine kinematics_compute_xi_ref_momenta

```

Generate kinematics, given a phase-space channel and a MC parameter set. The main result is the momentum array `p`, but we also fill the momentum entries in the structure-function chain and the Jacobian-factor array `f`. Regarding phase space, we fill only the parameter arrays for the selected channel.

```

<Kinematics: kinematics: TBP>+≡

```

```

    procedure :: compute_selected_channel => kinematics_compute_selected_channel
(Kinematics: procedures)+≡
    subroutine kinematics_compute_selected_channel &
        (k, mci_work, phs_channel, p, success)
        class(kinematics_t), intent(inout) :: k
        type(mci_work_t), intent(in) :: mci_work
        integer, intent(in) :: phs_channel
        type(vector4_t), dimension(:), intent(out) :: p
        logical, intent(out) :: success
        integer :: sf_channel
        k%selected_channel = phs_channel
        sf_channel = k%phs%config%get_sf_channel (phs_channel)
        call k%sf_chain%compute_kinematics (sf_channel, mci_work%get_x_strfun ())
        call k%sf_chain%get_out_momenta (p(1:k%n_in))
        call k%phs%set_incoming_momenta (p(1:k%n_in))
        call k%phs%compute_flux ()
        call k%phs%select_channel (phs_channel)
        call k%phs%evaluate_selected_channel (phs_channel, &
            mci_work%get_x_process ())

        select type (phs => k%phs)
        type is (phs_fks_t)
            if (debug_on) call msg_debug2 (D_REAL, "phase space is phs_FKS")
            if (phs%q_defined) then
                call phs%get_born_momenta (p)
                if (debug_on) then
                    call msg_debug2 (D_REAL, "q is defined")
                    call msg_debug2 (D_REAL, "get_born_momenta called")
                end if
                k%phs_factor = phs%get_overall_factor ()
                success = .true.
            else
                k%phs_factor = 0
                success = .false.
            end if
        class default
            if (phs%q_defined) then
                call k%phs%get_outgoing_momenta (p(k%n_in + 1 :))
                k%phs_factor = k%phs%get_overall_factor ()
                success = .true.
            else
                k%phs_factor = 0
                success = .false.
            end if
        end select
    end subroutine kinematics_compute_selected_channel

(Kinematics: kinematics: TBP)+≡
    procedure :: redo_sf_chain => kinematics_redo_sf_chain
(Kinematics: procedures)+≡
    subroutine kinematics_redo_sf_chain (kin, mci_work, phs_channel)
        class(kinematics_t), intent(inout) :: kin
        type(mci_work_t), intent(in) :: mci_work

```

```

integer, intent(in) :: phs_channel
real(default), dimension(:), allocatable :: x
integer :: sf_channel, n
real(default) :: xi, y
n = size (mci_work%get_x_strfun ())
if (n > 0) then
  allocate (x(n))
  x = mci_work%get_x_strfun ()
  sf_channel = kin%phs%config%get_sf_channel (phs_channel)
  call kin%sf_chain%compute_kinematics (sf_channel, x)
end if
end subroutine kinematics_redo_sf_chain

```

Complete kinematics by filling the non-selected phase-space parameter arrays.

```

<Kinematics: kinematics: TBP>+≡
  procedure :: compute_other_channels => kinematics_compute_other_channels

<Kinematics: procedures>+≡
  subroutine kinematics_compute_other_channels (k, mci_work, phs_channel)
    class(kinematics_t), intent(inout) :: k
    type(mci_work_t), intent(in) :: mci_work
    integer, intent(in) :: phs_channel
    integer :: c, c_sf
    call k%phs%evaluate_other_channels (phs_channel)
    do c = 1, k%n_channel
      c_sf = k%phs%config%get_sf_channel (c)
      k%f(c) = k%sf_chain%get_f (c_sf) * k%phs%get_f (c)
    end do
  end subroutine kinematics_compute_other_channels

```

Just fetch the outgoing momenta of the `sf_chain` subobject, which become the incoming (seed) momenta of the hard interaction.

This is a stripped down-version of the above which we use when recovering kinematics. Momenta are known, but no MC parameters yet.

(We do not use the `get_out_momenta` method of the chain, since this relies on the structure-function interactions, which are not necessary filled here. We do rely on the momenta of the last evaluator in the chain, however.)

```

<Kinematics: kinematics: TBP>+≡
  procedure :: get_incoming_momenta => kinematics_get_incoming_momenta

<Kinematics: procedures>+≡
  subroutine kinematics_get_incoming_momenta (k, p)
    class(kinematics_t), intent(in) :: k
    type(vector4_t), dimension(:), intent(out) :: p
    type(interaction_t), pointer :: int
    integer :: i
    int => k%sf_chain%get_out_int_ptr ()
    do i = 1, k%n_in
      p(i) = int%get_momentum (k%sf_chain%get_out_i (i))
    end do
  end subroutine kinematics_get_incoming_momenta

```

```

(Kinematics: kinematics: TBP)+≡
  procedure :: get_boost_to_lab => kinematics_get_boost_to_lab

(Kinematics: procedures)+≡
  function kinematics_get_boost_to_lab (kin) result (lt)
    type(lorentz_transformation_t) :: lt
    class(kinematics_t), intent(in) :: kin
    lt = kin%phs%get_lorentz_transformation ()
  end function kinematics_get_boost_to_lab

(Kinematics: kinematics: TBP)+≡
  procedure :: get_boost_to_cms => kinematics_get_boost_to_cms

(Kinematics: procedures)+≡
  function kinematics_get_boost_to_cms (kin) result (lt)
    type(lorentz_transformation_t) :: lt
    class(kinematics_t), intent(in) :: kin
    lt = inverse (kin%phs%get_lorentz_transformation ())
  end function kinematics_get_boost_to_cms

```

This inverts the remainder of the above `compute` method. We know the momenta and recover the rest, as far as needed. If we select a channel, we can complete the inversion and reconstruct the MC parameter set.

```

(Kinematics: kinematics: TBP)+≡
  procedure :: recover_mcpair => kinematics_recover_mcpair

(Kinematics: procedures)+≡
  subroutine kinematics_recover_mcpair (k, mci_work, phs_channel, p)
    class(kinematics_t), intent(inout) :: k
    type(mci_work_t), intent(inout) :: mci_work
    integer, intent(in) :: phs_channel
    type(vector4_t), dimension(:), intent(in) :: p
    integer :: c, c_sf
    real(default), dimension(:), allocatable :: x_sf, x_phs
    c = phs_channel
    c_sf = k%phs%config%get_sf_channel (c)
    k%selected_channel = c
    call k%sf_chain%recover_kinematics (c_sf)
    call k%phs%set_incoming_momenta (p(1:k%n_in))
    call k%phs%compute_flux ()
    call k%phs%set_outgoing_momenta (p(k%n_in+1:))
    call k%phs%inverse ()
    do c = 1, k%n_channel
      c_sf = k%phs%config%get_sf_channel (c)
      k%f(c) = k%sf_chain%get_f (c_sf) * k%phs%get_f (c)
    end do
    k%phs_factor = k%phs%get_overall_factor ()
    c = phs_channel
    c_sf = k%phs%config%get_sf_channel (c)
    allocate (x_sf (k%sf_chain%config%get_n_bound ()))
    allocate (x_phs (k%phs%config%get_n_par ()))
    call k%phs%select_channel (c)
    call k%sf_chain%get_mcpair (c_sf, x_sf)
    call k%phs%get_mcpair (c, x_phs)
  end subroutine kinematics_recover_mcpair

```

```

        call mci_work%set_x_strfun (x_sf)
        call mci_work%set_x_process (x_phs)
    end subroutine kinematics_recover_mcpair

```

This first part of `recover_mcpair`: just handle the `sfchain`.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: recover_sfchain => kinematics_recover_sfchain

<Kinematics: procedures>+≡
    subroutine kinematics_recover_sfchain (k, channel, p)
        class(kinematics_t), intent(inout) :: k
        integer, intent(in) :: channel
        type(vector4_t), dimension(:), intent(in) :: p
        k%selected_channel = channel
        call k%sf_chain%recover_kinematics (channel)
    end subroutine kinematics_recover_sfchain

```

Retrieve the MC input parameter array for a specific channel. We assume that the kinematics is complete, so this is known for all channels.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: get_mcpair => kinematics_get_mcpair

<Kinematics: procedures>+≡
    subroutine kinematics_get_mcpair (k, phs_channel, r)
        class(kinematics_t), intent(in) :: k
        integer, intent(in) :: phs_channel
        real(default), dimension(:), intent(out) :: r
        integer :: sf_channel, n_par_sf, n_par_phs
        sf_channel = k%phs%config%get_sf_channel (phs_channel)
        n_par_phs = k%phs%config%get_n_par ()
        n_par_sf = k%sf_chain%config%get_n_bound ()
        if (n_par_sf > 0) then
            call k%sf_chain%get_mcpair (sf_channel, r(1:n_par_sf))
        end if
        if (n_par_phs > 0) then
            call k%phs%get_mcpair (phs_channel, r(n_par_sf+1:))
        end if
    end subroutine kinematics_get_mcpair

```

Evaluate the structure function chain, assuming that kinematics is known.

The status must be precisely `SF_DONE_KINEMATICS`. We thus avoid evaluating the chain twice via different pointers to the same target.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: evaluate_sf_chain => kinematics_evaluate_sf_chain

<Kinematics: procedures>+≡
    subroutine kinematics_evaluate_sf_chain (k, fac_scale, negative_sf, sf_rescale)
        class(kinematics_t), intent(inout) :: k
        real(default), intent(in) :: fac_scale
        logical, intent(in), optional :: negative_sf
        class(sf_rescale_t), intent(inout), optional :: sf_rescale
        select case (k%sf_chain%get_status ())
        case (SF_DONE_KINEMATICS)

```

```

        call k%sf_chain%evaluate (fac_scale, negative_sf = negative_sf, sf_rescale = sf_rescale)
    end select
end subroutine kinematics_evaluate_sf_chain

```

Recover beam momenta, i.e., return the beam momenta stored in the current `sf_chain` to their source. This is a side effect.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: return_beam_momenta => kinematics_return_beam_momenta

<Kinematics: procedures>+≡
    subroutine kinematics_return_beam_momenta (k)
        class(kinematics_t), intent(in) :: k
        call k%sf_chain%return_beam_momenta ()
    end subroutine kinematics_return_beam_momenta

```

Check whether the phase space is configured in the center-of-mass frame. Relevant for using the proper momenta input for BLHA matrix elements.

```

<Kinematics: kinematics: TBP>+≡
    procedure :: lab_is_cm => kinematics_lab_is_cm

<Kinematics: procedures>+≡
    function kinematics_lab_is_cm (k) result (lab_is_cm)
        logical :: lab_is_cm
        class(kinematics_t), intent(in) :: k
        lab_is_cm = k%phs%config%lab_is_cm
    end function kinematics_lab_is_cm

```

```

<Kinematics: kinematics: TBP>+≡
    procedure :: modify_momenta_for_subtraction => kinematics_modify_momenta_for_subtraction

<Kinematics: procedures>+≡
    subroutine kinematics_modify_momenta_for_subtraction (k, p_in, p_out)
        class(kinematics_t), intent(inout) :: k
        type(vector4_t), intent(in), dimension(:) :: p_in
        type(vector4_t), intent(out), dimension(:), allocatable :: p_out
        allocate (p_out (size (p_in)))
        if (k%threshold) then
            select type (phs => k%phs)
            type is (phs_fks_t)
                p_out = phs%get_onshell_projected_momenta ()
            end select
        else
            p_out = p_in
        end if
    end subroutine kinematics_modify_momenta_for_subtraction

```

```

<Kinematics: kinematics: TBP>+≡
    procedure :: threshold_projection => kinematics_threshold_projection

<Kinematics: procedures>+≡
    subroutine kinematics_threshold_projection (k, pcm_work, nlo_type)
        class(kinematics_t), intent(inout) :: k
        type(pcm_nlo_workspace_t), intent(inout) :: pcm_work

```

```

integer, intent(in) :: nlo_type
real(default) :: sqrts, mtop
type(lorentz_transformation_t) :: L_to_cms
type(vector4_t), dimension(:), allocatable :: p_tot, p_onshell
integer :: n_tot
n_tot = k%phs%get_n_tot ()
allocate (p_tot (size (pcm_work%real_kinematics%p_born_cms%phs_point(1))))
select type (phs => k%phs)
type is (phs_fks_t)
    p_tot = pcm_work%real_kinematics%p_born_cms%phs_point(1)
class default
    p_tot(1 : k%n_in) = phs%p
    p_tot(k%n_in + 1 : n_tot) = phs%q
end select
sqrts = sum (p_tot (1:k%n_in))*1
mtop = mls_to_mpole (sqrts)
L_to_cms = get_boost_for_threshold_projection (p_tot, sqrts, mtop)
call pcm_work%real_kinematics%p_born_cms%set_momenta (1, p_tot)
p_onshell = pcm_work%real_kinematics%p_born_onshell%phs_point(1)
call threshold_projection_born (mtop, L_to_cms, p_tot, p_onshell)
pcm_work%real_kinematics%p_born_onshell%phs_point(1) = p_onshell
if (debug2_active (D_THRESHOLD)) then
    print *, 'On-shell projected Born: '
    call vector4_write_set (p_onshell)
end if
end subroutine kinematics_threshold_projection

```

(Kinematics: kinematics: TBP)+≡

```
procedure :: evaluate_radiation => kinematics_evaluate_radiation
```

(Kinematics: procedures)+≡

```

subroutine kinematics_evaluate_radiation (k, p_in, p_out, success)
class(kinematics_t), intent(inout) :: k
type(vector4_t), intent(in), dimension(:) :: p_in
type(vector4_t), intent(out), dimension(:), allocatable :: p_out
logical, intent(out) :: success
type(vector4_t), dimension(:), allocatable :: p_real
type(vector4_t), dimension(:), allocatable :: p_born
real(default) :: xi_max_offshell, xi_offshell, y_offshell, jac_rand_dummy, phi
select type (phs => k%phs)
type is (phs_fks_t)
    allocate (p_born (size (p_in)))
    if (k%threshold) then
        p_born = phs%get_onshell_projected_momenta ()
    else
        p_born = p_in
    end if
    if (.not. k%phs%lab_is_cm () .and. .not. k%threshold) then
        p_born = inverse (k%phs%lt_cm_to_lab) * p_born
    end if
    call phs%compute_xi_max (p_born, k%threshold)
    if (k%emitter >= 0) then
        allocate (p_real (size (p_born) + 1))
        allocate (p_out (size (p_born) + 1))
    end if
end subroutine

```



```

if (k%emitter <= k%n_in) then
  call phs%generate_isr (k%i_phs, p_real)
else
  if (k%threshold) then
    jac_rand_dummy = 1._default
    call compute_y_from_emitter (phs%generator%real_kinematics%x_rad (I_Y), &
      phs%generator%real_kinematics%p_born_cms%get_momenta(1), &
      k%n_in, k%emitter, .false., phs%generator%y_max, jac_rand_dummy, &
      y_offshell)
    call phs%compute_xi_max (k%emitter, k%i_phs, y_offshell, &
      phs%generator%real_kinematics%p_born_cms%get_momenta(1), &
      xi_max_offshell)
    xi_offshell = xi_max_offshell * phs%generator%real_kinematics%xi_tilde
    phi = phs%generator%real_kinematics%phi
    call phs%generate_fsr (k%emitter, k%i_phs, p_real, &
      xi_y_phi = [xi_offshell, y_offshell, phi], no_jacobians = .true.)
    call phs%generator%real_kinematics%p_real_cms%set_momenta (k%i_phs, p_real)
    call phs%generate_fsr_threshold (k%emitter, k%i_phs, p_real)
    if (debug2_active (D_SUBTRACTION)) &
      call generate_fsr_threshold_for_other_emitters (k%emitter, k%i_phs)
  else if (k%i_con > 0) then
    call phs%generate_fsr (k%emitter, k%i_phs, p_real, k%i_con)
  else
    call phs%generate_fsr (k%emitter, k%i_phs, p_real)
  end if
end if
success = check_scalar_products (p_real)
if (debug2_active (D_SUBTRACTION)) then
  call msg_debug2 (D_SUBTRACTION, "Real phase-space: ")
  call vector4_write_set (p_real)
end if
p_out = p_real
else
  allocate (p_out (size (p_in))); p_out = p_in
  success = .true.
end if
end select
contains
subroutine generate_fsr_threshold_for_other_emitters (emitter, i_phs)
  integer, intent(in) :: emitter, i_phs
  integer :: ii_phs, this_emitter
  select type (phs => k%phs)
  type is (phs_fks_t)
    do ii_phs = 1, size (phs%phs_identifiers)
      this_emitter = phs%phs_identifiers(ii_phs)%emitter
      if (ii_phs /= i_phs .and. this_emitter /= emitter) &
        call phs%generate_fsr_threshold (this_emitter, i_phs)
    end do
  end select
end subroutine
end subroutine kinematics_evaluate_radiation

```

30.10 Instances

```
<instances.f90>≡
  <File header>

  module instances

    <Use kinds>
    <Use strings>
    <Use debug>
    use io_units
    use format_utils, only: write_separator
    use constants
    use diagnostics
    use os_interface
    use numeric_utils
    use lorentz
    use mci_base
    use particles
    use sm_qcd, only: qcd_t
    use interactions
    use quantum_numbers
    use model_data
    use helicities
    use flavors
    use beam_structures
    use variables
    use pdg_arrays, only: is_quark
    use sf_base
    use physics_defs
    use process_constants
    use process_libraries
    use state_matrices
    use integration_results
    use phs_base
    use prc_core, only: prc_core_t, prc_core_state_t

    !!! We should depend less on these modules (move it to pcm_nlo_t e.g.)
    use phs_wood, only: phs_wood_t
    use phs_fks
    use blha_olp_interfaces, only: prc_blha_t
    use blha_config, only: BLHA_AMP_COLOR_C
    use prc_external, only: prc_external_t, prc_external_state_t
    use prc_threshold, only: prc_threshold_t
    use blha_olp_interfaces, only: blha_result_array_size
    use prc_openloops, only: prc_openloops_t, openloops_state_t
    use prc_recola, only: prc_recola_t
    use blha_olp_interfaces, only: blha_color_c_fill_offdiag, blha_color_c_fill_diag

    use ttv_formfactors, only: mis_to_mpole
    !!! local modules
    use parton_states
    use process_counter
    use pcm_base
```

```

use pcm
use process_config
use process_mci
use process
use kinematics

⟨Standard module head⟩

⟨Instances: public⟩

⟨Instances: types⟩

⟨Instances: interfaces⟩

contains

⟨Instances: procedures⟩

end module instances

```

30.10.1 Term instance

A `term_instance_t` object contains all data that describe a term. Each process component consists of one or more distinct terms which may differ in kinematics, but whose squared transition matrices have to be added pointwise.

The `active` flag is set when this term is connected to an active process component. Inactive terms are skipped for kinematics and evaluation.

The `amp` array stores the amplitude values when we get them from evaluating the associated matrix-element code.

The `int_hard` interaction describes the elementary hard process. It receives the momenta and the amplitude entries for each sampling point.

The `isolated` object holds the effective parton state for the elementary interaction. The amplitude entries are computed from `int_hard`.

The `connected` evaluator set convolutes this scattering matrix with the beam (and possibly structure-function) density matrix.

The `checked` flag is set once we have applied cuts on this term. The result of this is stored in the `passed` flag.

Although each `term_instance` carries a `weight`, this currently always keeps the value 1 and is only used to be given to routines to fulfill their signature.

⟨Instances: types⟩≡

```

type :: term_instance_t
  type(process_term_t), pointer :: config => null ()
  class(pcm_t), pointer :: pcm => null ()
  class(pcm_workspace_t), pointer :: pcm_work => null ()
  logical :: active = .false.
  complex(default), dimension(:), allocatable :: amp
  type(interaction_t) :: int_hard
  type(isolated_state_t) :: isolated
  type(connected_state_t) :: connected
  class(prc_core_state_t), allocatable :: core_state
  logical :: checked = .false.
  logical :: passed = .false.

```

```

real(default) :: scale = 0
real(default) :: fac_scale = 0
real(default) :: ren_scale = 0
real(default) :: es_scale = 0
real(default), allocatable :: alpha_qcd_forced
real(default) :: weight = 1
type(vector4_t), dimension(:), allocatable :: p_seed
type(vector4_t), dimension(:), allocatable :: p_hard
integer :: nlo_type = BORN
integer, dimension(:), allocatable :: same_kinematics
logical :: negative_sf = .false.
contains
  <Instances: term instance: TBP>
end type term_instance_t

```

<Instances: term instance: TBP>≡

```

procedure :: write => term_instance_write

```

<Instances: procedures>≡

```

subroutine term_instance_write (term, unit, kin, show_eff_state, testflag)
  class(term_instance_t), intent(in) :: term
  integer, intent(in), optional :: unit
  type(kinematics_t), intent(in), optional :: kin
  logical, intent(in), optional :: show_eff_state
  logical, intent(in), optional :: testflag
  integer :: u
  logical :: state
  u = given_output_unit (unit)
  state = .true.; if (present (show_eff_state)) state = show_eff_state
  if (term%active) then
    if (associated (term%config)) then
      write (u, "(1x,A,I0,A,I0,A)") "Term #", term%config%i_term, &
        " (component #", term%config%i_component, ")"
    else
      write (u, "(1x,A)") "Term [undefined]"
    end if
  else
    write (u, "(1x,A,I0,A)") "Term #", term%config%i_term, &
      " [inactive]"
  end if
  if (term%checked) then
    write (u, "(3x,A,L1)") "passed cuts" = ", term%passed
  end if
  if (term%passed) then
    write (u, "(3x,A,ES19.12)") "overall scale" = ", term%scale
    write (u, "(3x,A,ES19.12)") "factorization scale" = ", term%fac_scale
    write (u, "(3x,A,ES19.12)") "renormalization scale" = ", term%ren_scale
    if (allocated (term%alpha_qcd_forced)) then
      write (u, "(3x,A,ES19.12)") "alpha(QCD) forced" = ", &
        term%alpha_qcd_forced
    end if
    write (u, "(3x,A,ES19.12)") "reweighting factor" = ", term%weight
  end if
  !!! This used to be a member of term_instance

```

```

    if (present (kin)) then
        call kin%write (u)
    end if
    call write_separator (u)
    write (u, "(1x,A)" "Amplitude (transition matrix of the &
        &hard interaction):"
    call write_separator (u)
    call term%int_hard%basic_write (u, testflag = testflag)
    if (state .and. term%isolated%has_trace) then
        call write_separator (u)
        write (u, "(1x,A)" "Evaluators for the hard interaction:"
        call term%isolated%write (u, testflag = testflag)
    end if
    if (state .and. term%connected%has_trace) then
        call write_separator (u)
        write (u, "(1x,A)" "Evaluators for the connected process:"
        call term%connected%write (u, testflag = testflag)
    end if
end subroutine term_instance_write

```

The interactions and evaluators must be finalized.

```

<Instances: term instance: TBP>+≡
    procedure :: final => term_instance_final

<Instances: procedures>+≡
    subroutine term_instance_final (term)
        class(term_instance_t), intent(inout) :: term
        if (allocated (term%amp)) deallocate (term%amp)
        if (allocated (term%core_state)) deallocate (term%core_state)
        if (allocated (term%alpha_qcd_forced)) &
            deallocate (term%alpha_qcd_forced)
        if (allocated (term%p_seed)) deallocate (term%p_seed)
        if (allocated (term%p_hard)) deallocate (term%p_hard)
        call term%connected%final ()
        call term%isolated%final ()
        call term%int_hard%final ()
        term%pcm => null ()
        term%pcm_work => null ()
    end subroutine term_instance_final

```

For a new term object, we configure the structure-function interface, the phase space, the matrix-element (interaction) interface, etc.

```

<Instances: term instance: TBP>+≡
    procedure :: configure => term_instance_configure

<Instances: procedures>+≡
    subroutine term_instance_configure (term_instance, process, i, pcm_work, sf_chain, kin)
        class(term_instance_t), intent(out), target :: term_instance
        type(process_t), intent(in), target :: process
        integer, intent(in) :: i
        class(pcm_workspace_t), intent(in), target :: pcm_work
        type(sf_chain_t), intent(in), target :: sf_chain
        type(kinematics_t), intent(inout), target :: kin
        type(process_term_t) :: term

```

```

integer :: i_component
logical :: requires_extended_sf
term = process%get_term_ptr (i)
i_component = term%i_component
if (i_component /= 0) then
  call term_instance%init &
    (process%get_pcm_ptr (), pcm_work, process%get_nlo_type_component (i_component))
  requires_extended_sf = term_instance%nlo_type == NLO_DGLAP .or. &
    (term_instance%nlo_type == NLO_REAL .and. process%get_i_sub (i) == i)
  call term_instance%setup_dynamics (process, i, kin, &
    real_finite = process%component_is_real_finite (i_component))
  select type (phs => kin%phs)
  type is (phs_fks_t)
    call term_instance%set_emitter (kin)
    call term_instance%setup_fks_kinematics (kin, &
      process%get_var_list_ptr (), &
      process%get_beam_config_ptr ())
  end select
  select type (pcm => term_instance%pcm)
  type is (pcm_nlo_t)
    call kin%set_threshold (pcm%settings%factorization_mode)
  end select
  call term_instance%setup_expressions (process%get_meta (), process%get_config ())
end if
end subroutine term_instance_configure

```

First part of term-instance configuration: initialize by assigning pointers to the overall pcm and the associated pcm_workspace objects.

(Instances: term instance: TBP)+≡

```

procedure :: init => term_instance_init

```

(Instances: procedures)+≡

```

subroutine term_instance_init (term_instance, pcm, pcm_work, nlo_type)
  class(term_instance_t), intent(out) :: term_instance
  class(pcm_t), intent(in), target :: pcm
  class(pcm_workspace_t), intent(in), target :: pcm_work
  integer, intent(in) :: nlo_type
  term_instance%pcm => pcm
  term_instance%pcm_work => pcm_work
  term_instance%nlo_type = nlo_type
end subroutine term_instance_init

```

The second part of term-instance configuration concerns dynamics, i.e., the interface to the matrix-element (interaction), and the parton-state objects that combine all kinematics and matrix-element data for evaluation.

The hard interaction (incoming momenta) is linked to the structure function instance. In the isolated state, we either set pointers to both, or we create modified copies (**rearrange**) as effective structure-function chain and interaction, respectively.

Finally, we set up the **subevt** component that will be used for evaluating observables, collecting particles from the trace evaluator in the effective connected state. Their quantum numbers must be determined by following back source links and set explicitly, since they are already eliminated in that trace.

The `rearrange` parts are still commented out; they could become relevant for a NLO algorithm.

(Instances: term instance: TBP)+≡

```
procedure :: setup_dynamics => term_instance_setup_dynamics
```

(Instances: procedures)+≡

```
subroutine term_instance_setup_dynamics (term, process, i_term, kin, real_finite)
  class(term_instance_t), intent(inout), target :: term
  type(process_t), intent(in), target :: process
  integer, intent(in) :: i_term
  type(kinematics_t), intent(in) :: kin
  logical, intent(in), optional :: real_finite
  class(prc_core_t), pointer :: core => null ()
  type(process_beam_config_t) :: beam_config
  type(interaction_t), pointer :: sf_chain_int
  type(interaction_t), pointer :: src_int
  type(quantum_numbers_mask_t), dimension(:), allocatable :: mask_in
  type(state_matrix_t), pointer :: state_matrix
  type(flavor_t), dimension(:), allocatable :: flv_int, flv_src, f_in, f_out
  integer, dimension(:,:), allocatable :: flv_born, flv_real
  type(flavor_t), dimension(:,:), allocatable :: flv_pdf
  type(quantum_numbers_t), dimension(:,:), allocatable :: qn_pdf
  integer :: n_in, n_vir, n_out, n_tot, n_sub
  integer :: n_flv_born, n_flv_real, n_flv_total
  integer :: i, j
  logical :: me_already_squared, keep_fs_flavors
  logical :: decrease_n_tot
  logical :: requires_extended_sf
  me_already_squared = .false.
  keep_fs_flavors = .false.
  term%config => process%get_term_ptr (i_term)
  term%int_hard = term%config%int
  core => process%get_core_term (i_term)
  term%negative_sf = process%get_negative_sf ()
  call core%allocate_workspace (term%core_state)
  select type (core)
  class is (prc_external_t)
    call reduce_interaction (term%int_hard, &
      core%includes_polarization (), .true., .false.)
    me_already_squared = .true.
    allocate (term%amp (term%int_hard%get_n_matrix_elements ()))
  class default
    allocate (term%amp (term%config%n_allowed))
  end select
  if (allocated (term%core_state)) then
    select type (core_state => term%core_state)
    type is (openloops_state_t)
      call core_state%init_threshold (process%get_model_ptr ())
    end select
  end if
  term%amp = cmplx (0, 0, default)
  decrease_n_tot = term%nlo_type == NLO_REAL .and. &
    term%config%i_term_global /= term%config%i_sub
  if (present (real_finite)) then
```

```

        if (real_finite) decrease_n_tot = .false.
    end if
    if (decrease_n_tot) then
        allocate (term%p_seed (term%int_hard%get_n_tot () - 1))
    else
        allocate (term%p_seed (term%int_hard%get_n_tot ()))
    end if
    allocate (term%p_hard (term%int_hard%get_n_tot ()))
    sf_chain_int => kin%sf_chain%get_out_int_ptr ()
    n_in = term%int_hard%get_n_in ()
    do j = 1, n_in
        i = kin%sf_chain%get_out_i (j)
        call term%int_hard%set_source_link (j, sf_chain_int, i)
    end do
    call term%isolated%init (kin%sf_chain, term%int_hard)
    allocate (mask_in (n_in))
    mask_in = kin%sf_chain%get_out_mask ()
    select type (phs => kin%phs)
        type is (phs_wood_t)
            if (me_already_squared) then
                call term%isolated%setup_identity_trace &
                    (core, mask_in, .true., .false.)
            else
                call term%isolated%setup_square_trace &
                    (core, mask_in, term%config%col, .false.)
            end if
        type is (phs_fks_t)
            select case (phs%mode)
                case (PHS_MODE_ADDITIONAL_PARTICLE)
                    if (me_already_squared) then
                        call term%isolated%setup_identity_trace &
                            (core, mask_in, .true., .false.)
                    else
                        keep_fs_flavors = term%config%data%n_flv > 1
                        call term%isolated%setup_square_trace &
                            (core, mask_in, term%config%col, &
                                keep_fs_flavors)
                    end if
                case (PHS_MODE_COLLINEAR_REMNANT)
                    if (me_already_squared) then
                        call term%isolated%setup_identity_trace &
                            (core, mask_in, .true., .false.)
                    else
                        call term%isolated%setup_square_trace &
                            (core, mask_in, term%config%col, .false.)
                    end if
            end select
        class default
            call term%isolated%setup_square_trace &
                (core, mask_in, term%config%col, .false.)
    end select
    if (term%nlo_type == NLO_VIRTUAL .or. (term%nlo_type == NLO_REAL .and. &
        term%config%i_term_global == term%config%i_sub) .or. &
        term%nlo_type == NLO_MISMATCH) then

```



```

        n_sub = term%get_n_sub ()
    else if (term%nlo_type == NLO_DGLAP) then
        n_sub = n_beams_rescaled + term%get_n_sub ()
    else
        !!! No integration of real subtraction in interactions yet
        n_sub = 0
    end if
    keep_fs_flavors = keep_fs_flavors .or. me_already_squared
    requires_extended_sf = term%nlo_type == NLO_DGLAP .or. &
        (term%is_subtraction () .and. process%pcm_contains_pdfs ())
    call term%connected%setup_connected_trace (term%isolated, &
        undo_helicities = undo_helicities (core, me_already_squared), &
        keep_fs_flavors = keep_fs_flavors, &
        requires_extended_sf = requires_extended_sf)
    associate (int_eff => term%isolated%int_eff)
        state_matrix => int_eff%get_state_matrix_ptr ()
        n_tot = int_eff%get_n_tot ()
        flv_int = quantum_numbers_get_flavor &
            (state_matrix%get_quantum_number (1))
        allocate (f_in (n_in))
        f_in = flv_int(1:n_in)
        deallocate (flv_int)
    end associate
    n_in = term%connected%trace%get_n_in ()
    n_vir = term%connected%trace%get_n_vir ()
    n_out = term%connected%trace%get_n_out ()
    allocate (f_out (n_out))
    do j = 1, n_out
        call term%connected%trace%find_source &
            (n_in + n_vir + j, src_int, i)
        if (associated (src_int)) then
            state_matrix => src_int%get_state_matrix_ptr ()
            flv_src = quantum_numbers_get_flavor &
                (state_matrix%get_quantum_number (1))
            f_out(j) = flv_src(i)
            deallocate (flv_src)
        end if
    end do

    beam_config = process%get_beam_config ()

    call term%connected%setup_subevt (term%isolated%sf_chain_eff, &
        beam_config%data%flv, f_in, f_out)
    call term%connected%setup_var_list &
        (process%get_var_list_ptr (), beam_config%data)
    ! Does connected%trace never have any helicity qn?
    call term%init_interaction_qn_index (core, term%connected%trace, n_sub, &
        process%get_model_ptr (), is_polarized = .false.)
    call term%init_interaction_qn_index (core, term%int_hard, n_sub, process%get_model_ptr ())
    if (requires_extended_sf) then
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
            n_in = pcm%region_data%get_n_in ()
            flv_born = pcm%region_data%get_flv_states_born ()

```

```

        flv_real = pcm%region_data%get_flv_states_real ()
        n_flv_born = pcm%region_data%get_n_flv_born ()
        n_flv_real = pcm%region_data%get_n_flv_real ()
        n_flv_total = n_flv_born + n_flv_real
        allocate (flv_pdf(n_in, n_flv_total), &
                 qn_pdf(n_in, n_flv_total))
        call flv_pdf(:, :n_flv_born)%init (flv_born(:n_in, :))
        call flv_pdf(:, n_flv_born + 1:n_flv_total)%init (flv_real(:n_in, :))
        call qn_pdf%init (flv_pdf)
        call sf_chain_int%init_qn_index (qn_pdf, n_flv_born, n_flv_real)
    end select
end if
contains

function undo_helicities (core, me_squared) result (val)
    logical :: val
    class(prc_core_t), intent(in) :: core
    logical, intent(in) :: me_squared
    select type (core)
    class is (prc_external_t)
        val = me_squared .and. .not. core%includes_polarization ()
    class default
        val = .false.
    end select
end function undo_helicities

subroutine reduce_interaction (int, polarized_beams, keep_fs_flavors, &
                             keep_colors)
    type(interaction_t), intent(inout) :: int
    logical, intent(in) :: polarized_beams
    logical, intent(in) :: keep_fs_flavors, keep_colors
    type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
    logical, dimension(:), allocatable :: mask_f, mask_c, mask_h
    integer :: n_tot, n_in
    n_in = int%get_n_in (); n_tot = int%get_n_tot ()
    allocate (qn_mask (n_tot))
    allocate (mask_f (n_tot), mask_c (n_tot), mask_h (n_tot))
    mask_c = .not. keep_colors
    mask_f (1 : n_in) = .false.
    if (keep_fs_flavors) then
        mask_f (n_in + 1 : ) = .false.
    else
        mask_f (n_in + 1 : ) = .true.
    end if
    if (polarized_beams) then
        mask_h (1 : n_in) = .false.
    else
        mask_h (1 : n_in) = .true.
    end if
    mask_h (n_in + 1 : ) = .true.
    call qn_mask%init (mask_f, mask_c, mask_h)
    call int%reduce_state_matrix (qn_mask, keep_order = .true.)
end subroutine reduce_interaction
end subroutine term_instance_setup_dynamics

```

Set up index mapping from state matrix to index pair `i_flg`, `i_sub`.

(Instances: public)≡

```
public :: setup_interaction_qn_index
```

(Instances: procedures)+≡

```
subroutine setup_interaction_qn_index (int, data, qn_config, n_sub, is_polarized)
  class(interaction_t), intent(inout) :: int
  class(process_constants_t), intent(in) :: data
  type(quantum_numbers_t), dimension(:, :), intent(in) :: qn_config
  integer, intent(in) :: n_sub
  logical, intent(in) :: is_polarized
  integer :: i
  type(quantum_numbers_t), dimension(:, :), allocatable :: qn_hel
  if (is_polarized) then
    call setup_interaction_qn_hel (int, data, qn_hel)
    call int%init_qn_index (qn_config, n_sub, qn_hel)
    call int%set_qn_index_helicity_flip (.true.)
  else
    call int%init_qn_index (qn_config, n_sub)
  end if
end subroutine setup_interaction_qn_index
```

Set up beam polarisation quantum numbers, if beam polarisation is required.

We retrieve the full helicity information from `term%config%data` and reduce the information only to the initial state. Afterwards, we uniquify the initial state polarization by applying an index (hash) table.

The helicity information is fed into an array of quantum numbers to assign flavor, helicity and subtraction indices correctly to their matrix element.

(Instances: public)+≡

```
public :: setup_interaction_qn_hel
```

(Instances: procedures)+≡

```
subroutine setup_interaction_qn_hel (int, data, qn_hel)
  class(interaction_t), intent(in) :: int
  class(process_constants_t), intent(in) :: data
  type(quantum_numbers_t), dimension(:, :), allocatable, intent(out) :: qn_hel
  type(helicity_t), dimension(:, :), allocatable :: hel
  integer, dimension(:, :), allocatable :: index_table
  integer, dimension(:, :), allocatable :: hel_state
  integer :: i, j, n_hel_unique
  associate (n_in => int%get_n_in (), n_tot => int%get_n_tot ())
    allocate (hel_state (n_tot, data%get_n_hel ()), &
      source = data%hel_state)
    allocate (index_table (data%get_n_hel ()), &
      source = 0)
    forall (j=1:data%get_n_hel (), i=n_in+1:n_tot) hel_state(i, j) = 0
    n_hel_unique = 0
    HELICITY: do i = 1, data%get_n_hel ()
      do j = 1, data%get_n_hel ()
        if (index_table (j) == 0) then
          index_table(j) = i; n_hel_unique = n_hel_unique + 1
        cycle HELICITY
      end do
    end do
  end associate
end subroutine setup_interaction_qn_hel
```

```

        else if (all (hel_state(:, i) == &
            hel_state(:, index_table(j)))) then
            cycle HELICITY
        end if
    end do
end do HELICITY
allocate (qn_hel (n_tot, n_hel_unique))
allocate (hel (n_tot))
do j = 1, n_hel_unique
    call hel%init (hel_state(:, index_table(j)))
    call qn_hel(:, j)%init (hel)
end do
end associate
end subroutine setup_interaction_qn_hel

```

(Instances: term instance: TBP)+≡

```

procedure :: init_interaction_qn_index => term_instance_init_interaction_qn_index

```

(Instances: procedures)+≡

```

subroutine term_instance_init_interaction_qn_index (term, core, int, n_sub, &
    model, is_polarized)
    class(term_instance_t), intent(inout), target :: term
    class(prc_core_t), intent(in) :: core
    class(interaction_t), intent(inout) :: int
    integer, intent(in) :: n_sub
    class(model_data_t), intent(in) :: model
    logical, intent(in), optional :: is_polarized
    logical :: polarized
    type(quantum_numbers_t), dimension(:, :), allocatable :: qn_config
    integer, dimension(:, :), allocatable :: flv_born
    type(flavor_t), dimension(:, :), allocatable :: flv
    integer :: i
    select type (core)
    class is (prc_external_t)
        if (present (is_polarized)) then
            polarized = is_polarized
        else
            polarized = core%includes_polarization ()
        end if
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            associate (is_born => .not. (term%nlo_type == NLO_REAL .and. &
                .not. term%is_subtraction ()))
                select type (pcm => term%pcm)
                type is (pcm_nlo_t)
                    qn_config = pcm%get_qn (is_born)
                end select
                call setup_interaction_qn_index (int, term%config%data, &
                    qn_config, n_sub, polarized)
            end associate
        class default
            call term%config%data%get_flv_state (flv_born)
            allocate (flv (size (flv_born, dim = 1)))
            allocate (qn_config (size (flv_born, dim = 1), size (flv_born, dim = 2)))

```

```

do i = 1, core%data%n_flv
  call flv%init (flv_born(:,i), model)
  call qn_config(:, i)%init (flv)
end do
call setup_interaction_qn_index (int, term%config%data, &
  qn_config, n_sub, polarized)
end select
class default
  call int%init_qn_index ()
end select
end subroutine term_instance_init_interaction_qn_index

```

(Instances: term instance: TBP)+≡

```

procedure :: setup_fks_kinematics => term_instance_setup_fks_kinematics

```

(Instances: procedures)+≡

```

subroutine term_instance_setup_fks_kinematics (term, kin, var_list, beam_config)
  class(term_instance_t), intent(inout), target :: term
  type(kinematics_t), intent(inout) :: kin
  type(var_list_t), intent(in) :: var_list
  type(process_beam_config_t), intent(in) :: beam_config
  integer :: mode
  logical :: singular_jacobian
  if (.not. (term%nlo_type == NLO_REAL .or. term%nlo_type == NLO_DGLAP .or. &
    term%nlo_type == NLO_MISMATCH)) return
  singular_jacobian = var_list%get_lval (var_str ("?powheg_use_singular_jacobian"))
  if (term%nlo_type == NLO_REAL) then
    mode = check_generator_mode (GEN_REAL_PHASE_SPACE)
  else if (term%nlo_type == NLO_MISMATCH) then
    mode = check_generator_mode (GEN_SOFT_MISMATCH)
  else
    mode = PHS_MODE_UNDEFINED
  end if
  select type (phs => kin%phs)
  type is (phs_fks_t)
    select type (pcm => term%pcm)
    type is (pcm_nlo_t)
      select type (pcm_work => term%pcm_work)
      type is (pcm_nlo_workspace_t)
        call pcm%setup_phs_generator (pcm_work, &
          phs%generator, phs%config%sqrts, mode, singular_jacobian)
        if (beam_config%has_structure_function ()) then
          pcm_work%isr_kinematics%isr_mode = SQRTS_VAR
        else
          pcm_work%isr_kinematics%isr_mode = SQRTS_FIXED
        end if
        if (debug_on) call msg_debug (D_PHASESPACE, "isr_mode: ", pcm_work%isr_kinematics%isr_mode)
      end select
    end select
  class default
    call msg_fatal ("Phase space should be an FKS phase space!")
  end select
contains
  function check_generator_mode (gen_mode_default) result (gen_mode)

```

```

integer :: gen_mode
integer, intent(in) :: gen_mode_default
select type (pcm => term%pcm)
type is (pcm_nlo_t)
  associate (settings => pcm%settings)
    if (settings%test_coll_limit .and. settings%test_anti_coll_limit) &
      call msg_fatal ("You cannot check the collinear and anti-collinear limit "&
        &"at the same time!")
    if (settings%test_soft_limit .and. .not. settings%test_coll_limit &
      .and. .not. settings%test_anti_coll_limit) then
      gen_mode = GEN_SOFT_LIMIT_TEST
    else if (.not. settings%test_soft_limit .and. settings%test_coll_limit) then
      gen_mode = GEN_COLL_LIMIT_TEST
    else if (.not. settings%test_soft_limit .and. settings%test_anti_coll_limit) then
      gen_mode = GEN_ANTI_COLL_LIMIT_TEST
    else if (settings%test_soft_limit .and. settings%test_coll_limit) then
      gen_mode = GEN_SOFT_COLL_LIMIT_TEST
    else if (settings%test_soft_limit .and. settings%test_anti_coll_limit) then
      gen_mode = GEN_SOFT_ANTI_COLL_LIMIT_TEST
    else
      gen_mode = gen_mode_default
    end if
  end associate
end select
end function check_generator_mode
end subroutine term_instance_setup_fks_kinematics

```

Set up seed kinematics, starting from the MC parameter set given as argument. As a result, the `k_seed` kinematics object is evaluated (except for the structure-function matrix-element evaluation, which we postpone until we know the factorization scale), and we have a valid `p_seed` momentum array.

```

<Instances: term instance: TBP>+≡
  procedure :: compute_seed_kinematics => term_instance_compute_seed_kinematics

<Instances: procedures>+≡
  subroutine term_instance_compute_seed_kinematics &
    (term, kin, mci_work, phs_channel, success)
    class(term_instance_t), intent(inout), target :: term
    type(kinematics_t), intent(inout) :: kin
    type(mci_work_t), intent(in) :: mci_work
    integer, intent(in) :: phs_channel
    logical, intent(out) :: success
    call kin%compute_selected_channel &
      (mci_work, phs_channel, term%p_seed, success)
  end subroutine term_instance_compute_seed_kinematics

<Instances: term instance: TBP>+≡
  procedure :: evaluate_projections => term_instance_evaluate_projections

<Instances: procedures>+≡
  subroutine term_instance_evaluate_projections (term, kin)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(inout) :: kin
    if (kin%threshold .and. term%nlo_type > BORN) then

```

```

    if (debug2_active (D_THRESHOLD)) &
        print *, 'Evaluate on-shell projection: ', &
            char (component_status (term%nlo_type))
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
        call kin%threshold_projection (pcm_work, term%nlo_type)
    end select
end if
end subroutine term_instance_evaluate_projections

```

Compute the momenta in the hard interactions, one for each term that constitutes this process component. In simple cases this amounts to just copying momenta. In more advanced cases, we may generate distinct sets of momenta from the seed kinematics.

The interactions in the term instances are accessed individually. We may choose to calculate all terms at once together with the seed kinematics, use `component%core_state` for storage, and just fill the interactions here.

(Instances: term instance: TBP)+≡

```

    procedure :: compute_hard_kinematics => &
        term_instance_compute_hard_kinematics

```

(Instances: procedures)+≡

```

    subroutine term_instance_compute_hard_kinematics &
        (term, kin, recover, skip_term, success)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(inout) :: kin
    integer, intent(in), optional :: skip_term
    logical, intent(in), optional :: recover
    logical, intent(out) :: success
    type(vector4_t), dimension(:), allocatable :: p
    if (allocated (term%core_state)) &
        call term%core_state%reset_new_kinematics ()
    if (present (skip_term)) then
        if (term%config%i_term_global == skip_term) return
    end if

    if (present (recover)) then
        if (recover) return
    end if
    if (term%nlo_type == NLO_REAL .and. kin%emitter >= 0) then
        call kin%evaluate_radiation (term%p_seed, p, success)
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
            if (pcm%dalitz_plot%active) then
                if (kin%emitter > kin%n_in) then
                    if (p(kin%emitter)**2 > tiny_07) &
                        call pcm%register_dalitz_plot (kin%emitter, p)
                end if
            end if
        end select
    else if (is_subtraction_component (kin%emitter, term%nlo_type)) then
        call kin%modify_momenta_for_subtraction (term%p_seed, p)
        success = .true.
    end if

```

```

else
  allocate (p (size (term%p_seed))); p = term%p_seed
  success = .true.
end if
call term%int_hard%set_momenta (p)
if (debug_on) then
  call msg_debug2 (D_REAL, "inside compute_hard_kinematics")
  if (debug2_active (D_REAL)) call vector4_write_set (p)
end if
end subroutine term_instance_compute_hard_kinematics

```

Here, we invert this. We fetch the incoming momenta which reside in the appropriate `sf_chain` object, stored within the `k_seed` subobject. On the other hand, we have the outgoing momenta of the effective interaction. We rely on the process core to compute the remaining seed momenta and to fill the momenta within the hard interaction. (The latter is trivial if hard and effective interaction coincide.)

After this is done, the incoming momenta in the trace evaluator that corresponds to the hard (effective) interaction, are still left undefined. We remedy this by calling `receive_kinematics` once.

```

<Instances: term instance: TBP>+≡
  procedure :: recover_seed_kinematics => &
    term_instance_recover_seed_kinematics

<Instances: procedures>+≡
  subroutine term_instance_recover_seed_kinematics (term, kin, p_seed_ref)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(in) :: kin
    integer :: n_in
    type(vector4_t), dimension(:), intent(in), optional :: p_seed_ref
    n_in = kin%n_in
    call kin%get_incoming_momenta (term%p_seed(1:n_in))
    associate (int_eff => term%isolated%int_eff)
      call int_eff%set_momenta (term%p_seed(1:n_in), outgoing = .false.)
      if (present (p_seed_ref)) then
        term%p_seed(n_in + 1 : ) = p_seed_ref
      else
        term%p_seed(n_in + 1 : ) = int_eff%get_momenta (outgoing = .true.)
      end if
    end associate
    call term%isolated%receive_kinematics ()
  end subroutine term_instance_recover_seed_kinematics

```

Compute the integration parameters for all channels except the selected one.
JRR: Obsolete now.

```

<XXX Instances: term instance: TBP>≡
  procedure :: compute_other_channels => &
    term_instance_compute_other_channels

<XXX Instances: procedures>≡
  subroutine term_instance_compute_other_channels &
    (term, mci_work, phs_channel)
    class(term_instance_t), intent(inout), target :: term

```



```

type(mci_work_t), intent(in) :: mci_work
integer, intent(in) :: phs_channel
call term%k_term%compute_other_channels (mci_work, phs_channel)
end subroutine term_instance_compute_other_channels

```

Recover beam momenta, i.e., return the beam momenta as currently stored in the kinematics subobject to their source. This is a side effect. JRR: Obsolete now.

```

<XXX Instances: term instance: TBP>+≡
  procedure :: return_beam_momenta => term_instance_return_beam_momenta

<XXX Instances: procedures>+≡
  subroutine term_instance_return_beam_momenta (term)
    class(term_instance_t), intent(in) :: term
    call term%k_term%return_beam_momenta ()
  end subroutine term_instance_return_beam_momenta

```

Applies the real partition by computing the real partition function $F(\Phi)$ and multiplying either $\mathcal{R}_{\text{sin}} = \mathcal{R} \cdot F$ or $\mathcal{R}_{\text{fin}} = \mathcal{R} \cdot (1 - F)$.

```

<Instances: term instance: TBP>+≡
  procedure :: apply_real_partition => term_instance_apply_real_partition

<Instances: procedures>+≡
  subroutine term_instance_apply_real_partition (term, kin, process)
    class(term_instance_t), intent(inout) :: term
    type(kinematics_t), intent(in) :: kin
    type(process_t), intent(in) :: process
    real(default) :: f, sqme
    integer :: i_component
    integer :: i_amp, n_amps, qn_index
    logical :: is_subtraction
    i_component = term%config%i_component
    if (process%component_is_selected (i_component) .and. &
        process%get_component_nlo_type (i_component) == NLO_REAL) then
      is_subtraction = process%get_component_type (i_component) == COMP_REAL_SING &
        .and. kin%emitter < 0
      if (is_subtraction) return
      select case (process%get_component_type (i_component))
      case (COMP_REAL_FIN)
        call term%connected%trace%set_duplicate_flv_zero()
      end select
      select type (pcm => process%get_pcm_ptr ())
      type is (pcm_nlo_t)
        f = pcm%real_partition%get_f (term%p_hard)
      end select
      n_amps = term%connected%trace%get_n_matrix_elements ()
      do i_amp = 1, n_amps
        qn_index = term%connected%trace%get_qn_index (i_amp, i_sub = 0)
        sqme = real (term%connected%trace%get_matrix_element (qn_index))
        if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "term_instance_apply_real_partition")
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
          select case (process%get_component_type (i_component))
          case (COMP_REAL_FIN, COMP_REAL_SING)

```

```

        select case (process%get_component_type (i_component))
        case (COMP_REAL_FIN)
            if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "Real finite")
            sqme = sqme * (one - f)
        case (COMP_REAL_SING)
            if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "Real singular")
            sqme = sqme * f
        end select
    end select
end select
if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "apply_damping: sqme", sqme)
call term%connected%trace%set_matrix_element (qn_index, cmplx (sqme, zero, default))
end do
end if
end subroutine term_instance_apply_real_partition

```

(Instances: term instance: TBP)+≡

```

    procedure :: get_p_hard => term_instance_get_p_hard

```

(Instances: procedures)+≡

```

    pure function term_instance_get_p_hard (term_instance) result (p_hard)
        type(vector4_t), dimension(:), allocatable :: p_hard
        class(term_instance_t), intent(in) :: term_instance
        allocate (p_hard (size (term_instance%p_hard)))
        p_hard = term_instance%p_hard
    end function term_instance_get_p_hard

```

(Instances: term instance: TBP)+≡

```

    procedure :: set_emitter => term_instance_set_emitter

```

(Instances: procedures)+≡

```

    subroutine term_instance_set_emitter (term, kin)
        class(term_instance_t), intent(inout) :: term
        type(kinematics_t), intent(inout) :: kin
        integer :: i_phs
        logical :: set_emitter
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
            select type (phs => kin%phs)
            type is (phs_fks_t)
                !!! Without resonances, i_alr = i_phs
                i_phs = term%config%i_term
                kin%i_phs = i_phs
                set_emitter = i_phs <= pcm%region_data%n_phs .and. term%nlo_type == NLO_REAL
                if (set_emitter) then
                    kin%emitter = phs%phs_identifiers(i_phs)%emitter
                    select type (pcm => term%pcm)
                    type is (pcm_nlo_t)
                        if (allocated (pcm%region_data%i_phs_to_i_con)) &
                            kin%i_con = pcm%region_data%i_phs_to_i_con (i_phs)
                    end select
                end if
            end select
        end select
    end subroutine

```

```
end subroutine term_instance_set_emitter
```

For initializing the expressions, we need the local variable list and the parse trees.

```
(Instances: term instance: TBP)+≡
  procedure :: setup_expressions => term_instance_setup_expressions
(Instances: procedures)+≡
  subroutine term_instance_setup_expressions (term, meta, config)
    class(term_instance_t), intent(inout), target :: term
    type(process_metadata_t), intent(in), target :: meta
    type(process_config_data_t), intent(in) :: config
    if (allocated (config%ef_cuts)) &
      call term%connected%setup_cuts (config%ef_cuts)
    if (allocated (config%ef_scale)) &
      call term%connected%setup_scale (config%ef_scale)
    if (allocated (config%ef_fac_scale)) &
      call term%connected%setup_fac_scale (config%ef_fac_scale)
    if (allocated (config%ef_ren_scale)) &
      call term%connected%setup_ren_scale (config%ef_ren_scale)
    if (allocated (config%ef_weight)) &
      call term%connected%setup_weight (config%ef_weight)
  end subroutine term_instance_setup_expressions
```

Prepare the extra evaluators that we need for processing events.

The matrix elements we get from OpenLoops and GoSam are already squared and summed over color and helicity. They should not be squared again.

```
(Instances: term instance: TBP)+≡
  procedure :: setup_event_data => term_instance_setup_event_data
(Instances: procedures)+≡
  subroutine term_instance_setup_event_data (term, kin, core, model)
    class(term_instance_t), intent(inout), target :: term
    type(kinematics_t), intent(in) :: kin
    class(prc_core_t), intent(in) :: core
    class(model_data_t), intent(in), target :: model
    integer :: n_in
    logical :: mask_color
    type(quantum_numbers_mask_t), dimension(:), allocatable :: mask_in
    n_in = term%int_hard%get_n_in ()
    allocate (mask_in (n_in))
    mask_in = kin%sf_chain%get_out_mask ()
    call setup_isolated (term%isolated, core, model, mask_in, term%config%col)
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
      mask_color = pcm_work%is_fixed_order_nlo_events ()
    class default
      mask_color = .false.
    end select
    call setup_connected (term%connected, term%isolated, core, &
      term%nlo_type, mask_color)
  contains
    subroutine setup_isolated (isolated, core, model, mask, color)
      type(isolated_state_t), intent(inout), target :: isolated
```

```

class(prc_core_t), intent(in) :: core
class(model_data_t), intent(in), target :: model
type(quantum_numbers_mask_t), intent(in), dimension(:) :: mask
integer, intent(in), dimension(:) :: color
select type (core)
class is (prc_blha_t)
    call isolated%matrix%init_identity(isolated%int_eff)
    isolated%has_matrix = .true.
class default
    call isolated%setup_square_matrix (core, model, mask, color)
end select
!!! TODO (PS-09-10-20) We should not square the flows
!!! if they come from BLHA either
call isolated%setup_square_flows (core, model, mask)
end subroutine setup_isolated

subroutine setup_connected (connected, isolated, core, nlo_type, mask_color)
type(connected_state_t), intent(inout), target :: connected
type(isolated_state_t), intent(in), target :: isolated
class(prc_core_t), intent(in) :: core
integer, intent(in) :: nlo_type
logical, intent(in) :: mask_color
type(quantum_numbers_mask_t), dimension(:), allocatable :: mask
call connected%setup_connected_matrix (isolated)
if (term%nlo_type == NLO_VIRTUAL .or. (term%nlo_type == NLO_REAL &
    .and. term%config%i_term_global == term%config%i_sub) &
    .or. term%nlo_type == NLO_DGLAP) then
    !!! We do not care about the subtraction matrix elements in
    !!! connected%matrix, because all entries there are supposed
    !!! to be squared. To be able to match with flavor quantum numbers,
    !!! we remove the subtraction quantum entries from the state matrix.
    allocate (mask (connected%matrix%get_n_tot()))
    call mask%set_sub (1)
    call connected%matrix%reduce_state_matrix (mask, keep_order = .true.)
end if
call term%init_interaction_qn_index (core, connected%matrix, 0, model, &
    is_polarized = .false.)
select type (core)
class is (prc_blha_t)
    call connected%setup_connected_flows &
        (isolated, mask_color = mask_color)
class default
    call connected%setup_connected_flows (isolated)
end select
call connected%setup_state_flv (isolated%get_n_out ())
end subroutine setup_connected
end subroutine term_instance_setup_event_data

```

Color-correlated matrix elements should be obtained from the external BLHA provider. According to the standard, the matrix elements output is a one-dimensional array. For FKS subtraction, we require the matrix B_{ij} . BLHA prescribes a mapping $(i, j) \rightarrow k$, where k is the index of the matrix element in the output array. It focusses on the off-diagonal entries, i.e. $i \neq j$. The subroutine

`blha_color_c_fill_offdiag` realizes this mapping. The diagonal entries can simply be obtained as the product of the Born matrix element and either C_A or C_F , which is achieved by `blha_color_c_fill_diag`. For simple processes, i.e. those with only one color line, it is $B_{ij} = C_F \cdot B$. For those, we keep the possibility of computing color correlations by a multiplication of the Born matrix element with C_F . It is triggered by the `use_internal_color_correlations` flag and should be used only for testing purposes. However, it is also used for the threshold computation where the process is well-defined and fixed.

(Instances: term instance: TBP)+≡

```
procedure :: evaluate_color_correlations => &
    term_instance_evaluate_color_correlations
```

(Instances: procedures)+≡

```
subroutine term_instance_evaluate_color_correlations (term, core)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
    integer :: i_flv_born
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
            if (debug_on) call msg_debug2 (D_SUBTRACTION, &
                "term_instance_evaluate_color_correlations: " // &
                "use_internal_color_correlations:", &
                pcm%settings%use_internal_color_correlations)
            if (debug_on) call msg_debug2 (D_SUBTRACTION, "fac_scale", term%fac_scale)
            do i_flv_born = 1, pcm%region_data%n_flv_born
                select case (term%nlo_type)
                case (NLO_REAL)
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        pcm_work%real_sub%sqme_born (i_flv_born), &
                        pcm_work%real_sub%sqme_born_color_c (:, :, i_flv_born))
                case (NLO_MISMATCH)
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        pcm_work%soft_mismatch%sqme_born (i_flv_born), &
                        pcm_work%soft_mismatch%sqme_born_color_c (:, :, i_flv_born))
                case (NLO_VIRTUAL)
                    !!! This is just a copy of the above with a different offset and can for sure be u
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        -one, pcm_work%virtual%sqme_color_c (:, :, i_flv_born))
                case (NLO_DGLAP)
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        pcm_work%dglap_remnant%sqme_born (i_flv_born), &
                        pcm_work%dglap_remnant%sqme_color_c_extra (:, :, i_flv_born))
                end select
            end do
        end select
    end select
contains
    function get_trivial_cf_factors (n_tot, flv, factorization_mode) result (beta_ij)
        integer, intent(in) :: n_tot, factorization_mode
        integer, intent(in), dimension(:) :: flv
        real(default), dimension(n_tot, n_tot) :: beta_ij
        if (factorization_mode == NO_FACTORIZATION) then
```

```

        beta_ij = get_trivial_cf_factors_default (n_tot, flv)
    else
        beta_ij = get_trivial_cf_factors_threshold (n_tot, flv)
    end if
end function get_trivial_cf_factors

function get_trivial_cf_factors_default (n_tot, flv) result (beta_ij)
    integer, intent(in) :: n_tot
    integer, intent(in), dimension(:) :: flv
    real(default), dimension(n_tot, n_tot) :: beta_ij
    integer :: i, j
    beta_ij = zero
    if (count (is_quark (flv)) == 2) then
        do i = 1, n_tot
            do j = 1, n_tot
                if (is_quark(flv(i)) .and. is_quark(flv(j))) then
                    if (i == j) then
                        beta_ij(i,j) = -cf
                    else
                        beta_ij(i,j) = cf
                    end if
                end if
            end do
        end do
    end if
end function get_trivial_cf_factors_default

function get_trivial_cf_factors_threshold (n_tot, flv) result (beta_ij)
    integer, intent(in) :: n_tot
    integer, intent(in), dimension(:) :: flv
    real(default), dimension(n_tot, n_tot) :: beta_ij
    integer :: i
    beta_ij = zero
    do i = 1, 4
        beta_ij(i,i) = -cf
    end do
    beta_ij(1,2) = cf; beta_ij(2,1) = cf
    beta_ij(3,4) = cf; beta_ij(4,3) = cf
end function get_trivial_cf_factors_threshold

subroutine transfer_me_array_to_bij (pcm, i_flv, &
    sqme_born, sqme_color_c)
    type(pcm_nlo_t), intent(in) :: pcm
    integer, intent(in) :: i_flv
    real(default), intent(in) :: sqme_born
    real(default), dimension(:,:), intent(inout) :: sqme_color_c
    logical :: special_case_interferences
    integer :: i_color_c, i_sub, n_offset
    real(default), dimension(:), allocatable :: sqme
    if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "transfer_me_array_to_bij")
    if (pcm%settings%use_internal_color_correlations) then
        !!! A negative value for sqme_born indicates that the Born matrix
        !!! element is multiplied at a different place, e.g. in the case
        !!! of the virtual component

```

```

sqme_color_c = get_trivial_cf_factors &
    (pcm%region_data%get_n_legs_born (), &
    pcm%region_data%get_flv_states_born (i_flv), &
    pcm%settings%factorization_mode)
if (sqme_born > zero) then
    sqme_color_c = sqme_born * sqme_color_c
else if (sqme_born == zero) then
    sqme_color_c = zero
end if
else
    special_case_interferences = pcm%region_data%nlo_correction_type == "EW"
    n_offset = 0
    if (term%nlo_type == NLO_VIRTUAL) then
        n_offset = 1
    else if (pcm%has_pdfs .and. (term%is_subtraction () &
        .or. term%nlo_type == NLO_DGLAP)) then
        n_offset = n_beams_rescaled
    end if
    allocate (sqme (term%get_n_sub_color ()), source = zero)
    do i_sub = 1, term%get_n_sub_color ()
        sqme(i_sub) = real(term%connected%trace%get_matrix_element ( &
            term%connected%trace%get_qn_index (i_flv, i_sub = i_sub + n_offset)), &
            default)
    end do
    call blha_color_c_fill_offdiag (pcm%region_data%n_legs_born, &
        sqme, sqme_color_c)
    call blha_color_c_fill_diag (real(term%connected%trace%get_matrix_element ( &
        term%connected%trace%get_qn_index (i_flv, i_sub = 0)), default), &
        pcm%region_data%get_flv_states_born (i_flv), &
        sqme_color_c, special_case_interferences)
end if
end subroutine transfer_me_array_to_bij
end subroutine term_instance_evaluate_color_correlations

```

(Instances: term instance: TBP)+≡

```

procedure :: evaluate_charge_correlations => &
    term_instance_evaluate_charge_correlations

```

(Instances: procedures)+≡

```

subroutine term_instance_evaluate_charge_correlations (term, core)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
    integer :: i_flv_born
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
            do i_flv_born = 1, pcm%region_data%n_flv_born
                select case (term%nlo_type)
                case (NLO_REAL)
                    call transfer_me_array_to_bij (pcm, i_flv_born, &
                        pcm_work%real_sub%sqme_born (i_flv_born), &
                        pcm_work%real_sub%sqme_born_charge_c (:, :, i_flv_born))
                case (NLO_MISMATCH)

```

```

        call transfer_me_array_to_bij (pcm, i_flv_born, &
            pcm_work%soft_mismatch%sqme_born (i_flv_born), &
            pcm_work%soft_mismatch%sqme_born_charge_c (:, :, i_flv_born))
    case (NLO_VIRTUAL)
        call transfer_me_array_to_bij (pcm, i_flv_born, &
            one, pcm_work%virtual%sqme_charge_c (:, :, i_flv_born))
    end select
end do
end select
end select
contains
subroutine transfer_me_array_to_bij (pcm, i_flv, sqme_born, sqme_charge_c)
    type(pcm_nlo_t), intent(in) :: pcm
    integer, intent(in) :: i_flv
    real(default), intent(in) :: sqme_born
    real(default), dimension(:,:), intent(inout) :: sqme_charge_c
    integer :: n_legs_born, i, j
    real(default), dimension(:), allocatable :: sigma
    real(default), dimension(:), allocatable :: Q
    n_legs_born = pcm%region_data%n_legs_born
    associate (flv_born => pcm%region_data%flv_born(i_flv))
        allocate (sigma (n_legs_born), Q (size (flv_born%charge)))
        Q = flv_born%charge
        sigma(1:flv_born%n_in) = -one
        sigma(flv_born%n_in + 1: ) = one
    end associate
    do i = 1, n_legs_born
        do j = 1, n_legs_born
            sqme_charge_c(i, j) = sigma(i) * sigma(j) * Q(i) * Q(j) * (-one)
        end do
    end do
    sqme_charge_c = sqme_charge_c * sqme_born
end subroutine transfer_me_array_to_bij
end subroutine term_instance_evaluate_charge_correlations

```

The information about spin correlations is not stored in the `nlo_settings` because it is only available after the `fks_regions` have been created.

(Instances: term instance: TBP)+≡

```
procedure :: evaluate_spin_correlations => term_instance_evaluate_spin_correlations
```

(Instances: procedures)+≡

```

subroutine term_instance_evaluate_spin_correlations (term, core)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(inout) :: core
    integer :: i_flv, i_sub, i_emitter, emitter
    integer :: n_flv, n_sub_color, n_sub_spin, n_offset, i, j
    real(default), dimension(1:3, 1:3) :: sqme_spin_c
    real(default), dimension(:), allocatable :: sqme_spin_c_all
    real(default), dimension(:), allocatable :: sqme_spin_c_arr
    if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
        "term_instance_evaluate_spin_correlations")
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
        if (pcm_work%real_sub%requires_spin_correlations () &

```



```

        .and. term%nlo_type == NLO_REAL) then
select type (core)
type is (prc_openloops_t)
    select type (pcm => term%pcm)
    type is (pcm_nlo_t)
        n_flv = term%connected%trace%get_qn_index_n_flv ()
        n_sub_color = term%get_n_sub_color ()
        n_sub_spin = term%get_n_sub_spin ()
        n_offset = 0; if(pcm%has_pdfs) n_offset = n_beams_rescaled
        allocate (sqme_spin_c_arr(6))
        do i_flv = 1, n_flv
            allocate (sqme_spin_c_all(n_sub_spin))
            do i_sub = 1, n_sub_spin
                sqme_spin_c_all(i_sub) = real(term%connected%trace%get_matrix_element &
                    (term%connected%trace%get_qn_index (i_flv, &
                        i_sub = i_sub + n_offset + n_sub_color)), default)
            end do
            do i_emitter = 1, pcm%region_data%n_emitters
                emitter = pcm%region_data%emitters(i_emitter)
                if (emitter > 0) then
                    call split_array (sqme_spin_c_all, sqme_spin_c_arr)
                    do j = 1, size (sqme_spin_c, dim=2)
                        do i = j, size (sqme_spin_c, dim=1)
                            !!! Restoring the symmetric matrix packed into a 1-dim array
                            !!! c.f. [[prc_openloops_compute_sqme_spin_c]]
                            sqme_spin_c(i,j) = sqme_spin_c_arr(j + i * (i - 1) / 2)
                            if (i /= j) sqme_spin_c(j,i) = sqme_spin_c(i,j)
                        end do
                    end do
                    pcm_work%real_sub%sqme_born_spin_c(:, :, emitter, i_flv) = sqme_spin_c
                end if
            end do
            deallocate (sqme_spin_c_all)
        end do
    end select
class default
    call msg_fatal ("Spin correlations so far only supported by OpenLoops.")
end select
end if
end select
end subroutine term_instance_evaluate_spin_correlations

```

@

(Instances: term instance: TBP)+≡

```
procedure :: apply_fks => term_instance_apply_fks
```

(Instances: procedures)+≡

```

subroutine term_instance_apply_fks (term, kin, alpha_s_sub, alpha_qed_sub)
class(term_instance_t), intent(inout) :: term
class(kinematics_t), intent(inout) :: kin
real(default), intent(in) :: alpha_s_sub, alpha_qed_sub
real(default), dimension(:), allocatable :: sqme
integer :: i, i_phs, emitter
logical :: is_subtraction

```

```

select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    if (term%connected%has_matrix) then
      allocate (sqme (pcm%get_n_alr ()))
    else
      allocate (sqme (1))
    end if
    sqme = zero
    select type (phs => kin%phs)
    type is (phs_fks_t)
      if (pcm%has_pdfs .and. &
        pcm%settings%use_internal_color_correlations) then
        call msg_fatal ("Color correlations for proton processes " // &
          "so far only supported by OpenLoops.")
      end if
      call pcm_work%set_real_and_isr_kinematics &
        (phs%phs_identifiers, kin%phs%get_sqrts ())
      if (kin%emitter < 0) then
        call pcm_work%set_subtraction_event ()
        do i_phs = 1, pcm%region_data%n_phs
          emitter = phs%phs_identifiers(i_phs)%emitter
          call pcm_work%real_sub%compute (emitter, &
            i_phs, alpha_s_sub, alpha_qed_sub, term%connected%has_matrix, sqme)
        end do
      else
        call pcm_work%set_radiation_event ()
        emitter = kin%emitter; i_phs = kin%i_phs
        do i = 1, term%connected%trace%get_qn_index_n_flv ()
          pcm_work%real_sub%sqme_real_non_sub (i, i_phs) = &
            real (term%connected%trace%get_matrix_element ( &
              term%connected%trace%get_qn_index (i)))
        end do
        call pcm_work%real_sub%compute (emitter, i_phs, alpha_s_sub, &
          alpha_qed_sub, term%connected%has_matrix, sqme)
      end if
    end select
  end select
end select
if (term%connected%has_trace) &
  call term%connected%trace%set_only_matrix_element &
    (1, cmplx (sum(sqme), 0, default))
select type (pcm => term%pcm)
type is (pcm_nlo_t)
  is_subtraction = kin%emitter < 0
  if (term%connected%has_matrix) &
    call refill_evaluator (cmplx (sqme * term%weight, 0, default), &
      pcm%get_qn (is_subtraction), &
      pcm%region_data%get_flavor_indices (is_subtraction), &
      term%connected%matrix)
  if (term%connected%has_flows) &
    call refill_evaluator (cmplx (sqme * term%weight, 0, default), &
      pcm%get_qn (is_subtraction), &

```

```

        pcm%region_data%get_flavor_indices (is_subtraction), &
        term%connected%flows)
    end select
end subroutine term_instance_apply_fks

```

(Instances: term instance: TBP)+≡

```

    procedure :: evaluate_sqme_virt => term_instance_evaluate_sqme_virt

```

(Instances: procedures)+≡

```

subroutine term_instance_evaluate_sqme_virt (term, alpha_s, alpha_qed)
    class(term_instance_t), intent(inout) :: term
    real(default), intent(in) :: alpha_s, alpha_qed
    real(default), dimension(2) :: alpha_coupling
    type(vector4_t), dimension(:), allocatable :: p_born
    real(default), dimension(:), allocatable :: sqme_virt
    integer :: i_flv
    if (term%nlo_type /= NLO_VIRTUAL) call msg_fatal &
        ("Trying to evaluate virtual matrix element with unsuited term_instance.")
    if (debug2_active (D_VIRTUAL)) then
        call msg_debug2 (D_VIRTUAL, "Evaluating virtual-subtracted matrix elements")
        print *, 'ren_scale: ', term%ren_scale
        print *, 'fac_scale: ', term%fac_scale
        print *, 'ES scale: ', term%es_scale
    end if
    select type (pcm => term%pcm)
    type is (pcm_nlo_t)
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            alpha_coupling = [alpha_s, alpha_qed]
            if (debug2_active (D_VIRTUAL)) then
                print *, 'alpha_s: ', alpha_coupling (1)
                print *, 'alpha_qed: ', alpha_coupling (2)
            end if
            allocate (p_born (pcm%region_data%n_legs_born))
            if (pcm%settings%factorization_mode == FACTORIZATION_THRESHOLD) then
                p_born = pcm_work%real_kinematics%p_born_onshell%get_momenta(1)
            else
                p_born = term%int_hard%get_momenta ()
            end if
            call pcm_work%set_momenta_and_scales_virtual &
                (p_born, term%ren_scale, term%fac_scale, term%es_scale)
            select type (pcm_work => term%pcm_work)
            type is (pcm_nlo_workspace_t)
                associate (virtual => pcm_work%virtual)
                    do i_flv = 1, term%connected%trace%get_qn_index_n_flv ()
                        virtual%sqme_born(i_flv) = &
                            real (term%connected%trace%get_matrix_element ( &
                                term%connected%trace%get_qn_index (i_flv, i_sub = 0)))
                        virtual%sqme_virt_fin(i_flv) = &
                            real (term%connected%trace%get_matrix_element ( &
                                term%connected%trace%get_qn_index (i_flv, i_sub = 1)))
                    end do
                end associate
            end select
        end select
    end select

```

```

        call pcm_work%compute_sqme_virt (term%pcm, term%p_hard, alpha_coupling, &
            term%connected%has_matrix, sqme_virt)
        call term%connected%trace%set_only_matrix_element &
            (1, cmplx (sum(sqme_virt), 0, default))
        if (term%connected%has_matrix) &
            call refill_evaluator (cmplx (sqme_virt * term%weight, 0, default), &
                pcm%get_qn (.true.), &
                remove_duplicates_from_int_array ( &
                    pcm%region_data%get_flavor_indices (.true.)), &
                    term%connected%matrix)
        if (term%connected%has_flows) &
            call refill_evaluator (cmplx (sqme_virt * term%weight, 0, default), &
                pcm%get_qn (.true.), &
                remove_duplicates_from_int_array ( &
                    pcm%region_data%get_flavor_indices (.true.)), &
                    term%connected%flows)
    end select
end select
end subroutine term_instance_evaluate_sqme_virt

```

(Instances: term instance: TBP)+=

```

    procedure :: evaluate_sqme_mismatch => term_instance_evaluate_sqme_mismatch

```

(Instances: procedures)+=

```

    subroutine term_instance_evaluate_sqme_mismatch (term, alpha_s)
        class(term_instance_t), intent(inout) :: term
        real(default), intent(in) :: alpha_s
        real(default), dimension(:), allocatable :: sqme_mism
        if (term%nlo_type /= NLO_MISMATCH) call msg_fatal &
            ("Trying to evaluate soft mismatch with unsuited term_instance.")
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            call pcm_work%compute_sqme_mismatch &
                (term%pcm, alpha_s, term%connected%has_matrix, sqme_mism)
        end select
        call term%connected%trace%set_only_matrix_element &
            (1, cmplx (sum (sqme_mism) * term%weight, 0, default))
        if (term%connected%has_matrix) then
            select type (pcm => term%pcm)
            type is (pcm_nlo_t)
                if (term%connected%has_matrix) &
                    call refill_evaluator (cmplx (sqme_mism * term%weight, 0, default), &
                        pcm%get_qn (.true.), &
                        remove_duplicates_from_int_array ( &
                            pcm%region_data%get_flavor_indices (.true.)), &
                            term%connected%matrix)
                if (term%connected%has_flows) &
                    call refill_evaluator (cmplx (sqme_mism * term%weight, 0, default), &
                        pcm%get_qn (.true.), &
                        remove_duplicates_from_int_array ( &
                            pcm%region_data%get_flavor_indices (.true.)), &
                            term%connected%flows)
            end select
        end if
    end if

```

```
end subroutine term_instance_evaluate_sqme_mismatch
```

(Instances: term instance: TBP)+≡

```
procedure :: evaluate_sqme_dglap => term_instance_evaluate_sqme_dglap
```

(Instances: procedures)+≡

```
subroutine term_instance_evaluate_sqme_dglap (term, alpha_s, alpha_qed)
  class(term_instance_t), intent(inout) :: term
  real(default), intent(in) :: alpha_s, alpha_qed
  real(default), dimension(2) :: alpha_coupling
  real(default), dimension(:), allocatable :: sqme_dglap
  integer :: i_flv
  if (term%nlo_type /= NLO_DGLAP) call msg_fatal &
    ("Trying to evaluate DGLAP remnant with unsuited term_instance.")
  if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "term_instance_evaluate_sqme_dglap")
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
      alpha_coupling = [alpha_s, alpha_qed]
      if (debug2_active (D_PROCESS_INTEGRATION)) then
        associate (n_flv => pcm_work%dglap_remnant%reg_data%n_flv_born)
          print *, "size(sqme_born) = ", size (pcm_work%dglap_remnant%sqme_born)
          call term%connected%trace%write ()
        end associate
      end if
      call pcm_work%compute_sqme_dglap_remnant (pcm, alpha_coupling, &
        term%connected%has_matrix, sqme_dglap)
    end select
  end select
  call term%connected%trace%set_only_matrix_element &
    (1, cmplx (sum (sqme_dglap) * term%weight, 0, default))
  if (term%connected%has_matrix) then
    select type (pcm => term%pcm)
    type is (pcm_nlo_t)
      call refill_evaluator (cmplx (sqme_dglap * term%weight, 0, default), &
        pcm%get_qn (.true.), &
        remove_duplicates_from_int_array ( &
          pcm%region_data%get_flavor_indices (.true.)), &
        term%connected%matrix)
      if (term%connected%has_flows) then
        call refill_evaluator (cmplx (sqme_dglap * term%weight, 0, default), &
          pcm%get_qn (.true.), &
          remove_duplicates_from_int_array ( &
            pcm%region_data%get_flavor_indices (.true.)), &
          term%connected%flows)
      end if
    end select
  end if
end subroutine term_instance_evaluate_sqme_dglap
```

Reset the term instance: clear the parton-state expressions and deactivate.

(Instances: term instance: TBP)+≡

```
procedure :: reset => term_instance_reset
```

```

<Instances: procedures>+≡
  subroutine term_instance_reset (term)
    class(term_instance_t), intent(inout) :: term
    call term%connected%reset_expressions ()
    if (allocated (term%alpha_qcd_forced)) deallocate (term%alpha_qcd_forced)
    term%active = .false.
  end subroutine term_instance_reset

```

Force an α_s value that should be used in the matrix-element calculation.

```

<Instances: term instance: TBP>+≡
  procedure :: set_alpha_qcd_forced => term_instance_set_alpha_qcd_forced

<Instances: procedures>+≡
  subroutine term_instance_set_alpha_qcd_forced (term, alpha_qcd)
    class(term_instance_t), intent(inout) :: term
    real(default), intent(in) :: alpha_qcd
    if (allocated (term%alpha_qcd_forced)) then
      term%alpha_qcd_forced = alpha_qcd
    else
      allocate (term%alpha_qcd_forced, source = alpha_qcd)
    end if
  end subroutine term_instance_set_alpha_qcd_forced

```

Complete the kinematics computation for the effective parton states.

We assume that the `compute_hard_kinematics` method of the process component instance has already been called, so the `int_hard` contains the correct hard kinematics. The duty of this procedure is first to compute the effective kinematics and store this in the `int_eff` effective interaction inside the `isolated` parton state. The effective kinematics may differ from the kinematics in the hard interaction. It may involve parton recombination or parton splitting. The `rearrange_partons` method is responsible for this part.

We may also call a method to compute the effective structure-function chain at this point. This is not implemented yet.

In the simple case that no rearrangement is necessary, as indicated by the `rearrange` flag, the effective interaction is a pointer to the hard interaction, and we can skip the rearrangement method. Similarly for the effective structure-function chain.

The final step of kinematics setup is to transfer the effective kinematics to the evaluators and to the `subevt`.

```

<Instances: term instance: TBP>+≡
  procedure :: compute_eff_kinematics => &
    term_instance_compute_eff_kinematics

<Instances: procedures>+≡
  subroutine term_instance_compute_eff_kinematics (term)
    class(term_instance_t), intent(inout) :: term
    term%checked = .false.
    term%passed = .false.
    call term%isolated%receive_kinematics ()
    call term%connected%receive_kinematics ()
  end subroutine term_instance_compute_eff_kinematics

```

Inverse. Reconstruct the connected state from the momenta in the trace evaluator (which we assume to be set), then reconstruct the isolated state as far as possible. The second part finalizes the momentum configuration, using the incoming seed momenta

```

<Instances: term instance: TBP>+≡
  procedure :: recover_hard_kinematics => &
    term_instance_recover_hard_kinematics

<Instances: procedures>+≡
  subroutine term_instance_recover_hard_kinematics (term)
    class(term_instance_t), intent(inout) :: term
    term%checked = .false.
    term%passed = .false.
    call term%connected%send_kinematics ()
    call term%isolated%send_kinematics ()
  end subroutine term_instance_recover_hard_kinematics

```

Check the term whether it passes cuts and, if successful, evaluate scales and weights. The factorization scale is also given to the term kinematics, enabling structure-function evaluation.

```

<Instances: term instance: TBP>+≡
  procedure :: evaluate_expressions => &
    term_instance_evaluate_expressions

<Instances: procedures>+≡
  subroutine term_instance_evaluate_expressions (term, scale_forced)
    class(term_instance_t), intent(inout) :: term
    real(default), intent(in), allocatable, optional :: scale_forced
    call term%connected%evaluate_expressions (term%passed, &
      term%scale, term%fac_scale, term%ren_scale, term%weight, &
      scale_forced, force_evaluation = .true.)
    term%checked = .true.
  end subroutine term_instance_evaluate_expressions

```

Evaluate the trace: first evaluate the hard interaction, then the trace evaluator. We use the `evaluate_interaction` method of the process component which generated this term. The `subevt` and cut expressions are not yet filled.

The `component` argument is `intent(inout)` because the `compute_amplitude` method may modify the `core_state` workspace object.

```

<Instances: term instance: TBP>+≡
  procedure :: evaluate_interaction => term_instance_evaluate_interaction

<Instances: procedures>+≡
  subroutine term_instance_evaluate_interaction (term, core, kin)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(in), pointer :: core
    type(kinematics_t), intent(inout) :: kin
    if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
      "term_instance_evaluate_interaction")
    if (kin%only_cm_frame .and. (.not. kin%lab_is_cm())) then
      term%p_hard = kin%get_boost_to_cms () * term%int_hard%get_momenta ()
    else
      term%p_hard = term%int_hard%get_momenta ()
    end if
  end subroutine term_instance_evaluate_interaction

```

```

end if
select type (core)
class is (prc_external_t)
    call term%evaluate_interaction_userdef (core, kin)
class default
    call term%evaluate_interaction_default (core)
end select
call term%int_hard%set_matrix_element (term%amp)
end subroutine term_instance_evaluate_interaction

```

(Instances: term instance: TBP)+≡

```

procedure :: evaluate_interaction_default &
=> term_instance_evaluate_interaction_default

```

(Instances: procedures)+≡

```

subroutine term_instance_evaluate_interaction_default (term, core)
class(term_instance_t), intent(inout) :: term
class(prc_core_t), intent(in) :: core
integer :: i
do i = 1, term%config%n_allowed
    term%amp(i) = core%compute_amplitude (term%config%i_term, term%p_hard, &
        term%config%flv(i), term%config%hel(i), term%config%col(i), &
        term%fac_scale, term%ren_scale, term%alpha_qcd_forced, &
        term%core_state)
end do
select type (pcm_work => term%pcm_work)
type is (pcm_nlo_workspace_t)
    call pcm_work%set_fac_scale (term%fac_scale)
end select
end subroutine term_instance_evaluate_interaction_default

```

(Instances: term instance: TBP)+≡

```

procedure :: evaluate_interaction_userdef &
=> term_instance_evaluate_interaction_userdef

```

(Instances: procedures)+≡

```

subroutine term_instance_evaluate_interaction_userdef (term, core, kin)
class(term_instance_t), intent(inout) :: term
class(prc_core_t), intent(inout) :: core
type(kinematics_t), intent(inout) :: kin
if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
    "term_instance_evaluate_interaction_userdef")
select type (core_state => term%core_state)
type is (openloops_state_t)
    select type (core)
    type is (prc_openloops_t)
        call core%compute_alpha_s (core_state, term%ren_scale)
        if (allocated (core_state%threshold_data)) &
            call evaluate_threshold_parameters (core_state, core, kin%phs%get_sqrts ())
    end select
class is (prc_external_state_t)
    select type (core)
    class is (prc_external_t)
        call core%compute_alpha_s (core_state, term%ren_scale)

```



```

        end select
    end select
    call evaluate_threshold_interaction ()
    if (term%nlo_type == NLO_VIRTUAL) then
        call term%evaluate_interaction_userdef_loop (core)
    else
        call term%evaluate_interaction_userdef_tree (core)
    end if
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
        call pcm_work%set_fac_scale (term%fac_scale)
    end select

contains
    subroutine evaluate_threshold_parameters (core_state, core, sqrts)
        type(openloops_state_t), intent(inout) :: core_state
        type(prc_openloops_t), intent(inout) :: core
        real(default), intent(in) :: sqrts
        real(default) :: mtop, wtop
        mtop = mls_to_mpole (sqrts)
        wtop = core_state%threshold_data%compute_top_width &
            (mtop, core_state%alpha_qcd)
        call core%set_mass_and_width (6, mtop, wtop)
    end subroutine

    subroutine evaluate_threshold_interaction ()
        integer :: leg
        select type (core)
        type is (prc_threshold_t)
            if (term%nlo_type > BORN) then
                select type (pcm_work => term%pcm_work)
                type is (pcm_nlo_workspace_t)
                    if (kin%emitter >= 0) then
                        call core%set_offshell_momenta &
                            (pcm_work%real_kinematics%p_real_cms%get_momenta(term%config%i_term))
                        leg = thr_leg (kin%emitter)
                        call core%set_leg (leg)
                        call core%set_onshell_momenta &
                            (pcm_work%real_kinematics%p_real_onshell(leg)%get_momenta(term%config%i_te
                    else
                        call core%set_leg (0)
                        call core%set_offshell_momenta &
                            (pcm_work%real_kinematics%p_born_cms%get_momenta(1))
                    end if
                end select
            else
                call core%set_leg (-1)
                call core%set_offshell_momenta (term%p_hard)
            end if
        end select
    end subroutine evaluate_threshold_interaction
end subroutine term_instance_evaluate_interaction_userdef

```

Retrieve the matrix elements from a matrix element provider and place them

into `term%amp`.

For the handling of NLO calculations, FKS applies a book keeping handling flavor and/or particle type (e.g. for QCD: quark/gluon and quark flavor) in order to calculate the subtraction terms. Therefore, we have to insert the calculated matrix elements correctly into the state matrix where each entry corresponds to a set of quantum numbers. We apply a mapping `hard_qn_ind` from a list of quantum numbers provided by FKS to the hard process `int_hard`.

The calculated matrix elements are insert into `term%amp` in the following way. The first `n_born` particles are the matrix element of the hard process. In non-trivial beams, we store another `n_beams_rescaled` copies of these matrix elements as the first `n_beams_rescaled` subtractions. This is a remnant from times before the method `term_instance_set_sf_factors` and these entries are not used anymore. However, eliminating these entries involves deeper changes in how the connection tables for the evaluator product are set up and should therefore be part of a larger refactoring of the interactions & state matrices. The next $n_{\text{born}} \times n_{\text{sub_color}}$ are color-correlated Born matrix elements, with then again the next $n_{\text{born}} \times n_{\text{emitters}} \times n_{\text{sub_spin}}$ being spin-correlated Born matrix elements.

If two or more flavor structures would produce the same amplitude we only compute one and use the `eqv_index` determined by the `prc_core` and just copy the result to improve performance.

(Instances: term instance: TBP)+≡

```
procedure :: evaluate_interaction_userdef_tree &
=> term_instance_evaluate_interaction_userdef_tree
```

(Instances: procedures)+≡

```
subroutine term_instance_evaluate_interaction_userdef_tree (term, core)
class(term_instance_t), intent(inout) :: term
class(prc_core_t), intent(inout) :: core
real(default) :: sqme
real(default), dimension(:), allocatable :: sqme_color_c
real(default), dimension(:), allocatable :: sqme_spin_c
real(default), dimension(6) :: sqme_spin_c_tmp
integer :: n_flv, n_hel, n_sub_color, n_sub_spin, n_pdf_off
integer :: i_flv, i_hel, i_sub, i_color_c, i_color_c_eqv, i_spin_c, i_spin_c_eqv
integer :: i_flv_eqv, i_hel_eqv
integer :: emitter, i_emitter
logical :: bad_point, bp
logical, dimension(:,:), allocatable :: eqv_me_evaluated
if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, &
"term_instance_evaluate_interaction_userdef_tree")
allocate (sqme_color_c (blha_result_array_size &
(term%int_hard%get_n_tot (), BLHA_AMP_COLOR_C)))
n_flv = term%int_hard%get_qn_index_n_flv ()
n_hel = term%int_hard%get_qn_index_n_hel ()
n_sub_color = term%get_n_sub_color ()
n_sub_spin = term%get_n_sub_spin ()
allocate (eqv_me_evaluated(n_flv,n_hel))
eqv_me_evaluated = .false.
do i_flv = 1, n_flv
do i_hel = 1, n_hel
i_flv_eqv = core%data%eqv_flv_index(i_flv)
i_hel_eqv = core%data%eqv_hel_index(i_hel)
```

```

if (.not. eqv_me_evaluated(i_flv_eqv, i_hel_eqv)) then
select type (core)
class is (prc_external_t)
  call core%update_alpha_s (term%core_state, term%ren_scale)
  call core%compute_sqme (i_flv, i_hel, term%p_hard, term%ren_scale, &
    sqme, bad_point)
  call term%pcm_work%set_bad_point (bad_point)
  associate (i_int => term%int_hard%get_qn_index &
    (i_flv = i_flv, i_hel = i_hel, i_sub = 0))
    term%amp(i_int) = cmplx (sqme, 0, default)
  end associate
end select
n_pdf_off = 0
if (term%pcm%has_pdfs .and. &
  (term%is_subtraction () .or. term%nlo_type == NLO_DGLAP)) then
  n_pdf_off = n_pdf_off + n_beams_rescaled
  do i_sub = 1, n_pdf_off
    term%amp(term%int_hard%get_qn_index (i_flv, i_hel, i_sub)) = &
      term%amp(term%int_hard%get_qn_index (i_flv, i_hel, i_sub = 0))
  end do
end if
if (term%pcm%has_pdfs .and. term%nlo_type == NLO_DGLAP) then
  sqme_color_c = zero
  select type (pcm => term%pcm)
  type is (pcm_nlo_t)
    if (pcm%settings%nlo_correction_type == "EW" .and. &
      pcm%region_data%alphas_power > 0) then
      select type (core)
      class is (prc_blha_t)
        call core%compute_sqme_color_c_raw (i_flv, i_hel, &
          term%p_hard, term%ren_scale, sqme_color_c, bad_point)
        call term%pcm_work%set_bad_point (bad_point)
      class is (prc_recola_t)
        call core%compute_sqme_color_c_raw (i_flv, i_hel, &
          term%p_hard, term%ren_scale, sqme_color_c, bad_point)
        call term%pcm_work%set_bad_point (bad_point)
      end select
    end if
  end select
  do i_sub = 1, n_sub_color
    i_color_c = term%int_hard%get_qn_index &
      (i_flv, i_hel, i_sub + n_pdf_off)
    term%amp(i_color_c) = cmplx (sqme_color_c(i_sub), 0, default)
  end do
end if
if ((term%nlo_type == NLO_REAL .and. term%is_subtraction ()) .or. &
  term%nlo_type == NLO_MISMATCH) then
  sqme_color_c = zero
  select type (core)
  class is (prc_blha_t)
    call core%compute_sqme_color_c_raw (i_flv, i_hel, &
      term%p_hard, term%ren_scale, sqme_color_c, bad_point)
    call term%pcm_work%set_bad_point (bad_point)
  class is (prc_recola_t)

```

```

        call core%compute_sqme_color_c_raw (i_flv, i_hel, &
            term%p_hard, term%ren_scale, sqme_color_c, bad_point)
        call term%pcm_work%set_bad_point (bad_point)
    end select
    do i_sub = 1, n_sub_color
        i_color_c = term%int_hard%get_qn_index &
            (i_flv, i_hel, i_sub + n_pdf_off)
        term%amp(i_color_c) = cmplx (sqme_color_c(i_sub), 0, default)
    end do
    if (n_sub_spin > 0) then
        bad_point = .false.
        allocate (sqme_spin_c(0))
        select type (core)
        type is (prc_openloops_t)
            select type (pcm => term%pcm)
            type is (pcm_nlo_t)
                do i_emitter = 1, pcm%region_data%n_emitters
                    emitter = pcm%region_data%emitters(i_emitter)
                    if (emitter > 0) then
                        call core%compute_sqme_spin_c &
                            (i_flv, &
                                i_hel, &
                                emitter, &
                                term%p_hard, &
                                term%ren_scale, &
                                sqme_spin_c_tmp, &
                                bp)
                        sqme_spin_c = [sqme_spin_c, sqme_spin_c_tmp]
                        bad_point = bad_point .or. bp
                    end if
                end do
            end select
        do i_sub = 1, n_sub_spin
            i_spin_c = term%int_hard%get_qn_index (i_flv, i_hel, &
                i_sub + n_pdf_off + n_sub_color)
            term%amp(i_spin_c) = cmplx &
                (sqme_spin_c(i_sub), 0, default)
        end do
    end select
    deallocate (sqme_spin_c)
end if
end if
eqv_me_evaluated(i_flv_eqv, i_hel_eqv) = .true.
else
    associate (i_int => term%int_hard%get_qn_index &
        (i_flv = i_flv, i_hel = i_hel, i_sub = 0), &
        i_int_eqv => term%int_hard%get_qn_index &
        (i_flv = i_flv_eqv, i_hel = i_hel_eqv, i_sub = 0))
        term%amp(i_int) = term%amp(i_int_eqv)
    end associate
    n_pdf_off = 0
    if (term%pcm%has_pdfs .and. &
        (term%is_subtraction () .or. term%nlo_type == NLO_DGLAP)) then
        n_pdf_off = n_pdf_off + n_beams_rescaled
    end if
end if

```

```

do i_sub = 1, n_pdf_off
  term%amp(term%int_hard%get_qn_index (i_flv, i_hel, i_sub)) = &
    term%amp(term%int_hard%get_qn_index (i_flv, i_hel, i_sub = 0))
end do
end if
if (term%pcm%has_pdfs .and. term%nlo_type == NLO_DGLAP) then
  do i_sub = 1, n_sub_color
    i_color_c = term%int_hard%get_qn_index &
      (i_flv, i_hel, i_sub + n_pdf_off)
    i_color_c_eqv = term%int_hard%get_qn_index &
      (i_flv_eqv, i_hel_eqv, i_sub + n_pdf_off)
    term%amp(i_color_c) = term%amp(i_color_c_eqv)
  end do
end if
if ((term%nlo_type == NLO_REAL .and. term%is_subtraction ()) .or. &
  term%nlo_type == NLO_MISMATCH) then
  do i_sub = 1, n_sub_color
    i_color_c = term%int_hard%get_qn_index &
      (i_flv, i_hel, i_sub + n_pdf_off)
    i_color_c_eqv = term%int_hard%get_qn_index &
      (i_flv_eqv, i_hel_eqv, i_sub + n_pdf_off)
    term%amp(i_color_c) = term%amp(i_color_c_eqv)
  end do
  do i_sub = 1, n_sub_spin
    i_spin_c = term%int_hard%get_qn_index (i_flv, i_hel, &
      i_sub + n_pdf_off + n_sub_color)
    i_spin_c_eqv = term%int_hard%get_qn_index (i_flv_eqv, i_hel_eqv, &
      i_sub + n_pdf_off + n_sub_color)
    term%amp(i_spin_c) = term%amp(i_spin_c_eqv)
  end do
end if
end if
end do
end do
end subroutine term_instance_evaluate_interaction_userdef_tree

```

Same as for `term_instance_evaluate_interaction_userdef_tree`, but for the integrated-subtraction and finite one-loop terms. We only need color-correlated Born matrix elements, but an additional entry per flavor structure for the finite one-loop contribution. We thus have $2 + n_{sub_color}$ entries in the `term%amp` for each `i_flv` and `i_hel` combination.

If two or more flavor structures would produce the same amplitude we only compute one and use the `eqv_index` determined by the `prc_core` and just copy the result to improve performance.

(Instances: term instance: TBP)+≡

```

procedure :: evaluate_interaction_userdef_loop &
=> term_instance_evaluate_interaction_userdef_loop

```

(Instances: procedures)+≡

```

subroutine term_instance_evaluate_interaction_userdef_loop (term, core)
  class(term_instance_t), intent(inout) :: term
  class(prc_core_t), intent(in) :: core
  integer :: n_hel, n_sub, n_flv

```

```

integer :: i, i_flv, i_hel, i_sub, i_virt, i_color_c, i_color_c_eqv
integer :: i_flv_eqv, i_hel_eqv
real(default), dimension(4) :: sqme_virt
real(default), dimension(:), allocatable :: sqme_color_c
logical :: bad_point
logical, dimension(:,:), allocatable :: eqv_me_evaluated
if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, &
    "term_instance_evaluate_interaction_userdef_loop")
allocate (sqme_color_c (blha_result_array_size &
    (term%int_hard%get_n_tot (), BLHA_AMP_COLOR_C)))
n_flv = term%int_hard%get_qn_index_n_flv ()
n_hel = term%int_hard%get_qn_index_n_hel ()
n_sub = term%int_hard%get_qn_index_n_sub ()
allocate (eqv_me_evaluated(n_flv,n_hel))
eqv_me_evaluated = .false.
i_virt = 1
do i_flv = 1, n_flv
    do i_hel = 1, n_hel
        i_flv_eqv = core%data%eqv_flv_index(i_flv)
        i_hel_eqv = core%data%eqv_hel_index(i_hel)
        if (.not. eqv_me_evaluated(i_flv_eqv, i_hel_eqv)) then
            select type (core)
            class is (prc_external_t)
                call core%compute_sqme_virt (i_flv, i_hel, term%p_hard, &
                    term%ren_scale, term%es_scale, &
                    term%pcm%blha_defaults%loop_method, &
                    sqme_virt, bad_point)
                call term%pcm_work%set_bad_point (bad_point)
            end select
            associate (i_born => term%int_hard%get_qn_index (i_flv, i_hel = i_hel, i_sub = 0), &
                i_loop => term%int_hard%get_qn_index (i_flv, i_hel = i_hel, i_sub = i_virt))
                term%amp(i_loop) = cmplx (sqme_virt(3), 0, default)
                term%amp(i_born) = cmplx (sqme_virt(4), 0, default)
            end associate
            select type (pcm => term%pcm)
            type is (pcm_nlo_t)
                select type (core)
                class is (prc_blha_t)
                    call core%compute_sqme_color_c_raw (i_flv, i_hel, &
                        term%p_hard, term%ren_scale, &
                        sqme_color_c, bad_point)
                    call term%pcm_work%set_bad_point (bad_point)
                    do i_sub = 1 + i_virt, n_sub
                        i_color_c = term%int_hard%get_qn_index &
                            (i_flv, i_hel = i_hel, i_sub = i_sub)
                        ! Index shift: i_sub - i_virt
                        term%amp(i_color_c) = &
                            cmplx (sqme_color_c(i_sub - i_virt), 0, default)
                    end do
                end select
            type is (prc_recola_t)
                call core%compute_sqme_color_c_raw (i_flv, i_hel, &
                    term%p_hard, term%ren_scale, sqme_color_c, bad_point)
                call term%pcm_work%set_bad_point (bad_point)
                do i_sub = 1 + i_virt, n_sub

```

```

        i_color_c = term%int_hard%get_qn_index &
            (i_flv, i_hel = i_hel, i_sub = i_sub)
        ! Index shift: i_sub - i_virt
        term%amp(i_color_c) = &
            cmplx (sqme_color_c(i_sub - i_virt), 0, default)
    end do
end select
end select
eqv_me_evaluated(i_flv_eqv, i_hel_eqv) = .true.
else
    associate (i_born => term%int_hard%get_qn_index (i_flv, i_hel = i_hel, i_sub = 0), &
        i_loop => term%int_hard%get_qn_index (i_flv, i_hel = i_hel, i_sub = i_virt), &
        i_born_eqv => term%int_hard%get_qn_index &
            (i_flv_eqv, i_hel = i_hel_eqv, i_sub = 0), &
        i_loop_eqv => term%int_hard%get_qn_index &
            (i_flv_eqv, i_hel = i_hel_eqv, i_sub = 1))
        term%amp(i_loop) = term%amp(i_loop_eqv)
        term%amp(i_born) = term%amp(i_born_eqv)
    end associate
    do i_sub = 1 + i_virt, n_sub
        i_color_c = term%int_hard%get_qn_index &
            (i_flv, i_hel = i_hel, i_sub = i_sub)
        i_color_c_eqv = term%int_hard%get_qn_index &
            (i_flv_eqv, i_hel = i_hel_eqv, i_sub = i_sub)
        ! Index shift: i_sub - i_virt
        term%amp(i_color_c) = term%amp(i_color_c_eqv)
    end do
end if
end do
end do
end subroutine term_instance_evaluate_interaction_userdef_loop

```

Evaluate the trace. First evaluate the structure-function chain (i.e., the density matrix of the incoming partons). Do this twice, in case the sf-chain instances within `kin` and `isolated` differ. Next, evaluate the hard interaction, then compute the convolution with the initial state.

(Instances: term instance: TBP)+≡

```

    procedure :: evaluate_trace => term_instance_evaluate_trace

```

(Instances: procedures)+≡

```

    subroutine term_instance_evaluate_trace (term, kin)
        class(term_instance_t), intent(inout) :: term
        type(kinematics_t), intent(inout) :: kin
        call kin%evaluate_sf_chain (term%fac_scale, term%negative_sf)
        call term%evaluate_scaled_sf_chains (kin)
        call term%isolated%evaluate_sf_chain (term%fac_scale)
        call term%isolated%evaluate_trace ()
        call term%connected%evaluate_trace ()
    end subroutine term_instance_evaluate_trace

```

Include rescaled structure functions due to NLO calculation. We rescale the structure function for the real subtraction `sf_rescale_collinear`, the collinear counter terms `sf_rescale_dglap_t` and for the case, in which we have an emit-

ter in the initial state, we rescale the kinematics for it using `sf_rescale_real_t`.
References: arXiv:0709.2092, (2.35)-(2.42).

Obviously, it is completely irrelevant, which beam is treated. It becomes problematic when handling `e`, `p`-beams.

(Instances: term instance: TBP)+≡

```
procedure :: evaluate_scaled_sf_chains => term_instance_evaluate_scaled_sf_chains
```

(Instances: procedures)+≡

```
subroutine term_instance_evaluate_scaled_sf_chains (term, kin)
  class(term_instance_t), intent(inout) :: term
  type(kinematics_t), intent(inout) :: kin
  class(sf_rescale_t), allocatable :: sf_rescale
  if (.not. term%pcm%has_pdfs) return
  if (term%nlo_type == NLO_REAL) then
    if (term%is_subtraction ()) then
      allocate (sf_rescale_collinear_t :: sf_rescale)
      select type (pcm_work => term%pcm_work)
      type is (pcm_nlo_workspace_t)
        select type (sf_rescale)
        type is (sf_rescale_collinear_t)
          call sf_rescale%set (pcm_work%real_kinematics%xi_tilde)
        end select
      end select
      call kin%sf_chain%evaluate (term%fac_scale, term%negative_sf, sf_rescale)
      deallocate (sf_rescale)
    else if (kin%emitter >= 0 .and. kin%emitter <= kin%n_in) then
      allocate (sf_rescale_real_t :: sf_rescale)
      select type (pcm_work => term%pcm_work)
      type is (pcm_nlo_workspace_t)
        select type (sf_rescale)
        type is (sf_rescale_real_t)
          call sf_rescale%set (pcm_work%real_kinematics%xi_tilde * &
                               pcm_work%real_kinematics%xi_max (kin%i_phs), &
                               pcm_work%real_kinematics%y (kin%i_phs))
        end select
      end select
      call kin%sf_chain%evaluate (term%fac_scale, term%negative_sf, sf_rescale)
      deallocate (sf_rescale)
    else
      call kin%sf_chain%evaluate (term%fac_scale, term%negative_sf)
    end if
  else if (term%nlo_type == NLO_DGLAP) then
    allocate (sf_rescale_dglap_t :: sf_rescale)
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
      select type (sf_rescale)
      type is (sf_rescale_dglap_t)
        call sf_rescale%set (pcm_work%isr_kinematics%z)
      end select
    end select
    call kin%sf_chain%evaluate (term%fac_scale, term%negative_sf, sf_rescale)
    deallocate (sf_rescale)
  end if
end subroutine term_instance_evaluate_scaled_sf_chains
```


Evaluate the extra data that we need for processing the object as a physical event.

```

<Instances: term instance: TBP>+≡
  procedure :: evaluate_event_data => term_instance_evaluate_event_data

<Instances: procedures>+≡
  subroutine term_instance_evaluate_event_data (term)
    class(term_instance_t), intent(inout) :: term
    logical :: only_momenta
    only_momenta = term%nlo_type > BORN
    call term%isolated%evaluate_event_data (only_momenta)
    call term%connected%evaluate_event_data (only_momenta)
  end subroutine term_instance_evaluate_event_data

<Instances: term instance: TBP>+≡
  procedure :: set_fac_scale => term_instance_set_fac_scale

<Instances: procedures>+≡
  subroutine term_instance_set_fac_scale (term, fac_scale)
    class(term_instance_t), intent(inout) :: term
    real(default), intent(in) :: fac_scale
    term%fac_scale = fac_scale
  end subroutine term_instance_set_fac_scale

```

Return data that might be useful for external processing. The factorization scale:

```

<Instances: term instance: TBP>+≡
  procedure :: get_fac_scale => term_instance_get_fac_scale

<Instances: procedures>+≡
  function term_instance_get_fac_scale (term) result (fac_scale)
    class(term_instance_t), intent(in) :: term
    real(default) :: fac_scale
    fac_scale = term%fac_scale
  end function term_instance_get_fac_scale

```

We take the strong coupling from the process core. The value is calculated when a new event is requested, so we should call it only after the event has been evaluated. If it is not available there (a negative number is returned), we take the value stored in the term configuration, which should be determined by the model. If the model does not provide a value, the result is zero.

```

<Instances: term instance: TBP>+≡
  procedure :: get_alpha_s => term_instance_get_alpha_s

<Instances: procedures>+≡
  function term_instance_get_alpha_s (term, core) result (alpha_s)
    class(term_instance_t), intent(in) :: term
    class(prc_core_t), intent(in) :: core
    real(default) :: alpha_s
    alpha_s = core%get_alpha_s (term%core_state)
    if (alpha_s < zero) alpha_s = term%config%alpha_s
  end function term_instance_get_alpha_s

```

The second helicity for `helicities` comes with a minus sign because `OpenLoops` inverts the helicity index of antiparticles.

(Instances: term instance: TBP)+≡

```
procedure :: get_helicities_for_openloops => term_instance_get_helicities_for_openloops
```

(Instances: procedures)+≡

```
subroutine term_instance_get_helicities_for_openloops (term, helicities)
  class(term_instance_t), intent(in) :: term
  integer, dimension(:,:), allocatable, intent(out) :: helicities
  type(helicity_t), dimension(:), allocatable :: hel
  type(quantum_numbers_t), dimension(:,:), allocatable :: qn
  type(quantum_numbers_mask_t) :: qn_mask
  integer :: h, i, j, n_in
  call qn_mask%set_sub (1)
  call term%isolated%trace%get_quantum_numbers_mask (qn_mask, qn)
  n_in = term%int_hard%get_n_in ()
  allocate (helicities (size (qn, dim=1), n_in))
  allocate (hel (n_in))
  do i = 1, size (qn, dim=1)
    do j = 1, n_in
      hel(j) = qn(i, j)%get_helicity ()
      call hel(j)%diagonalize ()
      call hel(j)%get_indices (h, h)
      helicities (i, j) = h
    end do
  end do
end subroutine term_instance_get_helicities_for_openloops
```

(Instances: term instance: TBP)+≡

```
procedure :: get_i_term_global => term_instance_get_i_term_global
```

(Instances: procedures)+≡

```
elemental function term_instance_get_i_term_global (term) result (i_term)
  integer :: i_term
  class(term_instance_t), intent(in) :: term
  i_term = term%config%i_term_global
end function term_instance_get_i_term_global
```

(Instances: term instance: TBP)+≡

```
procedure :: is_subtraction => term_instance_is_subtraction
```

(Instances: procedures)+≡

```
elemental function term_instance_is_subtraction (term) result (sub)
  logical :: sub
  class(term_instance_t), intent(in) :: term
  sub = term%config%i_term_global == term%config%i_sub
end function term_instance_is_subtraction
```

Retrieve `n_sub` which was calculated in `process_term_setup_interaction`.

(Instances: term instance: TBP)+≡

```
procedure :: get_n_sub => term_instance_get_n_sub
procedure :: get_n_sub_color => term_instance_get_n_sub_color
procedure :: get_n_sub_spin => term_instance_get_n_sub_spin
```

```

<Instances: procedures>+≡
function term_instance_get_n_sub (term) result (n_sub)
  integer :: n_sub
  class(term_instance_t), intent(in) :: term
  n_sub = term%config%n_sub
end function term_instance_get_n_sub

function term_instance_get_n_sub_color (term) result (n_sub_color)
  integer :: n_sub_color
  class(term_instance_t), intent(in) :: term
  n_sub_color = term%config%n_sub_color
end function term_instance_get_n_sub_color

function term_instance_get_n_sub_spin (term) result (n_sub_spin)
  integer :: n_sub_spin
  class(term_instance_t), intent(in) :: term
  n_sub_spin = term%config%n_sub_spin
end function term_instance_get_n_sub_spin

```

30.10.2 The process instance

NOTE: The description below represents the intended structure after refactoring and disentangling the FKS-NLO vs. LO algorithm dependencies.

A process instance contains all process data that depend on the sampling point and thus change often. In essence, it is an event record at the elementary (parton) level. We do not call it such, to avoid confusion with the actual event records. If decays are involved, the latter are compositions of several elementary processes (i.e., their instances).

We implement the process instance as an extension of the `mci_sampler_t` that we need for computing integrals and generate events.

The base type contains: the `integrand`, the `selected_channel`, the two-dimensional array `x` of parameters, and the one-dimensional array `f` of Jacobians. These subobjects are public and used for communicating with the multi-channel integrator.

The `process` pointer accesses the process of which this record is an instance. It is required whenever the calculation needs invariant configuration data, therefore the process should stay in memory for the whole lifetime of its instances.

The `pcm` pointer is a shortcut to the `pcm` (process-component manager) component of the associated process, which we need wherever the calculation depends on the overall algorithm.

The `pcm_work` component is the workspace for the `pcm` object referenced above.

The `evaluation_status` code is used to check the current status. In particular, failure at various stages is recorded there.

The `count` object records process evaluations, broken down according to status.

The `sqme` value is the single real number that results from evaluating and tracing the kinematics and matrix elements. This is the number that is handed over to an integration routine.

The **weight** value is the event weight. It is defined when an event has been generated from the process instance, either weighted or unweighted. The value is the **sqme** value times Jacobian weights from the integration, or unity, respectively.

The **i_mci** index chooses a subset of components that are associated with a common parameter set and integrator, i.e., that are added coherently.

The **sf_chain** subobject is a realization of the beam and structure-function configuration in the **process** object. It is not used for calculation directly but serves as the template for the sf-chain instances that are contained in the **component** objects.

The **kinematics** array contains the set of phase-space points that are associated with the current calculation. The entries may correspond to different process components and terms. (TODO wk 19-02-22: Not implemented yet.)

TODO wk 19-02-22: May include extra arrays for storing (squared) amplitude data. The **term** data set may be reduced to just results, or be removed altogether.

The **term** subobjects are workspace for evaluating kinematics, matrix elements, cuts etc. The array entries correspond to the **term** configuration entries in the associated process object.

The **mci_work** subobject contains the array of real input parameters (random numbers) that generates the kinematical point. It also contains the workspace for the MC integrators. The active entry of the **mci_work** array is selected by the **i_mci** index above.

The **hook** pointer accesses a list of after evaluate objects which are evaluated after the matrix element.

```

<Instances: public>+≡
    public :: process_instance_t

<Instances: types>+≡
    type, extends (mci_sampler_t) :: process_instance_t
        type(process_t), pointer :: process => null ()
        class(pcm_t), pointer :: pcm => null ()
        class(pcm_workspace_t), allocatable :: pcm_work
        integer :: evaluation_status = STAT_UNDEFINED
        real(default) :: sqme = 0
        real(default) :: weight = 0
        real(default) :: excess = 0
        integer :: n_dropped = 0
        integer :: i_mci = 0
        integer :: selected_channel = 0
        type(sf_chain_t) :: sf_chain
        type(kinematics_t), dimension(:), allocatable :: kin
        type(term_instance_t), dimension(:), allocatable :: term
        type(mci_work_t), dimension(:), allocatable :: mci_work
        class(process_instance_hook_t), pointer :: hook => null ()
    contains
        <Instances: process instance: TBP>
    end type process_instance_t

```

Wrapper type for storing pointers to process instance objects in arrays.

```

<Instances: public>+≡
    public :: process_instance_ptr_t

```

```

<Instances: types>+≡
  type :: process_instance_ptr_t
  type(process_instance_t), pointer :: p => null ()
end type process_instance_ptr_t

```

The process hooks are first-in-last-out list of objects which are evaluated after the phase space and matrixelement are evaluated. It is possible to retrieve the sampler object and read the sampler information.

The hook object are part of the `process_instance` and therefore, share a common lifetime. A data transfer, after the usual lifetime of the `process_instance`, is not provided, as such the finalisation procedure has to take care of this! E.g. write the object to file from which later the collected information can then be retrieved.

```

<Instances: public>+≡
  public :: process_instance_hook_t

<Instances: types>+≡
  type, abstract :: process_instance_hook_t
  class(process_instance_hook_t), pointer :: next => null ()
  contains
    procedure(process_instance_hook_init), deferred :: init
    procedure(process_instance_hook_final), deferred :: final
    procedure(process_instance_hook_evaluate), deferred :: evaluate
  end type process_instance_hook_t

```

We have to provide a `init`, a `final` procedure and, for after evaluation, the `evaluate` procedure.

The `init` procedures accesses `var_list` and current `instance` object.

```

<Instances: public>+≡
  public :: process_instance_hook_final, process_instance_hook_evaluate

<Instances: interfaces>≡
  abstract interface
    subroutine process_instance_hook_init (hook, var_list, instance)
      import :: process_instance_hook_t, var_list_t, process_instance_t
      class(process_instance_hook_t), intent(inout), target :: hook
      type(var_list_t), intent(in) :: var_list
      class(process_instance_t), intent(in), target :: instance
    end subroutine process_instance_hook_init

    subroutine process_instance_hook_final (hook)
      import :: process_instance_hook_t
      class(process_instance_hook_t), intent(inout) :: hook
    end subroutine process_instance_hook_final

    subroutine process_instance_hook_evaluate (hook, instance)
      import :: process_instance_hook_t, process_instance_t
      class(process_instance_hook_t), intent(inout) :: hook
      class(process_instance_t), intent(in), target :: instance
    end subroutine process_instance_hook_evaluate
  end interface

```

The output routine contains a header with the most relevant information about the process, copied from `process_metadata_write`. We mark the active components by an asterisk.

The next section is the MC parameter input. The following sections are written only if the evaluation status is beyond setting the parameters, or if the `verbose` option is set.

```

<Instances: process instance: TBP>≡
  procedure :: write_header => process_instance_write_header
  procedure :: write => process_instance_write

<Instances: procedures>+≡
  subroutine process_instance_write_header (object, unit, testflag)
    class(process_instance_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    if (associated (object%process)) then
      call object%process%write_meta (u, testflag)
    else
      write (u, "(1x,A)") "Process instance [undefined process]"
      return
    end if
    write (u, "(3x,A)", advance = "no") "status = "
    select case (object%evaluation_status)
    case (STAT_INITIAL);           write (u, "(A)") "initialized"
    case (STAT_ACTIVATED);         write (u, "(A)") "activated"
    case (STAT_BEAM_MOMENTA);      write (u, "(A)") "beam momenta set"
    case (STAT_FAILED_KINEMATICS); write (u, "(A)") "failed kinematics"
    case (STAT_SEED_KINEMATICS);   write (u, "(A)") "seed kinematics"
    case (STAT_HARD_KINEMATICS);   write (u, "(A)") "hard kinematics"
    case (STAT_EFF_KINEMATICS);    write (u, "(A)") "effective kinematics"
    case (STAT_FAILED_CUTS);       write (u, "(A)") "failed cuts"
    case (STAT_PASSED_CUTS);       write (u, "(A)") "passed cuts"
    case (STAT_EVALUATED_TRACE);   write (u, "(A)") "evaluated trace"
    call write_separator (u)
    write (u, "(3x,A,ES19.12)") "sqme = ", object%sqme
    case (STAT_EVENT_COMPLETE);   write (u, "(A)") "event complete"
    call write_separator (u)
    write (u, "(3x,A,ES19.12)") "sqme = ", object%sqme
    write (u, "(3x,A,ES19.12)") "weight = ", object%weight
    if (.not. vanishes (object%excess)) &
      write (u, "(3x,A,ES19.12)") "excess = ", object%excess
    case default;                 write (u, "(A)") "undefined"
    end select
    if (object%i_mci /= 0) then
      call write_separator (u)
      call object%mc_work(object%i_mci)%write (u, testflag)
    end if
    call write_separator (u, 2)
  end subroutine process_instance_write_header

  subroutine process_instance_write (object, unit, testflag)

```

```

class(process_instance_t), intent(in) :: object
integer, intent(in), optional :: unit
logical, intent(in), optional :: testflag
integer :: u, i
u = given_output_unit (unit)
call object%write_header (u)
if (object%evaluation_status >= STAT_BEAM_MOMENTA) then
  call object%sf_chain%write (u)
  call write_separator (u, 2)
  if (object%evaluation_status >= STAT_SEED_KINEMATICS) then
    if (object%evaluation_status >= STAT_HARD_KINEMATICS) then
      call write_separator (u, 2)
      write (u, "(1x,A)") "Active terms:"
      if (any (object%term%active)) then
        do i = 1, size (object%term)
          if (object%term(i)%active) then
            call write_separator (u)
            call object%term(i)%write (u, &
              kin = object%kin(i), &
              show_eff_state = &
              object%evaluation_status >= STAT_EFF_KINEMATICS, &
              testflag = testflag)
          end if
        end do
      end if
    end if
  end if
  call write_separator (u, 2)
end if
end if
end subroutine process_instance_write

```

Initialization connects the instance with a process. All initial information is transferred from the process object. The process object contains templates for the interaction subobjects (beam and term), but no evaluators. The initialization routine creates evaluators for the matrix element trace, other evaluators are left untouched.

Before we start generating, we double-check if the process library has been updated after the process was initialized (`check_library_sanity`). This may happen if between integration and event generation the library has been recompiled, so all links become broken.

The `instance` object must have the `target` attribute (also in any caller) since the initialization routine assigns various pointers to subobject of `instance`.

(Instances: process instance: TBP)+≡

```

procedure :: init => process_instance_init

```

(Instances: procedures)+≡

```

subroutine process_instance_init (instance, process)
  class(process_instance_t), intent(out), target :: instance
  type(process_t), intent(inout), target :: process
  integer :: i
  class(pcm_t), pointer :: pcm
  type(process_term_t), pointer :: term
  type(var_list_t), pointer :: var_list

```

```

integer :: i_born, i_real, i_real_fin, i_component
if (debug_on) call msg_debug (D_PROCESS_INTEGRATION, "process_instance_init")
instance%process => process
instance%pcm => process%get_pcm_ptr ()
call instance%process%check_library_sanity ()
call instance%setup_sf_chain (process%get_beam_config_ptr ())
allocate (instance%mc_i_work (process%get_n_mci ()))
do i = 1, size (instance%mc_i_work)
    call instance%process%init_mci_work (instance%mc_i_work(i), i)
end do
call instance%process%reset_selected_cores ()
pcm => instance%process%get_pcm_ptr ()
call pcm%allocate_workspace (instance%pcm_work)
select type (pcm)
type is (pcm_nlo_t)
    !!! The process is kept when the integration is finalized, but not the
    !!! process_instance. Thus, we check whether pcm has been initialized
    !!! but set up the pcm_work each time.
    i_real_fin = process%get_associated_real_fin (1)
    if (.not. pcm%initialized) then
        i_born = pcm%get_i_core (pcm%i_born)
        i_real = pcm%get_i_core (pcm%i_real)
        call pcm%init_qn (process%get_model_ptr ())
        if (i_real_fin > 0) call pcm%allocate_ps_matching ()
        var_list => process%get_var_list_ptr ()
        if (var_list%get_sval (var_str ("dalitz_plot")) /= var_str ('')) &
            call pcm%activate_dalitz_plot (var_list%get_sval (var_str ("dalitz_plot")))
    end if
    pcm%initialized = .true.
    select type (pcm_work => instance%pcm_work)
    type is (pcm_nlo_workspace_t)
        call pcm_work%init_config (pcm, &
            process%component_can_be_integrated (), &
            process%get_nlo_type_component (), process%get_energy (), &
            i_real_fin, process%get_model_ptr ())
    end select
end select
! TODO wk-03-01 n_terms will eventually acquire a different meaning
allocate (instance%kin (process%get_n_terms ()))
do i = 1, process%get_n_terms ()
    term => process%get_term_ptr (i)
    i_component = term%i_component
    call instance%kin(i)%configure (pcm, instance%pcm_work, &
        instance%sf_chain, &
        process%get_beam_config_ptr (), &
        process%get_phs_config (i_component), &
        process%get_nlo_type_component (i_component), &
        term%i_sub == i)
end do
! TODO wk-03-01 n_terms will eventually acquire a different meaning
allocate (instance%term (process%get_n_terms ()))
do i = 1, process%get_n_terms ()
    call instance%term(i)%configure (process, i, instance%pcm_work, &
        instance%sf_chain, instance%kin(i))
end do

```



```

end do
call instance%set_i_mci_to_real_component ()
call instance%find_same_kinematics ()
instance%evaluation_status = STAT_INITIAL
end subroutine process_instance_init

```

Finalize all subobjects that may contain allocated pointers.

```

<Instances: process instance: TBP>+≡
  procedure :: final => process_instance_final

<Instances: procedures>+≡
  subroutine process_instance_final (instance)
    class(process_instance_t), intent(inout) :: instance
    class(process_instance_hook_t), pointer :: current
    integer :: i
    instance%process => null ()
    if (allocated (instance%mci_work)) then
      do i = 1, size (instance%mci_work)
        call instance%mci_work(i)%final ()
      end do
      deallocate (instance%mci_work)
    end if
    call instance%sf_chain%final ()
    if (allocated (instance%kin)) then
      do i = 1, size (instance%kin)
        call instance%kin(i)%final ()
      end do
      deallocate (instance%kin)
    end if
    if (allocated (instance%term)) then
      do i = 1, size (instance%term)
        call instance%term(i)%final ()
      end do
      deallocate (instance%term)
    end if
    call instance%pcm_work%final ()
    instance%evaluation_status = STAT_UNDEFINED
    do while (associated (instance%hook))
      current => instance%hook
      call current%final ()
      instance%hook => current%next
      deallocate (current)
    end do
    instance%hook => null ()
  end subroutine process_instance_final

```

Revert the process instance to initial state. We do not deallocate anything, just reset the state index and deactivate all components and terms.

We do not reset the choice of the MCI set `i_mci` unless this is required explicitly.

```

<Instances: process instance: TBP>+≡
  procedure :: reset => process_instance_reset

```

```

<Instances: procedures>+≡
subroutine process_instance_reset (instance, reset_mci)
  class(process_instance_t), intent(inout), target :: instance
  logical, intent(in), optional :: reset_mci
  integer :: i
  call instance%process%reset_selected_cores ()
  do i = 1, size (instance%term)
    call instance%term(i)%reset ()
  end do
  instance%term%checked = .false.
  instance%term%passed = .false.
  instance%kin%new_seed = .true.
  if (present (reset_mci)) then
    if (reset_mci) instance%i_mci = 0
  end if
  instance%selected_channel = 0
  instance%evaluation_status = STAT_INITIAL
end subroutine process_instance_reset

```

Integration and event generation

The sampler test should just evaluate the squared matrix element `n_calls` times, discarding the results, and return. This can be done before integration, e.g., for timing estimates.

```

<Instances: process instance: TBP>+≡
  procedure :: sampler_test => process_instance_sampler_test

<Instances: procedures>+≡
subroutine process_instance_sampler_test (instance, i_mci, n_calls)
  class(process_instance_t), intent(inout), target :: instance
  integer, intent(in) :: i_mci
  integer, intent(in) :: n_calls
  integer :: i_mci_work
  i_mci_work = instance%process%get_i_mci_work (i_mci)
  call instance%choose_mci (i_mci_work)
  call instance%reset_counter ()
  call instance%process%sampler_test (instance, n_calls, i_mci_work)
  call instance%process%set_counter_mci_entry (i_mci_work, instance%get_counter ())
end subroutine process_instance_sampler_test

```

Generate a weighted event. We select one of the available MCI integrators by its index `i_mci` and thus generate an event for the associated (group of) process component(s). The arguments exactly correspond to the initializer and finalizer above.

The resulting event is stored in the `process_instance` object, which also holds the workspace of the integrator.

Note: The `process` object contains the random-number state, which changes for each event. Otherwise, all volatile data are inside the `instance` object.

```

<Instances: process instance: TBP>+≡
  procedure :: generate_weighted_event => process_instance_generate_weighted_event

```

<Instances: procedures>+≡

```

subroutine process_instance_generate_weighted_event (instance, i_mci)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_mci
  integer :: i_mci_work
  i_mci_work = instance%process%get_i_mci_work (i_mci)
  call instance%choose_mci (i_mci_work)
  associate (mci_work => instance%mci_work(i_mci_work))
    call instance%process%generate_weighted_event &
      (i_mci_work, mci_work, instance, &
        instance%keep_failed_events ())
  end associate
end subroutine process_instance_generate_weighted_event

```

<Instances: process instance: TBP>+≡

```

procedure :: generate_unweighted_event => process_instance_generate_unweighted_event

```

<Instances: procedures>+≡

```

subroutine process_instance_generate_unweighted_event (instance, i_mci)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_mci
  integer :: i_mci_work
  i_mci_work = instance%process%get_i_mci_work (i_mci)
  call instance%choose_mci (i_mci_work)
  associate (mci_work => instance%mci_work(i_mci_work))
    call instance%process%generate_unweighted_event &
      (i_mci_work, mci_work, instance)
  end associate
end subroutine process_instance_generate_unweighted_event

```

This replaces the event generation methods for the situation that the process instance object has been filled by other means (i.e., reading and/or recalculating its contents). We just have to fill in missing MCI data, especially the event weight.

<Instances: process instance: TBP>+≡

```

procedure :: recover_event => process_instance_recover_event

```

<Instances: procedures>+≡

```

subroutine process_instance_recover_event (instance)
  class(process_instance_t), intent(inout) :: instance
  integer :: i_mci
  i_mci = instance%i_mci
  call instance%process%set_i_mci_work (i_mci)
  associate (mci_instance => instance%mci_work(i_mci)%mci)
    call mci_instance%fetch (instance, instance%selected_channel)
  end associate
end subroutine process_instance_recover_event

```

Activate the components and terms that correspond to a currently selected MCI parameter set.

<Instances: process instance: TBP>+≡

```

procedure :: activate => process_instance_activate

```

(Instances: procedures)+≡

```

subroutine process_instance_activate (instance)
  class(process_instance_t), intent(inout) :: instance
  integer :: i, j
  integer, dimension(:), allocatable :: i_term
  associate (mci_work => instance%mci_work(instance%i_mci))
    call instance%process%select_components (mci_work%get_active_components ())
  end associate
  associate (process => instance%process)
    do i = 1, instance%process%get_n_components ()
      if (instance%process%component_is_selected (i)) then
        allocate (i_term (size (process%get_component_i_terms (i))))
        i_term = process%get_component_i_terms (i)
        do j = 1, size (i_term)
          instance%term(i_term(j))%active = .true.
        end do
      end if
      if (allocated (i_term)) deallocate (i_term)
    end do
  end associate
  instance%evaluation_status = STAT_ACTIVATED
end subroutine process_instance_activate

```

(Instances: process instance: TBP)+≡

```

procedure :: find_same_kinematics => process_instance_find_same_kinematics

```

(Instances: procedures)+≡

```

subroutine process_instance_find_same_kinematics (instance)
  class(process_instance_t), intent(inout) :: instance
  integer :: i_term1, i_term2, k, n_same
  do i_term1 = 1, size (instance%term)
    if (.not. allocated (instance%term(i_term1)%same_kinematics)) then
      n_same = 1 !!! Index group includes the index of its term_instance
      do i_term2 = 1, size (instance%term)
        if (i_term1 == i_term2) cycle
        if (compare_md5s (i_term1, i_term2)) n_same = n_same + 1
      end do
      allocate (instance%term(i_term1)%same_kinematics (n_same))
      associate (same_kinematics1 => instance%term(i_term1)%same_kinematics)
        same_kinematics1 = 0
        k = 1
        do i_term2 = 1, size (instance%term)
          if (compare_md5s (i_term1, i_term2)) then
            same_kinematics1(k) = i_term2
            k = k + 1
          end if
        end do
        do k = 1, size (same_kinematics1)
          if (same_kinematics1(k) == i_term1) cycle
          i_term2 = same_kinematics1(k)
          allocate (instance%term(i_term2)%same_kinematics (n_same))
          instance%term(i_term2)%same_kinematics = same_kinematics1
        end do
      end associate
    end do
  end do
end subroutine process_instance_find_same_kinematics

```

```

        end if
    end do
contains
    function compare_md5s (i, j) result (same)
        logical :: same
        integer, intent(in) :: i, j
        character(32) :: md5sum_1, md5sum_2
        integer :: mode_1, mode_2
        mode_1 = 0; mode_2 = 0
        select type (phs => instance%kin(i)%phs%config)
        type is (phs_fks_config_t)
            md5sum_1 = phs%md5sum_born_config
            mode_1 = phs%mode
        class default
            md5sum_1 = phs%md5sum_phs_config
        end select
        select type (phs => instance%kin(j)%phs%config)
        type is (phs_fks_config_t)
            md5sum_2 = phs%md5sum_born_config
            mode_2 = phs%mode
        class default
            md5sum_2 = phs%md5sum_phs_config
        end select
        same = (md5sum_1 == md5sum_2) .and. (mode_1 == mode_2)
    end function compare_md5s
end subroutine process_instance_find_same_kinematics

```

(Instances: process instance: TBP)+≡

```

    procedure :: transfer_same_kinematics => process_instance_transfer_same_kinematics

```

(Instances: procedures)+≡

```

subroutine process_instance_transfer_same_kinematics (instance, i_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_term
    integer :: i, i_term_same
    associate (same_kinematics => instance%term(i_term)%same_kinematics)
    do i = 1, size (same_kinematics)
        i_term_same = same_kinematics(i)
        instance%term(i_term_same)%p_seed = instance%term(i_term)%p_seed
        associate (phs => instance%kin(i_term_same)%phs)
            call phs%set_lorentz_transformation &
                (instance%kin(i_term)%phs%get_lorentz_transformation ())
        select type (phs)
        type is (phs_fks_t)
            call phs%set_momenta (instance%term(i_term_same)%p_seed)
            if (i_term_same /= i_term) then
                call phs%set_reference_frames (.false.)
            end if
        end select
        end associate
        instance%kin(i_term_same)%new_seed = .false.
    end do
end associate
end subroutine process_instance_transfer_same_kinematics

```

```

<Instances: process instance: TBP>+≡
  procedure :: redo_sf_chains => process_instance_redo_sf_chains

<Instances: procedures>+≡
  subroutine process_instance_redo_sf_chains (instance, i_term, phs_channel)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in), dimension(:) :: i_term
    integer, intent(in) :: phs_channel
    integer :: i
    do i = 1, size (i_term)
      call instance%kin(i_term(i))%redo_sf_chain &
        (instance%mci_work(instance%i_mci), phs_channel)
    end do
  end subroutine process_instance_redo_sf_chains

```

Integrate the process, using a previously initialized process instance. We select one of the available MCI integrators by its index `i_mci` and thus integrate over (structure functions and) phase space for the associated (group of) process component(s).

```

<Instances: process instance: TBP>+≡
  procedure :: integrate => process_instance_integrate

<Instances: procedures>+≡
  subroutine process_instance_integrate (instance, i_mci, n_it, n_calls, &
    adapt_grids, adapt_weights, final, pacify)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_mci
    integer, intent(in) :: n_it
    integer, intent(in) :: n_calls
    logical, intent(in), optional :: adapt_grids
    logical, intent(in), optional :: adapt_weights
    logical, intent(in), optional :: final, pacify
    integer :: nlo_type, i_mci_work
    nlo_type = instance%process%get_component_nlo_type (i_mci)
    i_mci_work = instance%process%get_i_mci_work (i_mci)
    call instance%choose_mci (i_mci_work)
    call instance%reset_counter ()
    associate (mci_work => instance%mci_work(i_mci_work), &
      process => instance%process)
      call process%integrate (i_mci_work, mci_work, &
        instance, n_it, n_calls, adapt_grids, adapt_weights, &
        final, pacify, nlo_type = nlo_type)
      call process%set_counter_mci_entry (i_mci_work, instance%get_counter ())
    end associate
  end subroutine process_instance_integrate

```

Subroutine of the initialization above: initialize the beam and structure-function chain template. We establish pointers to the configuration data, so `beam_config` must have a `target` attribute.

The resulting chain is not used directly for calculation. It will acquire instances which are stored in the process-component instance objects.

```

<Instances: process instance: TBP>+≡

```

```

    procedure :: setup_sf_chain => process_instance_setup_sf_chain
  (Instances: procedures)+≡
    subroutine process_instance_setup_sf_chain (instance, config)
      class(process_instance_t), intent(inout) :: instance
      type(process_beam_config_t), intent(in), target :: config
      integer :: n_strfun
      n_strfun = config%n_strfun
      if (n_strfun /= 0) then
        call instance%sf_chain%init (config%data, config%sf)
      else
        call instance%sf_chain%init (config%data)
      end if
      if (config%sf_trace) then
        call instance%sf_chain%setup_tracing (config%sf_trace_file)
      end if
    end subroutine process_instance_setup_sf_chain

```

This initialization routine should be called only for process instances which we intend as a source for physical events. It initializes the evaluators in the parton states of the terms. They describe the (semi-)exclusive transition matrix and the distribution of color flow for the partonic process, convoluted with the beam and structure-function chain.

If the model is not provided explicitly, we may use the model instance that belongs to the process. However, an explicit model allows us to override particle settings.

```

  (Instances: process instance: TBP)+≡
    procedure :: setup_event_data => process_instance_setup_event_data
  (Instances: procedures)+≡
    subroutine process_instance_setup_event_data (instance, model, i_core)
      class(process_instance_t), intent(inout), target :: instance
      class(model_data_t), intent(in), optional, target :: model
      integer, intent(in), optional :: i_core
      class(model_data_t), pointer :: current_model
      integer :: i
      class(prc_core_t), pointer :: core => null ()
      if (present (model)) then
        current_model => model
      else
        current_model => instance%process%get_model_ptr ()
      end if
      do i = 1, size (instance%term)
        associate (term => instance%term(i), kin => instance%kin(i))
          if (associated (term%config)) then
            core => instance%process%get_core_term (i)
            call term%setup_event_data (kin, core, current_model)
          end if
        end associate
      end do
      core => null ()
    end subroutine process_instance_setup_event_data

```

Choose a MC parameter set and the corresponding integrator. The choice persists beyond calls of the `reset` method above. This method is automatically called here.

```

<Instances: process instance: TBP>+≡
  procedure :: choose_mci => process_instance_choose_mci

<Instances: procedures>+≡
  subroutine process_instance_choose_mci (instance, i_mci)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_mci
    instance%i_mci = i_mci
    call instance%reset ()
  end subroutine process_instance_choose_mci

```

Explicitly set a MC parameter set. Works only if we are in initial state. We assume that the length of the parameter set is correct.

After setting the parameters, activate the components and terms that correspond to the chosen MC parameter set.

The `warmup_flag` is used when a dummy phase-space point is computed for the warmup of e.g. OpenLoops helicities. The setting of the `evaluation_status` has to be avoided then.

```

<Instances: process instance: TBP>+≡
  procedure :: set_mcpair => process_instance_set_mcpair

<Instances: procedures>+≡
  subroutine process_instance_set_mcpair (instance, x, warmup_flag)
    class(process_instance_t), intent(inout) :: instance
    real(default), dimension(:), intent(in) :: x
    logical, intent(in), optional :: warmup_flag
    logical :: activate
    activate = .true.; if (present (warmup_flag)) activate = .not. warmup_flag
    if (instance%evaluation_status == STAT_INITIAL) then
      associate (mci_work => instance%mci_work(instance%i_mci))
        call mci_work%set (x)
      end associate
      if (activate) call instance%activate ()
    end if
  end subroutine process_instance_set_mcpair

```

Receive the beam momentum/momenta from a source interaction. This applies to a cascade decay process instance, where the ‘beam’ momentum varies event by event.

The master beam momentum array is contained in the main structure function chain subobject `sf_chain`. The sf-chain instance that reside in the components will take their beam momenta from there.

The procedure transforms the instance status into `STAT_BEAM_MOMENTA`. For process instance with fixed beam, this intermediate status is skipped.

```

<Instances: process instance: TBP>+≡
  procedure :: receive_beam_momenta => process_instance_receive_beam_momenta

<Instances: procedures>+≡
  subroutine process_instance_receive_beam_momenta (instance)
    class(process_instance_t), intent(inout) :: instance

```



```

    if (instance%evaluation_status >= STAT_INITIAL) then
        call instance%sf_chain%receive_beam_momenta ()
        instance%evaluation_status = STAT_BEAM_MOMENTA
    end if
end subroutine process_instance_receive_beam_momenta

```

Set the beam momentum/momenta explicitly. Otherwise, analogous to the previous procedure.

```

<Instances: process instance: TBP>+≡
    procedure :: set_beam_momenta => process_instance_set_beam_momenta

<Instances: procedures>+≡
    subroutine process_instance_set_beam_momenta (instance, p)
        class(process_instance_t), intent(inout) :: instance
        type(vector4_t), dimension(:), intent(in) :: p
        if (instance%evaluation_status >= STAT_INITIAL) then
            call instance%sf_chain%set_beam_momenta (p)
            instance%evaluation_status = STAT_BEAM_MOMENTA
        end if
    end subroutine process_instance_set_beam_momenta

```

Recover the initial beam momenta (those in the `sf_chain` component), given a valid (recovered) `sf_chain_instance` in one of the active components. We need to do this only if the lab frame is not the c.m. frame, otherwise those beams would be fixed anyway.

```

<Instances: process instance: TBP>+≡
    procedure :: recover_beam_momenta => process_instance_recover_beam_momenta

<Instances: procedures>+≡
    subroutine process_instance_recover_beam_momenta (instance, i_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_term
        if (.not. instance%process%lab_is_cm ()) then
            if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
                call instance%kin(i_term)%return_beam_momenta ()
            end if
        end if
    end subroutine process_instance_recover_beam_momenta

```

Explicitly choose MC integration channel. We assume here that the channel count is identical for all active components.

```

<Instances: process instance: TBP>+≡
    procedure :: select_channel => process_instance_select_channel

<Instances: procedures>+≡
    subroutine process_instance_select_channel (instance, channel)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: channel
        instance%selected_channel = channel
    end subroutine process_instance_select_channel

```

First step of process evaluation: set up seed kinematics. That is, for each active process component, compute a momentum array from the MC input parameters.

If `skip_term` is set, we skip the component that accesses this term. We can assume that the associated data have already been recovered, and we are just computing the rest.

```

<Instances: process instance: TBP>+=
  procedure :: compute_seed_kinematics => &
    process_instance_compute_seed_kinematics

<Instances: procedures>+=
  subroutine process_instance_compute_seed_kinematics &
    (instance, recover, skip_term)
    class(process_instance_t), intent(inout) :: instance
    logical, intent(in), optional :: recover
    integer, intent(in), optional :: skip_term
    integer :: channel, skip_component, i, j
    logical :: success
    integer, dimension(:), allocatable :: i_term
    channel = instance%selected_channel
    if (channel == 0) then
      call msg_bug ("Compute seed kinematics: undefined integration channel")
    end if
    if (present (skip_term)) then
      skip_component = instance%term(skip_term)%config%i_component
    else
      skip_component = 0
    end if
    if (present (recover)) then
      if (recover) return
    end if
    if (instance%evaluation_status >= STAT_ACTIVATED) then
      success = .true.
      do i = 1, instance%process%get_n_components ()
        if (i == skip_component) cycle
        if (instance%process%component_is_selected (i)) then
          allocate (i_term (size (instance%process%get_component_i_terms (i))))
          i_term = instance%process%get_component_i_terms (i)
          do j = 1, size (i_term)
            associate (term => instance%term(i_term(j)), kin => instance%kin(i_term(j)))
              if (kin%new_seed) then
                call term%compute_seed_kinematics (kin, &
                  instance%mc_i_work(instance%i_mci), channel, success)
                call instance%transfer_same_kinematics (i_term(j))
              end if
              if (.not. success) exit
            end select type (pcm => instance%pcm)
            class is (pcm_nlo_t)
              call term%evaluate_projections (kin)
              call kin%evaluate_radiation_kinematics &
                (instance%mc_i_work(instance%i_mci)%get_x_process ())
              call kin%generate_fsr_in ()
              call kin%compute_xi_ref_momenta (pcm%region_data, term%nlo_type)
            end select
          end associate
        end if
      end do
    end if
  end subroutine

```

```

        end do
    end if
    if (allocated (i_term)) deallocate (i_term)
end do
if (success) then
    instance%evaluation_status = STAT_SEED_KINEMATICS
else
    instance%evaluation_status = STAT_FAILED_KINEMATICS
end if
end if
associate (mci_work => instance%mci_work(instance%i_mci))
    select type (pcm_work => instance%pcm_work)
    class is (pcm_nlo_workspace_t)
        call pcm_work%set_x_rad (mci_work%get_x_process ())
    end select
end associate
end subroutine process_instance_compute_seed_kinematics

```

<Instances: process instance: TBP>+≡

```

    procedure :: get_x_process => process_instance_get_x_process

```

<Instances: procedures>+≡

```

    pure function process_instance_get_x_process (instance) result (x)
        real(default), dimension(:), allocatable :: x
        class(process_instance_t), intent(in) :: instance
        allocate (x(size (instance%mci_work(instance%i_mci)%get_x_process ())))
        x = instance%mci_work(instance%i_mci)%get_x_process ()
    end function process_instance_get_x_process

```

<Instances: process instance: TBP>+≡

```

    procedure :: get_active_component_type => process_instance_get_active_component_type

```

<Instances: procedures>+≡

```

    pure function process_instance_get_active_component_type (instance) &
        result (nlo_type)
        integer :: nlo_type
        class(process_instance_t), intent(in) :: instance
        nlo_type = instance%process%get_component_nlo_type (instance%i_mci)
    end function process_instance_get_active_component_type

```

Inverse: recover missing parts of the kinematics from the momentum configuration, which we know for a single term and component. Given a channel, reconstruct the MC parameter set.

<Instances: process instance: TBP>+≡

```

    procedure :: recover_mcpair => process_instance_recover_mcpair

```

<Instances: procedures>+≡

```

    subroutine process_instance_recover_mcpair (instance, i_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_term
        integer :: channel, i
        if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
            channel = instance%selected_channel
            if (channel == 0) then

```

```

        call msg_bug ("Recover MC parameters: undefined integration channel")
    end if
    call instance%kin(i_term)%recover_mcpair &
        (instance%mc_i_work(instance%i_mci), channel, instance%term(i_term)%p_seed)
    if (instance%term(i_term)%nlo_type == NLO_REAL) then
        do i = 1, size (instance%term)
            if (i /= i_term .and. instance%term(i)%nlo_type == NLO_REAL) then
                if (instance%term(i)%active) then
                    call instance%kin(i)%recover_mcpair &
                        (instance%mc_i_work(instance%i_mci), channel, &
                            instance%term(i)%p_seed)
                end if
            end if
        end do
    end if
end if
end subroutine process_instance_recover_mcpair

```

This is part of `recover_mcpair`, extracted for the case when there is no phase space and parameters to recover, but we still need the structure function kinematics for evaluation.

```

<Instances: process instance: TBP>+≡
    procedure :: recover_sfchain => process_instance_recover_sfchain

<Instances: procedures>+≡
    subroutine process_instance_recover_sfchain (instance, i_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_term
        integer :: channel
        if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
            channel = instance%selected_channel
            if (channel == 0) then
                call msg_bug ("Recover sfchain: undefined integration channel")
            end if
            call instance%kin(i_term)%recover_sfchain (channel, instance%term(i_term)%p_seed)
        end if
    end subroutine process_instance_recover_sfchain

```

Second step of process evaluation: compute all momenta, for all active components, from the seed kinematics.

```

<Instances: process instance: TBP>+≡
    procedure :: compute_hard_kinematics => &
        process_instance_compute_hard_kinematics

<Instances: procedures>+≡
    subroutine process_instance_compute_hard_kinematics (instance, recover, skip_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in), optional :: skip_term
        logical, intent(in), optional :: recover
        integer :: i
        logical :: success
        success = .true.
        if (instance%evaluation_status >= STAT_SEED_KINEMATICS) then
            do i = 1, size (instance%term)

```

```

        associate (term => instance%term(i), kin => instance%kin(i))
        if (term%active) then
            call term%compute_hard_kinematics &
                (kin, recover, skip_term, success)
            if (.not. success) exit
            !!! Ren scale is zero when this is commented out! Understand!
            if (term%nlo_type == NLO_REAL) &
                call kin%redo_sf_chain (instance%mc_work(instance%i_mci), &
                    instance%selected_channel)
            end if
        end associate
    end do
    if (success) then
        instance%evaluation_status = STAT_HARD_KINEMATICS
    else
        instance%evaluation_status = STAT_FAILED_KINEMATICS
    end if
end if
end if
end subroutine process_instance_compute_hard_kinematics

```

Inverse: recover seed kinematics. We know the beam momentum configuration and the outgoing momenta of the effective interaction, for one specific term.

(Instances: process instance: TBP)+≡

```

    procedure :: recover_seed_kinematics => &
        process_instance_recover_seed_kinematics

```

(Instances: procedures)+≡

```

    subroutine process_instance_recover_seed_kinematics (instance, i_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_term
    type(vector4_t), dimension(:), allocatable :: p_seed_ref
    integer :: i
    if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
        call instance%term(i_term)%recover_seed_kinematics (instance%kin(i_term))
        if (instance%term(i_term)%nlo_type == NLO_REAL) then
            allocate (p_seed_ref (instance%term(i_term)%isolated%int_eff%get_n_out ()))
            p_seed_ref = instance%term(i_term)%isolated%int_eff%get_momenta &
                (outgoing = .true.)
            do i = 1, size (instance%term)
                if (i /= i_term .and. instance%term(i)%nlo_type == NLO_REAL) then
                    if (instance%term(i)%active) then
                        call instance%term(i)%recover_seed_kinematics &
                            (instance%kin(i), p_seed_ref)
                    end if
                end if
            end do
        end if
    end if
end if
end subroutine process_instance_recover_seed_kinematics

```

Third step of process evaluation: compute the effective momentum configurations, for all active terms, from the hard kinematics.

(Instances: process instance: TBP)+≡

```

    procedure :: compute_eff_kinematics => &
        process_instance_compute_eff_kinematics
<Instances: procedures>+=
    subroutine process_instance_compute_eff_kinematics (instance, skip_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in), optional :: skip_term
        integer :: i
        if (instance%evaluation_status >= STAT_HARD_KINEMATICS) then
            do i = 1, size (instance%term)
                if (present (skip_term)) then
                    if (i == skip_term) cycle
                end if
                if (instance%term(i)%active) then
                    call instance%term(i)%compute_eff_kinematics ()
                end if
            end do
            instance%evaluation_status = STAT_EFF_KINEMATICS
        end if
    end subroutine process_instance_compute_eff_kinematics

```

Inverse: recover the hard kinematics from effective kinematics for one term, then compute effective kinematics for the other terms.

```

<Instances: process instance: TBP>+=
    procedure :: recover_hard_kinematics => &
        process_instance_recover_hard_kinematics
<Instances: procedures>+=
    subroutine process_instance_recover_hard_kinematics (instance, i_term)
        class(process_instance_t), intent(inout) :: instance
        integer, intent(in) :: i_term
        integer :: i
        if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
            call instance%term(i_term)%recover_hard_kinematics ()
            do i = 1, size (instance%term)
                if (i /= i_term) then
                    if (instance%term(i)%active) then
                        call instance%term(i)%compute_eff_kinematics ()
                    end if
                end if
            end do
            instance%evaluation_status = STAT_EFF_KINEMATICS
        end if
    end subroutine process_instance_recover_hard_kinematics

```

Fourth step of process evaluation: check cuts for all terms. Where successful, compute any scales and weights. Otherwise, deactivate the term. If any of the terms has passed, set the state to `STAT_PASSED_CUTS`.

The argument `scale_forced`, if present, will override the scale calculation in the term expressions.

```

<Instances: process instance: TBP>+=
    procedure :: evaluate_expressions => &
        process_instance_evaluate_expressions

```

(Instances: procedures)+≡

```

subroutine process_instance_evaluate_expressions (instance, scale_forced)
  class(process_instance_t), intent(inout) :: instance
  real(default), intent(in), allocatable, optional :: scale_forced
  integer :: i
  logical :: passed_real
  if (instance%evaluation_status >= STAT_EFF_KINEMATICS) then
    do i = 1, size (instance%term)
      if (instance%term(i)%active) then
        call instance%term(i)%evaluate_expressions (scale_forced)
      end if
    end do
    call evaluate_real_scales_and_cuts ()
    call set_ellis_sexton_scale ()
    if (.not. passed_real) then
      instance%evaluation_status = STAT_FAILED_CUTS
    else
      if (any (instance%term%passed)) then
        instance%evaluation_status = STAT_PASSED_CUTS
      else
        instance%evaluation_status = STAT_FAILED_CUTS
      end if
    end if
  end if
contains
  subroutine evaluate_real_scales_and_cuts ()
    integer :: i
    passed_real = .true.
    select type (pcm => instance%pcm)
    type is (pcm_nlo_t)
      do i = 1, size (instance%term)
        if (instance%term(i)%active .and. instance%term(i)%nlo_type == NLO_REAL) then
          if (pcm%settings%cut_all_real_sqmes) &
            passed_real = passed_real .and. instance%term(i)%passed
          if (pcm%settings%use_born_scale) &
            call replace_scales (instance%term(i))
        end if
      end do
    end select
  end subroutine evaluate_real_scales_and_cuts

  subroutine replace_scales (this_term)
    type(term_instance_t), intent(inout) :: this_term
    integer :: i_sub
    i_sub = this_term%config%i_sub
    if (this_term%config%i_term_global /= i_sub .and. i_sub > 0) then
      this_term%ren_scale = instance%term(i_sub)%ren_scale
      this_term%fac_scale = instance%term(i_sub)%fac_scale
    end if
  end subroutine replace_scales

  subroutine set_ellis_sexton_scale ()
    real(default) :: es_scale
    type(var_list_t), pointer :: var_list

```

```

integer :: i
var_list => instance%process%get_var_list_ptr ()
es_scale = var_list%get_rval (var_str ("ellis_sextton_scale"))
do i = 1, size (instance%term)
  if (instance%term(i)%active .and. instance%term(i)%nlo_type == NLO_VIRTUAL) then
    if (es_scale < zero) then
      instance%term(i)%es_scale = instance%term(i)%ren_scale
    else
      instance%term(i)%es_scale = es_scale
    end if
  end if
end do
end subroutine set_ellis_sextton_scale
end subroutine process_instance_evaluate_expressions

```

Fifth step of process evaluation: fill the parameters for the non-selected channels, that have not been used for seeding. We should do this after evaluating cuts, since we may save some expensive calculations if the phase space point fails the cuts.

If `skip_term` is set, we skip the component that accesses this term. We can assume that the associated data have already been recovered, and we are just computing the rest.

```

<Instances: process instance: TBP>+≡
  procedure :: compute_other_channels => &
    process_instance_compute_other_channels

<Instances: procedures>+≡
  subroutine process_instance_compute_other_channels (instance, skip_term)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in), optional :: skip_term
    integer :: channel, skip_component, i, j
    integer, dimension(:), allocatable :: i_term
    channel = instance%selected_channel
    if (channel == 0) then
      call msg_bug ("Compute other channels: undefined integration channel")
    end if
    if (present (skip_term)) then
      skip_component = instance%term(skip_term)%config%i_component
    else
      skip_component = 0
    end if
    if (instance%evaluation_status >= STAT_PASSED_CUTS) then
      do i = 1, instance%process%get_n_components ()
        if (i == skip_component) cycle
        if (instance%process%component_is_selected (i)) then
          allocate (i_term (size (instance%process%get_component_i_terms (i))))
          i_term = instance%process%get_component_i_terms (i)
          do j = 1, size (i_term)
            call instance%kin(i_term(j))%compute_other_channels &
              (instance%mci_work(instance%i_mci), channel)
          end do
        end if
      end do
      if (allocated (i_term)) deallocate (i_term)
    end if
  end subroutine

```



```

        end do
    end if
end subroutine process_instance_compute_other_channels

```

If not done otherwise, we flag the kinematics as new for the core state, such that the routine below will actually compute the matrix element and not just look it up.

```

<Instances: process instance: TBP>+≡
    procedure :: reset_core_kinematics => process_instance_reset_core_kinematics

<Instances: procedures>+≡
    subroutine process_instance_reset_core_kinematics (instance)
        class(process_instance_t), intent(inout) :: instance
        integer :: i
        if (instance%evaluation_status >= STAT_PASSED_CUTS) then
            do i = 1, size (instance%term)
                associate (term => instance%term(i))
                    if (term%active .and. term%passed) then
                        if (allocated (term%core_state)) &
                            call term%core_state%reset_new_kinematics ()
                    end if
                end associate
            end do
        end if
    end subroutine process_instance_reset_core_kinematics

```

Sixth step of process evaluation: evaluate the matrix elements, and compute the trace (summed over quantum numbers) for all terms. Finally, sum up the terms, iterating over all active process components.

```

<Instances: process instance: TBP>+≡
    procedure :: evaluate_trace => process_instance_evaluate_trace

<Instances: procedures>+≡
    subroutine process_instance_evaluate_trace (instance, recover)
        class(process_instance_t), intent(inout) :: instance
        logical, intent(in), optional :: recover
        class(prc_core_t), pointer :: core => null ()
        integer :: i, i_real_fin, i_core
        real(default) :: alpha_s, alpha_qed
        class(prc_core_t), pointer :: core_sub => null ()
        class(model_data_t), pointer :: model => null ()
        logical :: has_pdfs
        if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "process_instance_evaluate_trace")
        has_pdfs = instance%process%pcm_contains_pdfs ()
        instance%sqme = zero
        call instance%reset_matrix_elements ()
        if (instance%evaluation_status >= STAT_PASSED_CUTS) then
            do i = 1, size (instance%term)
                associate (term => instance%term(i), kin => instance%kin(i))
                    if (term%active .and. term%passed) then
                        core => instance%process%get_core_term (i)
                        select type (pcm => instance%process%get_pcm_ptr ())
                        class is (pcm_nlo_t)

```

```

        i_core = pcm%get_i_core (pcm%i_sub)
        core_sub => instance%process%get_core_ptr (i_core)
    end select
    call term%evaluate_interaction (core, kin)
    call term%evaluate_trace (kin)
    i_real_fin = instance%process%get_associated_real_fin (1)
    if (instance%process%uses_real_partition ()) &
        call term%apply_real_partition (kin, instance%process)
    if (term%config%i_component /= i_real_fin) then
        if ((term%nlo_type == NLO_REAL .and. kin%emitter < 0) &
            .or. term%nlo_type == NLO_MISMATCH &
            .or. term%nlo_type == NLO_DGLAP) &
            call term%set_born_sqmes (core)
        if (term%is_subtraction () .or. &
            term%nlo_type == NLO_DGLAP) &
            call term%set_sf_factors (kin, has_pdfs)
        if (term%nlo_type > BORN) then
            if (.not. (term%nlo_type == NLO_REAL .and. &
                kin%emitter >= 0)) then
                select type (pcm => term%pcm)
                type is (pcm_nlo_t)
                    if (char (pcm%settings%nlo_correction_type) == "QCD" .or. &
                        char (pcm%settings%nlo_correction_type) == "Full") &
                        call term%evaluate_color_correlations (core_sub)
                    if (char (pcm%settings%nlo_correction_type) == "EW" .or. &
                        char (pcm%settings%nlo_correction_type) == "Full") then
                        call term%evaluate_charge_correlations (core_sub)
                    select type (pcm => term%pcm)
                    type is (pcm_nlo_t)
                        associate (reg_data => pcm%region_data)
                            if (reg_data%alphas_power > 0) &
                                call term%evaluate_color_correlations (core_sub)
                        end associate
                    end select
                end if
            end select
        end if
        if (term%is_subtraction ()) then
            call term%evaluate_spin_correlations (core_sub)
        end if
    end if
    alpha_s = core%get_alpha_s (term%core_state)
    alpha_qed = core%get_alpha_qed ()
    if (term%nlo_type > BORN) then
        select type (pcm => term%pcm)
        type is (pcm_nlo_t)
            if (alpha_qed == -1 .and. (&
                char (pcm%settings%nlo_correction_type) == "EW" .or. &
                char (pcm%settings%nlo_correction_type) == "Full")) then
                call msg_bug("Attempting to compute EW corrections with alpha_qed = -1")
            end if
        end select
    end if
    if (present (recover)) then

```

```

        if (recover) return
    end if
    select case (term%nlo_type)
    case (NLO_REAL)
        call term%apply_fks (kin, alpha_s, alpha_qed)
    case (NLO_VIRTUAL)
        call term%evaluate_sqme_virt (alpha_s, alpha_qed)
    case (NLO_MISMATCH)
        call term%evaluate_sqme_mismatch (alpha_s)
    case (NLO_DGLAP)
        call term%evaluate_sqme_dglap (alpha_s, alpha_qed)
    end select
    end if
    end if
    core_sub => null ()
    instance%sqme = instance%sqme + real (sum (&
        term%connected%trace%get_matrix_element () * &
        term%weight))
    end associate
end do
core => null ()
if (instance%pcm_work%is_valid ()) then
    instance%evaluation_status = STAT_EVALUATED_TRACE
else
    instance%evaluation_status = STAT_FAILED_KINEMATICS
end if
else
    !!! Failed kinematics or failed cuts: set sqme to zero
    instance%sqme = zero
end if
end subroutine process_instance_evaluate_trace

```

(Instances: term instance: TBP)+≡

```

    procedure :: set_born_sqmes => term_instance_set_born_sqmes

```

(Instances: procedures)+≡

```

subroutine term_instance_set_born_sqmes (term, core)
    class(term_instance_t), intent(inout) :: term
    class(prc_core_t), intent(in) :: core
    integer :: i_flv, ii_flv
    real(default) :: sqme
    select type (pcm_work => term%pcm_work)
    type is (pcm_nlo_workspace_t)
        do i_flv = 1, term%connected%trace%get_qn_index_n_flv ()
            ii_flv = term%connected%trace%get_qn_index (i_flv, i_sub = 0)
            sqme = real (term%connected%trace%get_matrix_element (ii_flv))
            select case (term%nlo_type)
            case (NLO_REAL)
                pcm_work%real_sub%sqme_born(i_flv) = sqme
            case (NLO_MISMATCH)
                pcm_work%soft_mismatch%sqme_born(i_flv) = sqme
            case (NLO_DGLAP)
                pcm_work%dglap_remnant%sqme_born(i_flv) = sqme
            end select
        end do
    end select

```

```

        end do
    end select
end subroutine term_instance_set_born_sqmes

```

Calculates and then saves the ratio of the value of the (rescaled) real structure function chain of each ISR alpha region over the value of the corresponding underlying born flavor structure. In the case of emitter 0 we also need the rescaled ratio for emitter 1 and 2 in that region for the (soft-)collinear limits. If the emitter is 1 or 2 in some cases, e. g. for EW corrections where a photon in the proton is required, there can be the possibility of soft radiation off the initial state. For that purpose the unrescaled ratio is needed and as a default we always save these numbers in `sf_factors(:, 0)`. Although this procedure is implying functionality for general structure functions, it should be reviewed for anything else besides PDFs, as there might be complications in the details. The general idea of getting the ratio in this way should hold up in these cases as well, however.

```

<Instances: term instance: TBP>+≡
    procedure :: set_sf_factors => term_instance_set_sf_factors

<Instances: procedures>+≡
    subroutine term_instance_set_sf_factors (term, kin, has_pdfs)
        class(term_instance_t), intent(inout) :: term
        type(kinematics_t), intent(inout) :: kin
        logical, intent(in) :: has_pdfs
        type(interaction_t), pointer :: sf_chain_int
        real(default) :: factor_born, factor_real
        integer :: n_in, alr, em
        integer :: i_born, i_real
        select type (pcm_work => term%pcm_work)
        type is (pcm_nlo_workspace_t)
            if (.not. has_pdfs) then
                pcm_work%real_sub%sf_factors = one
                return
            end if
            select type (pcm => term%pcm)
            type is (pcm_nlo_t)
                sf_chain_int => kin%sf_chain%get_out_int_ptr ()
                associate (reg_data => pcm%region_data)
                    n_in = reg_data%get_n_in ()
                    do alr = 1, reg_data%n_regions
                        em = reg_data%regions(alr)%emitter
                        if (em <= n_in) then
                            i_born = reg_data%regions(alr)%uborn_index
                            i_real = reg_data%regions(alr)%real_index
                            factor_born = sf_chain_int%get_matrix_element &
                                (sf_chain_int%get_sf_qn_index_born (i_born, i_sub = 0))
                            factor_real = sf_chain_int%get_matrix_element &
                                (sf_chain_int%get_sf_qn_index_real (i_real, i_sub = em))
                            call set_factor (pcm_work, alr, em, factor_born, factor_real)
                            if (em == 0) then
                                do em = 1, 2
                                    factor_real = sf_chain_int%get_matrix_element &
                                        (sf_chain_int%get_sf_qn_index_real (i_real, i_sub = em))
                                end do
                            end if
                        end if
                    end do
                end associate
            end type is
        end select
    end subroutine

```

```

        call set_factor (pcm_work, alr, em, factor_born, factor_real)
    end do
    else
        factor_real = sf_chain_int%get_matrix_element &
            (sf_chain_int%get_sf_qn_index_real (i_real, i_sub = 0))
        call set_factor (pcm_work, alr, 0, factor_born, factor_real)
    end if
end if
end do
end associate
end select
end select
contains
subroutine set_factor (pcm_work, alr, em, factor_born, factor_real)
    type(pcm_nlo_workspace_t), intent(inout), target :: pcm_work
    integer, intent(in) :: alr, em
    real(default), intent(in) :: factor_born, factor_real
    real(default) :: factor
    if (any (vanishes ([factor_real, factor_born], tiny(1._default), tiny(1._default)))) then
        factor = zero
    else
        factor = factor_real / factor_born
    end if
    select case (term%nlo_type)
    case (NLO_REAL)
        pcm_work%real_sub%sf_factors(alr, em) = factor
    case (NLO_DGLAP)
        pcm_work%dglap_remnant%sf_factors(alr, em) = factor
    end select
end subroutine
end subroutine term_instance_set_sf_factors

```

(Instances: process instance: TBP)+≡

```

    procedure :: apply_real_partition => process_instance_apply_real_partition

```

(Instances: procedures)+≡

```

subroutine process_instance_apply_real_partition (instance)
    class(process_instance_t), intent(inout) :: instance
    integer :: i_component, i_term
    integer, dimension(:), allocatable :: i_terms
    associate (process => instance%process)
        i_component = process%get_first_real_component ()
        if (process%component_is_selected (i_component) .and. &
            process%get_component_nlo_type (i_component) == NLO_REAL) then
            allocate (i_terms (size (process%get_component_i_terms (i_component))))
            i_terms = process%get_component_i_terms (i_component)
            do i_term = 1, size (i_terms)
                call instance%term(i_terms(i_term))%apply_real_partition ( &
                    instance%kin(i_terms(i_term)), &
                    process)
            end do
        end if
        if (allocated (i_terms)) deallocate (i_terms)
    end associate

```

```

end subroutine process_instance_apply_real_partition

<Instances: process instance: TBP>+≡
  procedure :: set_i_mci_to_real_component => process_instance_set_i_mci_to_real_component
<Instances: procedures>+≡
  subroutine process_instance_set_i_mci_to_real_component (instance)
    class(process_instance_t), intent(inout) :: instance
    integer :: i_mci, i_component
    type(process_component_t), pointer :: component => null ()
    select type (pcm_work => instance%pcm_work)
    type is (pcm_nlo_workspace_t)
      if (allocated (pcm_work%i_mci_to_real_component)) then
        call msg_warning ("i_mci_to_real_component already allocated - replace it")
        deallocate (pcm_work%i_mci_to_real_component)
      end if
      allocate (pcm_work%i_mci_to_real_component (size (instance%mci_work)))
      do i_mci = 1, size (instance%mci_work)
        do i_component = 1, instance%process%get_n_components ()
          component => instance%process%get_component_ptr (i_component)
          if (component%i_mci /= i_mci) cycle
          select case (component%component_type)
          case (COMP_MASTER, COMP_REAL)
            pcm_work%i_mci_to_real_component (i_mci) = &
              component%config%get_associated_real ()
          case (COMP_REAL_FIN)
            pcm_work%i_mci_to_real_component (i_mci) = &
              component%config%get_associated_real_fin ()
          case (COMP_REAL_SING)
            pcm_work%i_mci_to_real_component (i_mci) = &
              component%config%get_associated_real_sing ()
          end select
        end do
      end do
      component => null ()
    end select
  end subroutine process_instance_set_i_mci_to_real_component

```

Final step of process evaluation: evaluate the matrix elements, and compute the trace (summed over quantum numbers) for all terms. Finally, sum up the terms, iterating over all active process components.

If **weight** is provided, we already know the kinematical event weight (the MCI weight which depends on the kinematics sampling algorithm, but not on the matrix element), so we do not need to take it from the MCI record.

```

<Instances: process instance: TBP>+≡
  procedure :: evaluate_event_data => process_instance_evaluate_event_data
<Instances: procedures>+≡
  subroutine process_instance_evaluate_event_data (instance, weight)
    class(process_instance_t), intent(inout) :: instance
    real(default), intent(in), optional :: weight
    integer :: i
    if (instance%evaluation_status >= STAT_EVALUATED_TRACE) then

```

```

do i = 1, size (instance%term)
  associate (term => instance%term(i))
    if (term%active) then
      call term%evaluate_event_data ()
    end if
  end associate
end do
if (present (weight)) then
  instance%weight = weight
else
  instance%weight = &
    instance%mc_i_work(instance%i_mci)%mc_i%get_event_weight ()
  instance%excess = &
    instance%mc_i_work(instance%i_mci)%mc_i%get_event_excess ()
end if
instance%n_dropped = &
  instance%mc_i_work(instance%i_mci)%mc_i%get_n_event_dropped ()
instance%evaluation_status = STAT_EVENT_COMPLETE
else
  !!! failed kinematics etc.: set weight to zero
  instance%weight = zero
  !!! Maybe we want to process and keep the event nevertheless
  if (instance%keep_failed_events ()) then
    do i = 1, size (instance%term)
      associate (term => instance%term(i))
        if (term%active) then
          call term%evaluate_event_data ()
        end if
      end associate
    end do
    !      do i = 1, size (instance%term)
    !        instance%term(i)%fac_scale = zero
    !      end do
    instance%evaluation_status = STAT_EVENT_COMPLETE
  end if
end if
end subroutine process_instance_evaluate_event_data

```

Computes the real-emission matrix element for externally supplied momenta for the term instance with index `i_term` and a phase space point set with index `i_phs`. In addition, for the real emission, each term instance corresponds to one emitter. Also, e.g. for Powheg, there is the possibility to supply an external α_s .

(Instances: process instance: TBP)+≡

```
procedure :: compute_sqme_rad => process_instance_compute_sqme_rad
```

(Instances: procedures)+≡

```

subroutine process_instance_compute_sqme_rad &
  (instance, i_term, i_phs, is_subtraction, alpha_s_external)
class(process_instance_t), intent(inout) :: instance
integer, intent(in) :: i_term, i_phs
logical, intent(in) :: is_subtraction
real(default), intent(in), optional :: alpha_s_external
class(prc_core_t), pointer :: core
integer :: i_real_fin

```

```

logical :: has_pdfs
has_pdfs = instance%process%pcm_contains_pdfs ()
if (debug_on) call msg_debug2 (D_PROCESS_INTEGRATION, "process_instance_compute_sqme_rad")
select type (pcm_work => instance%pcm_work)
type is (pcm_nlo_workspace_t)
  associate (term => instance%term(i_term), kin => instance%kin(i_term))
    core => instance%process%get_core_term (i_term)
    if (is_subtraction) then
      call pcm_work%set_subtraction_event ()
    else
      call pcm_work%set_radiation_event ()
    end if
    call term%int_hard%set_momenta (pcm_work%get_momenta &
      (term%pcm, i_phs = i_phs, born_phsp = is_subtraction))
    if (allocated (term%core_state)) &
      call term%core_state%reset_new_kinematics ()
    if (present (alpha_s_external)) &
      call term%set_alpha_qcd_forced (alpha_s_external)
    call term%compute_eff_kinematics ()
    call term%evaluate_expressions ()
    call term%evaluate_interaction (core, kin)
    call term%evaluate_trace (kin)
    if (term%is_subtraction ()) then
      call term%set_sf_factors (kin, has_pdfs)
      select type (pcm => instance%pcm)
      type is (pcm_nlo_t)
        if (char (pcm%settings%nlo_correction_type) == "QCD" .or. &
          char (pcm%settings%nlo_correction_type) == "Full") &
          call term%evaluate_color_correlations (core)
        if (char (pcm%settings%nlo_correction_type) == "EW" .or. &
          char (pcm%settings%nlo_correction_type) == "Full") &
          call term%evaluate_charge_correlations (core)
        end select
      call term%evaluate_spin_correlations (core)
    end if
    i_real_fin = instance%process%get_associated_real_fin (1)
    if (term%config%i_component /= i_real_fin) &
      call term%apply_fks (kin, core%get_alpha_s (term%core_state), &
        core%get_alpha_qed ())
    if (instance%process%uses_real_partition ()) &
      call instance%apply_real_partition ()
  end associate
end select
core => null ()
end subroutine process_instance_compute_sqme_rad

```

For unweighted event generation, we should reset the reported event weight to unity (signed) or zero. The latter case is appropriate for an event which failed for whatever reason.

```

<Instances: process instance: TBP>+≡
  procedure :: normalize_weight => process_instance_normalize_weight
<Instances: procedures>+≡
  subroutine process_instance_normalize_weight (instance)

```



```

class(process_instance_t), intent(inout) :: instance
if (.not. vanishes (instance%weight)) then
  instance%weight = sign (1._default, instance%weight)
end if
end subroutine process_instance_normalize_weight

```

This is a convenience routine that performs the computations of the steps 1 to 5 in a single step. The arguments are the input for `set_mcp`. After this, the evaluation status should be either `STAT_FAILED_KINEMATICS`, `STAT_FAILED_CUTS` or `STAT_EVALUATED_TRACE`.

Before calling this, we should call `choose_mci`.

```

<Instances: process instance: TBP>+≡
  procedure :: evaluate_sqme => process_instance_evaluate_sqme

<Instances: procedures>+≡
  subroutine process_instance_evaluate_sqme (instance, channel, x)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: channel
    real(default), dimension(:), intent(in) :: x
    call instance%reset ()
    call instance%set_mcp (x)
    call instance%select_channel (channel)
    call instance%compute_seed_kinematics ()
    call instance%compute_hard_kinematics ()
    call instance%compute_eff_kinematics ()
    call instance%evaluate_expressions ()
    call instance%compute_other_channels ()
    call instance%evaluate_trace ()
  end subroutine process_instance_evaluate_sqme

```

This is the inverse. Assuming that the final trace evaluator contains a valid momentum configuration, recover kinematics and recalculate the matrix elements and their trace.

To be precise, we first recover kinematics for the given term and associated component, then recalculate from that all other terms and active components. The `channel` is not really required to obtain the matrix element, but it allows us to reconstruct the exact MC parameter set that corresponds to the given phase space point.

Before calling this, we should call `choose_mci`.

```

<Instances: process instance: TBP>+≡
  procedure :: recover => process_instance_recover

<Instances: procedures>+≡
  subroutine process_instance_recover &
    (instance, channel, i_term, update_sqme, recover_phs, scale_forced)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: channel
    integer, intent(in) :: i_term
    logical, intent(in) :: update_sqme
    logical, intent(in) :: recover_phs
    real(default), intent(in), allocatable, optional :: scale_forced
    logical :: skip_phs, recover
    call instance%activate ()

```

```

instance%evaluation_status = STAT_EFF_KINEMATICS
call instance%recover_hard_kinematics (i_term)
call instance%recover_seed_kinematics (i_term)
call instance%select_channel (channel)
recover = instance%pcm_work%is_nlo ()
if (recover_phs) then
  call instance%recover_mcpair (i_term)
  call instance%recover_beam_momenta (i_term)
  call instance%compute_seed_kinematics &
    (recover = recover, skip_term = i_term)
  call instance%compute_hard_kinematics &
    (recover = recover, skip_term = i_term)
  call instance%compute_eff_kinematics (i_term)
  call instance%compute_other_channels (i_term)
else
  call instance%recover_sfchain (i_term)
end if
call instance%evaluate_expressions (scale_forced)
if (update_sqme) then
  call instance%reset_core_kinematics ()
  call instance%evaluate_trace (recover)
end if
end subroutine process_instance_recover

```

The `evaluate` method is required by the `sampler_t` base type of which the process instance is an extension.

The requirement is that after the process instance is evaluated, the integrand, the selected channel, the x array, and the f Jacobian array are exposed by the `sampler_t` object.

We allow for the additional hook to be called, if associated, for outlying object to access information from the current state of the `sampler`.

```

<Instances: process instance: TBP>+≡
  procedure :: evaluate => process_instance_evaluate

<Instances: procedures>+≡
  subroutine process_instance_evaluate (sampler, c, x_in, val, x, f)
    class(process_instance_t), intent(inout) :: sampler
    integer, intent(in) :: c
    real(default), dimension(:), intent(in) :: x_in
    real(default), intent(out) :: val
    real(default), dimension(:,:), intent(out) :: x
    real(default), dimension(:), intent(out) :: f
    call sampler%evaluate_sqme (c, x_in)
    if (sampler%is_valid ()) then
      call sampler%fetch (val, x, f)
    end if
    call sampler%record_call ()
    call sampler%evaluate_after_hook ()
  end subroutine process_instance_evaluate

```

The phase-space point is valid if the event has valid kinematics and has passed the cuts.

```

<Instances: process instance: TBP>+≡

```

```

    procedure :: is_valid => process_instance_is_valid
  <Instances: procedures>+≡
    function process_instance_is_valid (sampler) result (valid)
      class(process_instance_t), intent(in) :: sampler
      logical :: valid
      valid = sampler%evaluation_status >= STAT_PASSED_CUTS
    end function process_instance_is_valid

```

Add a process_instance_hook object..

```

  <Instances: process instance: TBP>+≡
    procedure :: append_after_hook => process_instance_append_after_hook
  <Instances: procedures>+≡
    subroutine process_instance_append_after_hook (sampler, new_hook)
      class(process_instance_t), intent(inout), target :: sampler
      class(process_instance_hook_t), intent(inout), target :: new_hook
      class(process_instance_hook_t), pointer :: last
      if (associated (new_hook%next)) then
        call msg_bug ("process_instance_append_after_hook: reuse of SAME hook object is forbidden.")
      end if
      if (associated (sampler%hook)) then
        last => sampler%hook
        do while (associated (last%next))
          last => last%next
        end do
        last%next => new_hook
      else
        sampler%hook => new_hook
      end if
    end subroutine process_instance_append_after_hook

```

Evaluate the after hook as first in, last out.

```

  <Instances: process instance: TBP>+≡
    procedure :: evaluate_after_hook => process_instance_evaluate_after_hook
  <Instances: procedures>+≡
    subroutine process_instance_evaluate_after_hook (sampler)
      class(process_instance_t), intent(in) :: sampler
      class(process_instance_hook_t), pointer :: current
      current => sampler%hook
      do while (associated(current))
        call current%evaluate (sampler)
        current => current%next
      end do
    end subroutine process_instance_evaluate_after_hook

```

The `rebuild` method should rebuild the kinematics section out of the `x_in` parameter set. The integrand value `val` should not be computed, but is provided as input.

```

  <Instances: process instance: TBP>+≡
    procedure :: rebuild => process_instance_rebuild

```

```

<Instances: procedures>+≡
subroutine process_instance_rebuild (sampler, c, x_in, val, x, f)
  class(process_instance_t), intent(inout) :: sampler
  integer, intent(in) :: c
  real(default), dimension(:), intent(in) :: x_in
  real(default), intent(in) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  call msg_bug ("process_instance_rebuild not implemented yet")
  x = 0
  f = 0
end subroutine process_instance_rebuild

```

This is another method required by the `sampler_t` base type: fetch the data that are relevant for the MCI record.

```

<Instances: process instance: TBP>+≡
  procedure :: fetch => process_instance_fetch

<Instances: procedures>+≡
subroutine process_instance_fetch (sampler, val, x, f)
  class(process_instance_t), intent(in) :: sampler
  real(default), intent(out) :: val
  real(default), dimension(:,:), intent(out) :: x
  real(default), dimension(:), intent(out) :: f
  integer, dimension(:), allocatable :: i_terms
  integer :: i, i_term_base, cc
  integer :: n_channel

  val = 0
  associate (process => sampler%process)
    FIND_COMPONENT: do i = 1, process%get_n_components ()
      if (sampler%process%component_is_selected (i)) then
        allocate (i_terms (size (process%get_component_i_terms (i))))
        i_terms = process%get_component_i_terms (i)
        i_term_base = i_terms(1)
        associate (k => sampler%kin(i_term_base))
          n_channel = k%n_channel
          do cc = 1, n_channel
            call k%get_mcpair (cc, x(:,cc))
          end do
          f = k%f
          val = sampler%sqme * k%phs_factor
        end associate
        if (allocated (i_terms)) deallocate (i_terms)
        exit FIND_COMPONENT
      end if
    end do FIND_COMPONENT
  end associate
end subroutine process_instance_fetch

```

Initialize and finalize event generation for the specified MCI entry.

```

<Instances: process instance: TBP>+≡
  procedure :: init_simulation => process_instance_init_simulation
  procedure :: final_simulation => process_instance_final_simulation

```

```

<Instances: procedures>+≡
  subroutine process_instance_init_simulation (instance, i_mci, &
    safety_factor, keep_failed_events)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_mci
    real(default), intent(in), optional :: safety_factor
    logical, intent(in), optional :: keep_failed_events
    call instance%mci_work(i_mci)%init_simulation (safety_factor, keep_failed_events)
  end subroutine process_instance_init_simulation

  subroutine process_instance_final_simulation (instance, i_mci)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_mci
    call instance%mci_work(i_mci)%final_simulation ()
  end subroutine process_instance_final_simulation

```

Accessing the process instance

Once the seed kinematics is complete, we can retrieve the MC input parameters for all channels, not just the seed channel.

Note: We choose the first active component. This makes sense only if the seed kinematics is identical for all active components.

```

<Instances: process instance: TBP>+≡
  procedure :: get_mcpair => process_instance_get_mcpair

<Instances: procedures>+≡
  subroutine process_instance_get_mcpair (instance, channel, x)
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: channel
    real(default), dimension(:), intent(out) :: x
    integer :: i
    if (instance%evaluation_status >= STAT_SEED_KINEMATICS) then
      do i = 1, size (instance%term)
        if (instance%term(i)%active) then
          call instance%kin(i)%get_mcpair (channel, x)
          return
        end if
      end do
      call msg_bug ("Process instance: get_mcpair: no active channels")
    else
      call msg_bug ("Process instance: get_mcpair: no seed kinematics")
    end if
  end subroutine process_instance_get_mcpair

```

Return true if the `sqme` value is known. This also implies that the event is kinematically valid and has passed all cuts.

```

<Instances: process instance: TBP>+≡
  procedure :: has_evaluated_trace => process_instance_has_evaluated_trace

<Instances: procedures>+≡
  function process_instance_has_evaluated_trace (instance) result (flag)
    class(process_instance_t), intent(in) :: instance

```

```

    logical :: flag
    flag = instance%evaluation_status >= STAT_EVALUATED_TRACE
end function process_instance_has_evaluated_trace

```

Return true if the event is complete. In particular, the event must be kinematically valid, passed all cuts, and the event data have been computed.

```

<Instances: process instance: TBP>+≡
    procedure :: is_complete_event => process_instance_is_complete_event

<Instances: procedures>+≡
    function process_instance_is_complete_event (instance) result (flag)
        class(process_instance_t), intent(in) :: instance
        logical :: flag
        flag = instance%evaluation_status >= STAT_EVENT_COMPLETE
    end function process_instance_is_complete_event

```

Select the term for the process instance that will provide the basic event record (used in `evt_trivial_make_particle_set`). It might be necessary to write out additional events corresponding to other terms (done in `evt_nlo`).

```

<Instances: process instance: TBP>+≡
    procedure :: select_i_term => process_instance_select_i_term

<Instances: procedures>+≡
    function process_instance_select_i_term (instance) result (i_term)
        integer :: i_term
        class(process_instance_t), intent(in) :: instance
        integer :: i_mci
        i_mci = instance%i_mci
        i_term = instance%process%select_i_term (i_mci)
    end function process_instance_select_i_term

```

Return pointer to the master beam interaction.

```

<Instances: process instance: TBP>+≡
    procedure :: get_beam_int_ptr => process_instance_get_beam_int_ptr

<Instances: procedures>+≡
    function process_instance_get_beam_int_ptr (instance) result (ptr)
        class(process_instance_t), intent(in), target :: instance
        type(interaction_t), pointer :: ptr
        ptr => instance%sf_chain%get_beam_int_ptr ()
    end function process_instance_get_beam_int_ptr

```

Return pointers to the matrix and flows interactions, given a term index.

```

<Instances: process instance: TBP>+≡
    procedure :: get_trace_int_ptr => process_instance_get_trace_int_ptr
    procedure :: get_matrix_int_ptr => process_instance_get_matrix_int_ptr
    procedure :: get_flows_int_ptr => process_instance_get_flows_int_ptr

<Instances: procedures>+≡
    function process_instance_get_trace_int_ptr (instance, i_term) result (ptr)
        class(process_instance_t), intent(in), target :: instance
        integer, intent(in) :: i_term
        type(interaction_t), pointer :: ptr

```

```

    ptr => instance%term(i_term)%connected%get_trace_int_ptr ()
end function process_instance_get_trace_int_ptr

function process_instance_get_matrix_int_ptr (instance, i_term) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    integer, intent(in) :: i_term
    type(interaction_t), pointer :: ptr
    ptr => instance%term(i_term)%connected%get_matrix_int_ptr ()
end function process_instance_get_matrix_int_ptr

function process_instance_get_flows_int_ptr (instance, i_term) result (ptr)
    class(process_instance_t), intent(in), target :: instance
    integer, intent(in) :: i_term
    type(interaction_t), pointer :: ptr
    ptr => instance%term(i_term)%connected%get_flows_int_ptr ()
end function process_instance_get_flows_int_ptr

```

Return the complete account of flavor combinations in the underlying interaction object, including beams, radiation, and hard interaction.

```

<Instances: process instance: TBP>+≡
    procedure :: get_state_flv => process_instance_get_state_flv

<Instances: procedures>+≡
    function process_instance_get_state_flv (instance, i_term) result (state_flv)
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
        type(state_flv_content_t) :: state_flv
        state_flv = instance%term(i_term)%connected%get_state_flv ()
    end function process_instance_get_state_flv

```

Return pointers to the parton states of a selected term.

```

<Instances: process instance: TBP>+≡
    procedure :: get_isolated_state_ptr => &
        process_instance_get_isolated_state_ptr
    procedure :: get_connected_state_ptr => &
        process_instance_get_connected_state_ptr

<Instances: procedures>+≡
    function process_instance_get_isolated_state_ptr (instance, i_term) &
        result (ptr)
        class(process_instance_t), intent(in), target :: instance
        integer, intent(in) :: i_term
        type(isolated_state_t), pointer :: ptr
        ptr => instance%term(i_term)%isolated
    end function process_instance_get_isolated_state_ptr

    function process_instance_get_connected_state_ptr (instance, i_term) &
        result (ptr)
        class(process_instance_t), intent(in), target :: instance
        integer, intent(in) :: i_term
        type(connected_state_t), pointer :: ptr
        ptr => instance%term(i_term)%connected
    end function process_instance_get_connected_state_ptr

```

Return the indices of the beam particles and incoming partons within the currently active state matrix, respectively.

(Instances: process instance: TBP)+≡

```
procedure :: get_beam_index => process_instance_get_beam_index
procedure :: get_in_index => process_instance_get_in_index
```

(Instances: procedures)+≡

```
subroutine process_instance_get_beam_index (instance, i_term, i_beam)
  class(process_instance_t), intent(in) :: instance
  integer, intent(in) :: i_term
  integer, dimension(:), intent(out) :: i_beam
  call instance%term(i_term)%connected%get_beam_index (i_beam)
end subroutine process_instance_get_beam_index

subroutine process_instance_get_in_index (instance, i_term, i_in)
  class(process_instance_t), intent(in) :: instance
  integer, intent(in) :: i_term
  integer, dimension(:), intent(out) :: i_in
  call instance%term(i_term)%connected%get_in_index (i_in)
end subroutine process_instance_get_in_index
```

Return squared matrix element and event weight, and event weight excess where applicable. `n_dropped` is a number that can be nonzero when a weighted event has been generated, dropping events with zero weight (failed cuts) on the fly.

(Instances: process instance: TBP)+≡

```
procedure :: get_sqme => process_instance_get_sqme
procedure :: get_weight => process_instance_get_weight
procedure :: get_excess => process_instance_get_excess
procedure :: get_n_dropped => process_instance_get_n_dropped
```

(Instances: procedures)+≡

```
function process_instance_get_sqme (instance, i_term) result (sqme)
  real(default) :: sqme
  class(process_instance_t), intent(in) :: instance
  integer, intent(in), optional :: i_term
  if (instance%evaluation_status >= STAT_EVALUATED_TRACE) then
    if (present (i_term)) then
      sqme = instance%term(i_term)%connected%trace%get_matrix_element (1)
    else
      sqme = instance%sqme
    end if
  else
    sqme = 0
  end if
end function process_instance_get_sqme

function process_instance_get_weight (instance) result (weight)
  real(default) :: weight
  class(process_instance_t), intent(in) :: instance
  if (instance%evaluation_status >= STAT_EVENT_COMPLETE) then
    weight = instance%weight
  else
    weight = 0
  end if
end if
```



```

end function process_instance_get_weight

function process_instance_get_excess (instance) result (excess)
  real(default) :: excess
  class(process_instance_t), intent(in) :: instance
  if (instance%evaluation_status >= STAT_EVENT_COMPLETE) then
    excess = instance%excess
  else
    excess = 0
  end if
end function process_instance_get_excess

function process_instance_get_n_dropped (instance) result (n_dropped)
  integer :: n_dropped
  class(process_instance_t), intent(in) :: instance
  if (instance%evaluation_status >= STAT_EVENT_COMPLETE) then
    n_dropped = instance%n_dropped
  else
    n_dropped = 0
  end if
end function process_instance_get_n_dropped

```

Return the currently selected MCI channel.

```

<Instances: process instance: TBP>+≡
  procedure :: get_channel => process_instance_get_channel

<Instances: procedures>+≡
  function process_instance_get_channel (instance) result (channel)
    integer :: channel
    class(process_instance_t), intent(in) :: instance
    channel = instance%selected_channel
  end function process_instance_get_channel

```

```

<Instances: process instance: TBP>+≡
  procedure :: set_fac_scale => process_instance_set_fac_scale

<Instances: procedures>+≡
  subroutine process_instance_set_fac_scale (instance, fac_scale)
    class(process_instance_t), intent(inout) :: instance
    real(default), intent(in) :: fac_scale
    integer :: i_term
    i_term = 1
    call instance%term(i_term)%set_fac_scale (fac_scale)
  end subroutine process_instance_set_fac_scale

```

Return factorization scale and strong coupling. We have to select a term instance.

```

<Instances: process instance: TBP>+≡
  procedure :: get_fac_scale => process_instance_get_fac_scale
  procedure :: get_alpha_s => process_instance_get_alpha_s

<Instances: procedures>+≡
  function process_instance_get_fac_scale (instance, i_term) result (fac_scale)
    class(process_instance_t), intent(in) :: instance

```

```

integer, intent(in) :: i_term
real(default) :: fac_scale
fac_scale = instance%term(i_term)%get_fac_scale ()
end function process_instance_get_fac_scale

function process_instance_get_alpha_s (instance, i_term) result (alpha_s)
real(default) :: alpha_s
class(process_instance_t), intent(in) :: instance
integer, intent(in) :: i_term
class(prc_core_t), pointer :: core => null ()
core => instance%process%get_core_term (i_term)
alpha_s = instance%term(i_term)%get_alpha_s (core)
core => null ()
end function process_instance_get_alpha_s

```

```

<Instances: process instance: TBP>+≡
procedure :: get_qcd => process_instance_get_qcd

<Instances: procedures>+≡
function process_instance_get_qcd (process_instance) result (qcd)
type(qcd_t) :: qcd
class(process_instance_t), intent(in) :: process_instance
qcd = process_instance%process%get_qcd ()
end function process_instance_get_qcd

```

Counter.

```

<Instances: process instance: TBP>+≡
procedure :: reset_counter => process_instance_reset_counter
procedure :: record_call => process_instance_record_call
procedure :: get_counter => process_instance_get_counter

<Instances: procedures>+≡
subroutine process_instance_reset_counter (process_instance)
class(process_instance_t), intent(inout) :: process_instance
call process_instance%mc_i_work(process_instance%i_mci)%reset_counter ()
end subroutine process_instance_reset_counter

subroutine process_instance_record_call (process_instance)
class(process_instance_t), intent(inout) :: process_instance
call process_instance%mc_i_work(process_instance%i_mci)%record_call &
(process_instance%evaluation_status)
end subroutine process_instance_record_call

pure function process_instance_get_counter (process_instance) result (counter)
class(process_instance_t), intent(in) :: process_instance
type(process_counter_t) :: counter
counter = process_instance%mc_i_work(process_instance%i_mci)%get_counter ()
end function process_instance_get_counter

```

Sum up the total number of calls for all MCI records.

```

<Instances: process instance: TBP>+≡
procedure :: get_actual_calls_total => process_instance_get_actual_calls_total

```

(Instances: procedures)+≡

```

pure function process_instance_get_actual_calls_total (process_instance) &
    result (n)
    class(process_instance_t), intent(in) :: process_instance
    integer :: n
    integer :: i
    type(process_counter_t) :: counter
    n = 0
    do i = 1, size (process_instance%mci_work)
        counter = process_instance%mci_work(i)%get_counter ()
        n = n + counter%total
    end do
end function process_instance_get_actual_calls_total

```

(Instances: process instance: TBP)+≡

```

procedure :: reset_matrix_elements => process_instance_reset_matrix_elements

```

(Instances: procedures)+≡

```

subroutine process_instance_reset_matrix_elements (instance)
    class(process_instance_t), intent(inout) :: instance
    integer :: i_term
    do i_term = 1, size (instance%term)
        call instance%term(i_term)%connected%trace%set_matrix_element (cmplx (0, 0, default))
        call instance%term(i_term)%connected%matrix%set_matrix_element (cmplx (0, 0, default))
    end do
end subroutine process_instance_reset_matrix_elements

```

(Instances: process instance: TBP)+≡

```

procedure :: get_test_phase_space_point &
    => process_instance_get_test_phase_space_point

```

(Instances: procedures)+≡

```

subroutine process_instance_get_test_phase_space_point (instance, &
    i_component, i_core, p)
    type(vector4_t), dimension(:), allocatable, intent(out) :: p
    class(process_instance_t), intent(inout) :: instance
    integer, intent(in) :: i_component, i_core
    real(default), dimension(:), allocatable :: x
    logical :: success
    integer :: i_term
    instance%i_mci = i_component
    i_term = instance%process%get_i_term (i_core)
    associate (term => instance%term(i_term), kin => instance%kin(i_term))
        allocate (x (instance%mci_work(i_component)%config%n_par))
        x = 0.5_default
        call instance%set_mcp (x, .true.)
        call instance%select_channel (1)
        call term%compute_seed_kinematics &
            (kin, instance%mci_work(i_component), 1, success)
        call kin%evaluate_radiation_kinematics &
            (instance%mci_work(instance%i_mci)%get_x_process ())
        call term%compute_hard_kinematics (kin, success = success)
        allocate (p (size (term%p_hard)))
        p = term%int_hard%get_momenta ()
    end associate
end subroutine process_instance_get_test_phase_space_point

```

```

        end associate
    end subroutine process_instance_get_test_phase_space_point

    <Instances: process instance: TBP>+≡
        procedure :: get_p_hard => process_instance_get_p_hard

    <Instances: procedures>+≡
        pure function process_instance_get_p_hard (process_instance, i_term) &
            result (p_hard)
            type(vector4_t), dimension(:), allocatable :: p_hard
            class(process_instance_t), intent(in) :: process_instance
            integer, intent(in) :: i_term
            allocate (p_hard (size (process_instance%term(i_term)%get_p_hard ())))
            p_hard = process_instance%term(i_term)%get_p_hard ()
        end function process_instance_get_p_hard

    <Instances: process instance: TBP>+≡
        procedure :: get_first_active_i_term => process_instance_get_first_active_i_term

    <Instances: procedures>+≡
        function process_instance_get_first_active_i_term (instance) result (i_term)
            integer :: i_term
            class(process_instance_t), intent(in) :: instance
            integer :: i
            i_term = 0
            do i = 1, size (instance%term)
                if (instance%term(i)%active) then
                    i_term = i
                    exit
                end if
            end do
        end function process_instance_get_first_active_i_term

    <Instances: process instance: TBP>+≡
        procedure :: get_real_of_mci => process_instance_get_real_of_mci

    <Instances: procedures>+≡
        function process_instance_get_real_of_mci (instance) result (i_real)
            integer :: i_real
            class(process_instance_t), intent(in) :: instance
            select type (pcm_work => instance%pcm_work)
                type is (pcm_nlo_workspace_t)
                    i_real = pcm_work%i_mci_to_real_component (instance%i_mci)
            end select
        end function process_instance_get_real_of_mci

    <Instances: process instance: TBP>+≡
        procedure :: get_connected_states => process_instance_get_connected_states

    <Instances: procedures>+≡
        function process_instance_get_connected_states (instance, i_component) result (connected)
            type(connected_state_t), dimension(:), allocatable :: connected
            class(process_instance_t), intent(in) :: instance
            integer, intent(in) :: i_component

```

```

        connected = instance%process%get_connected_states (i_component, &
            instance%term(:)%connected)
    end function process_instance_get_connected_states

```

Get the hadronic center-of-mass energy

```

<Instances: process instance: TBP>+≡
    procedure :: get_sqrts => process_instance_get_sqrts

<Instances: procedures>+≡
    function process_instance_get_sqrts (instance) result (sqrts)
        class(process_instance_t), intent(in) :: instance
        real(default) :: sqrts
        sqrts = instance%process%get_sqrts ()
    end function process_instance_get_sqrts

```

Get the polarizations

```

<Instances: process instance: TBP>+≡
    procedure :: get_polarization => process_instance_get_polarization

<Instances: procedures>+≡
    function process_instance_get_polarization (instance) result (pol)
        class(process_instance_t), intent(in) :: instance
        real(default), dimension(2) :: pol
        pol = instance%process%get_polarization ()
    end function process_instance_get_polarization

```

Get the beam spectrum

```

<Instances: process instance: TBP>+≡
    procedure :: get_beam_file => process_instance_get_beam_file

<Instances: procedures>+≡
    function process_instance_get_beam_file (instance) result (file)
        class(process_instance_t), intent(in) :: instance
        type(string_t) :: file
        file = instance%process%get_beam_file ()
    end function process_instance_get_beam_file

```

Get the process name

```

<Instances: process instance: TBP>+≡
    procedure :: get_process_name => process_instance_get_process_name

<Instances: procedures>+≡
    function process_instance_get_process_name (instance) result (name)
        class(process_instance_t), intent(in) :: instance
        type(string_t) :: name
        name = instance%process%get_id ()
    end function process_instance_get_process_name

```

Particle sets

Here we provide two procedures that convert the process instance from/to a particle set. The conversion applies to the trace evaluator which has no quantum-number information, thus it involves only the momenta and the parent-child relations. We keep virtual particles.

If `n_incoming` is provided, the status code of the first `n_incoming` particles will be reset to incoming. Otherwise, they would be classified as virtual.

Nevertheless, it is possible to reconstruct the complete structure from a particle set. The reconstruction implies a re-evaluation of the structure function and matrix-element codes.

The `i_term` index is needed for both input and output, to select among different active trace evaluators.

In both cases, the `instance` object must be properly initialized.

NB: The `recover_beams` option should be used only when the particle set originates from an external event file, and the user has asked for it. It should be switched off when reading from raw event file.

(Instances: process instance: TBP)+≡

```
procedure :: get_trace => process_instance_get_trace
procedure :: set_trace => process_instance_set_trace
```

(Instances: procedures)+≡

```
subroutine process_instance_get_trace (instance, pset, i_term, n_incoming)
  class(process_instance_t), intent(in), target :: instance
  type(particle_set_t), intent(out) :: pset
  integer, intent(in) :: i_term
  integer, intent(in), optional :: n_incoming
  type(interaction_t), pointer :: int
  logical :: ok
  int => instance%get_trace_int_ptr (i_term)
  call pset%init (ok, int, int, FM_IGNORE_HELICITY, &
    [0._default, 0._default], .false., .true., n_incoming)
end subroutine process_instance_get_trace
```

```
subroutine process_instance_set_trace &
  (instance, pset, i_term, recover_beams, check_match, success)
  class(process_instance_t), intent(inout), target :: instance
  type(particle_set_t), intent(in) :: pset
  integer, intent(in) :: i_term
  logical, intent(in), optional :: recover_beams, check_match
  logical, intent(out), optional :: success
  type(interaction_t), pointer :: int
  integer :: n_in
  int => instance%get_trace_int_ptr (i_term)
  n_in = instance%process%get_n_in ()
  call pset%fill_interaction (int, n_in, &
    recover_beams = recover_beams, &
    check_match = check_match, &
    state_flg = instance%get_state_flg (i_term), &
    success = success)
end subroutine process_instance_set_trace
```

This procedure allows us to override any QCD setting of the WHIZARD process and directly set the coupling value that comes together with a particle set.

(Instances: process instance: TBP)+≡

```
procedure :: set_alpha_qcd_forced => process_instance_set_alpha_qcd_forced
```

(Instances: procedures)+≡

```
subroutine process_instance_set_alpha_qcd_forced (instance, i_term, alpha_qcd)
  class(process_instance_t), intent(inout) :: instance
  integer, intent(in) :: i_term
  real(default), intent(in) :: alpha_qcd
  call instance%term(i_term)%set_alpha_qcd_forced (alpha_qcd)
end subroutine process_instance_set_alpha_qcd_forced
```

(Instances: process instance: TBP)+≡

```
procedure :: has_nlo_component => process_instance_has_nlo_component
```

(Instances: procedures)+≡

```
function process_instance_has_nlo_component (instance) result (nlo)
  class(process_instance_t), intent(in) :: instance
  logical :: nlo
  nlo = instance%process%is_nlo_calculation ()
end function process_instance_has_nlo_component
```

(Instances: process instance: TBP)+≡

```
procedure :: keep_failed_events => process_instance_keep_failed_events
```

(Instances: procedures)+≡

```
function process_instance_keep_failed_events (instance) result (keep)
  logical :: keep
  class(process_instance_t), intent(in) :: instance
  keep = instance%mc_i_work(instance%i_mci)%keep_failed_events
end function process_instance_keep_failed_events
```

(Instances: process instance: TBP)+≡

```
procedure :: get_term_indices => process_instance_get_term_indices
```

(Instances: procedures)+≡

```
function process_instance_get_term_indices (instance, nlo_type) result (i_term)
  integer, dimension(:), allocatable :: i_term
  class(process_instance_t), intent(in) :: instance
  integer :: nlo_type
  allocate (i_term (count (instance%term%nlo_type == nlo_type)))
  i_term = pack (instance%term%get_i_term_global (), instance%term%nlo_type == nlo_type)
end function process_instance_get_term_indices
```

(Instances: process instance: TBP)+≡

```
procedure :: get_boost_to_lab => process_instance_get_boost_to_lab
```

(Instances: procedures)+≡

```
function process_instance_get_boost_to_lab (instance, i_term) result (lt)
  type(lorentz_transformation_t) :: lt
  class(process_instance_t), intent(in) :: instance
  integer, intent(in) :: i_term
  lt = instance%kin(i_term)%get_boost_to_lab ()
end function process_instance_get_boost_to_lab
```

```

<Instances: process instance: TBP>+≡
    procedure :: get_boost_to_cms => process_instance_get_boost_to_cms

<Instances: procedures>+≡
    function process_instance_get_boost_to_cms (instance, i_term) result (lt)
        type(lorentz_transformation_t) :: lt
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
        lt = instance%kin(i_term)%get_boost_to_cms ()
    end function process_instance_get_boost_to_cms

<Instances: process instance: TBP>+≡
    procedure :: lab_is_cm => process_instance_lab_is_cm

<Instances: procedures>+≡
    function process_instance_lab_is_cm (instance, i_term) result (lab_is_cm)
        logical :: lab_is_cm
        class(process_instance_t), intent(in) :: instance
        integer, intent(in) :: i_term
        lab_is_cm = instance%kin(i_term)%phs%lab_is_cm ()
    end function process_instance_lab_is_cm

```

The `pacify` subroutine has the purpose of setting numbers to zero which are (by comparing with a `tolerance` parameter) considered equivalent with zero. We do this in some unit tests. Here, we apply this to the phase space subobject of the process instance.

```

<Instances: public>+≡
    public :: pacify

<Instances: interfaces>+≡
    interface pacify
        module procedure pacify_process_instance
    end interface pacify

<Instances: procedures>+≡
    subroutine pacify_process_instance (instance)
        type(process_instance_t), intent(inout) :: instance
        integer :: i
        do i = 1, size (instance%kin)
            call pacify (instance%kin(i)%phs)
        end do
    end subroutine pacify_process_instance

```

30.11 Unit tests

Test module, followed by the corresponding implementation module.

```

<processes_ut.f90>≡
    <File header>

    module processes_ut
        use unit_tests

```



```

    use processes_uti

    <Standard module head>

    <Processes: public test>

    <Processes: public test auxiliary>

contains

    <Processes: test driver>

end module processes_ut
<processes_uti.f90>≡
    <File header>

module processes_uti

    <Use kinds>
    <Use strings>
    use format_utils, only: write_separator
    use constants, only: TWOPI4
    use physics_defs, only: CONV
    use os_interface
    use sm_qcd
    use lorentz
    use pdg_arrays
    use model_data
    use models
    use var_base, only: vars_t
    use variables, only: var_list_t
    use model_testbed, only: prepare_model
    use particle_specifiers, only: new_prt_spec
    use flavors
    use interactions, only: reset_interaction_counter
    use particles
    use rng_base
    use mci_base
    use mci_none, only: mci_none_t
    use mci_midpoint
    use sf_mappings
    use sf_base
    use phs_base
    use phs_single
    use phs_forests, only: syntax_phs_forest_init, syntax_phs_forest_final
    use phs_wood, only: phs_wood_config_t
    use resonances, only: resonance_history_set_t
    use process_constants
    use prc_core_def, only: prc_core_def_t
    use prc_core
    use prc_test, only: prc_test_create_library
    use prc_template_me, only: template_me_def_t
    use process_libraries
    use prc_test_core

```

```

    use process_counter
    use process_config, only: process_term_t
    use process, only: process_t
    use instances, only: process_instance_t, process_instance_hook_t

    use rng_base_ut, only: rng_test_factory_t
    use sf_base_ut, only: sf_test_data_t
    use mci_base_ut, only: mci_test_t
    use phs_base_ut, only: phs_test_config_t

    <Standard module head>

    <Processes: public test auxiliary>

    <Processes: test declarations>

    <Processes: test types>

contains

    <Processes: tests>

    <Processes: test auxiliary>

end module processes_util

```

API: driver for the unit tests below.

```

<Processes: public test>≡
    public :: processes_test

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

```

Write an empty process object

The most trivial test is to write an uninitialized process object.

```

<Processes: execute tests>≡
    call test (processes_1, "processes_1", &
        "write an empty process object", &
        u, results)

<Processes: test declarations>≡
    public :: processes_1

<Processes: tests>≡
    subroutine processes_1 (u)
        integer, intent(in) :: u
        type(process_t) :: process

```

```

write (u, "(A)")  "* Test output: processes_1"
write (u, "(A)")  "* Purpose: display an empty process object"
write (u, "(A)")

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_1"

end subroutine processes_1

```

Initialize a process object

Initialize a process and display it.

```

<Processes: execute tests>+≡
  call test (processes_2, "processes_2", &
    "initialize a simple process object", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_2

<Processes: tests>+≡
  subroutine processes_2 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable :: process
    class(mci_t), allocatable :: mci_template
    class(phs_config_t), allocatable :: phs_config_template

    write (u, "(A)")  "* Test output: processes_2"
    write (u, "(A)")  "* Purpose: initialize a simple process object"
    write (u, "(A)")

    write (u, "(A)")  "* Build and load a test library with one process"
    write (u, "(A)")

    libname = "processes2"
    procname = libname

    call os_data%init ()
    call prc_test_create_library (libname, lib)

    write (u, "(A)")  "* Initialize a process object"
    write (u, "(A)")

    call model%init_test ()

    allocate (process)
    call process%init (procname, lib, os_data, model)

```

```

call process%set_run_id (var_str ("run_2"))
call process%setup_test_cores ()

allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

call process%setup_mci (dispatch_mci_empty)

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_2"

end subroutine processes_2

```

Trivial for testing: do not allocate the MCI record.

```

<Processes: test auxiliary>≡
subroutine dispatch_mci_empty (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
end subroutine dispatch_mci_empty

```

Compute a trivial matrix element

Initialize a process, retrieve some information and compute a matrix element.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

```

<Processes: execute tests>+≡
  call test (processes_3, "processes_3", &
    "retrieve a trivial matrix element", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_3

<Processes: tests>+≡
subroutine processes_3 (u)
  integer, intent(in) :: u
  type(process_library_t), target :: lib
  type(string_t) :: libname
  type(string_t) :: procname
  type(os_data_t) :: os_data
  type(model_t), target :: model

```

```

type(process_t), allocatable :: process
class(phs_config_t), allocatable :: phs_config_template
type(process_constants_t) :: data
type(vector4_t), dimension(:), allocatable :: p

write (u, "(A)")  "* Test output: processes_3"
write (u, "(A)")  "* Purpose: create a process &
                  &and compute a matrix element"
write (u, "(A)")

write (u, "(A)")  "* Build and load a test library with one process"
write (u, "(A)")

libname = "processes3"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)
call process%setup_test_cores ()

allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)
call process%setup_mci (dispatch_mci_test3)

write (u, "(A)")  "* Return the number of process components"
write (u, "(A)")

write (u, "(A,IO)")  "n_components = ", process%get_n_components ()

write (u, "(A)")
write (u, "(A)")  "* Return the number of flavor states"
write (u, "(A)")

data = process%get_constants (1)

write (u, "(A,IO)")  "n_flv(1) = ", data%n_flv

write (u, "(A)")
write (u, "(A)")  "* Return the first flavor state"
write (u, "(A)")

write (u, "(A,4(1x,IO))")  "flv_state(1) =", data%flv_state (:,1)

write (u, "(A)")
write (u, "(A)")  "* Set up kinematics &
                  &[arbitrary, the matrix element is constant]"

allocate (p (4))

```

```

write (u, "(A)")
write (u, "(A)")  "* Retrieve the matrix element"
write (u, "(A)")

write (u, "(A,F5.3,' + ',F5.3,' I')")  "me (1, p, 1, 1, 1) = ", &
    process%compute_amplitude (1, 1, 1, p, 1, 1, 1)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_3"

end subroutine processes_3

```

MCI record with some contents.

```

<Processes: test auxiliary>+≡
subroutine dispatch_mci_test3 (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
  allocate (mci_test_t :: mci)
  select type (mci)
  type is (mci_test_t)
    call mci%set_dimensions (2, 2)
    call mci%set_divisions (100)
  end select
end subroutine dispatch_mci_test3

```

Generate a process instance

Initialize a process and process instance, choose a sampling point and fill the process instance.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

```

<Processes: execute tests>+≡
call test (processes_4, "processes_4", &
    "create and fill a process instance (partonic event)", &
    u, results)

<Processes: test declarations>+≡
public :: processes_4

```

```

<Processes: tests>+≡
subroutine processes_4 (u)
  integer, intent(in) :: u
  type(process_library_t), target :: lib
  type(string_t) :: libname
  type(string_t) :: procname
  type(os_data_t) :: os_data
  type(model_t), target :: model
  type(process_t), allocatable, target :: process
  class(phs_config_t), allocatable :: phs_config_template
  real(default) :: sqrts
  type(process_instance_t), allocatable, target :: process_instance
  type(particle_set_t) :: pset

  write (u, "(A)")  "* Test output: processes_4"
  write (u, "(A)")  "*   Purpose: create a process &
      &and fill a process instance"
  write (u, "(A)")

  write (u, "(A)")  "* Build and initialize a test process"
  write (u, "(A)")

  libname = "processes4"
  procname = libname

  call os_data%init ()
  call prc_test_create_library (libname, lib)

  call reset_interaction_counter ()

  call model%init_test ()

  allocate (process)
  call process%init (procname, lib, os_data, model)

  call process%setup_test_cores ()
  allocate (phs_test_config_t :: phs_config_template)
  call process%init_components (phs_config_template)

  write (u, "(A)")  "* Prepare a trivial beam setup"
  write (u, "(A)")

  sqrts = 1000
  call process%setup_beams_sqrts (sqrts, i_core = 1)
  call process%configure_phs ()
  call process%setup_mci (dispatch_mci_empty)

  write (u, "(A)")  "* Complete process initialization"
  write (u, "(A)")

  call process%setup_terms ()
  call process%write (.false., u)

  write (u, "(A)")

```

```

write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inject a set of random numbers"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%set_mcpars ([0._default, 0._default])
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Set up hard kinematics"
write (u, "(A)")

call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()
call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()

write (u, "(A)")  "* Evaluate matrix element and square"
write (u, "(A)")

call process_instance%evaluate_trace ()
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)

call process_instance%activate ()

```



```

process_instance%evaluation_status = STAT_EFF_KINEMATICS
call process_instance%recover_hard_kinematics (i_term = 1)
call process_instance%recover_seed_kinematics (i_term = 1)
call process_instance%select_channel (1)
call process_instance%recover_mcpair (i_term = 1)

call process_instance%compute_seed_kinematics (skip_term = 1)
call process_instance%compute_hard_kinematics (skip_term = 1)
call process_instance%compute_eff_kinematics (skip_term = 1)

call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels (skip_term = 1)
call process_instance%evaluate_trace ()
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()
call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_4"

end subroutine processes_4

```

Structure function configuration

Configure structure functions (multi-channel) in a process object.

```

<Processes: execute tests>+≡
    call test (processes_7, "processes_7", &
        "process configuration with structure functions", &
        u, results)

<Processes: test declarations>+≡
    public :: processes_7

<Processes: tests>+≡
    subroutine processes_7 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_t), allocatable, target :: process
        class(phs_config_t), allocatable :: phs_config_template
        real(default) :: sqrts

```

```

type(pdg_array_t) :: pdg_in
class(sf_data_t), allocatable, target :: data
type(sf_config_t), dimension(:), allocatable :: sf_config
type(sf_channel_t), dimension(2) :: sf_channel

write (u, "(A)")  "* Test output: processes_7"
write (u, "(A)")  "* Purpose: initialize a process with &
                  &structure functions"
write (u, "(A)")

write (u, "(A)")  "* Build and initialize a process object"
write (u, "(A)")

libname = "processes7"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Set beam, structure functions, and mappings"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()

pdg_in = 25
allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (process%get_model_ptr (), pdg_in)
end select

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call process%init_sf_chain (sf_config)
deallocate (sf_config)

call process%test_allocate_sf_channels (3)

call sf_channel(1)%init (2)
call sf_channel(1)%activate_mapping ([1,2])
call process%set_sf_channel (2, sf_channel(1))

```

```

call sf_channel(2)%init (2)
call sf_channel(2)%set_s_mapping ([1,2])
call process%set_sf_channel (3, sf_channel(2))

call process%setup_mci (dispatch_mci_empty)

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_7"

end subroutine processes_7

```

Evaluating a process with structure function

Configure structure functions (single-channel) in a process object, create an instance, compute kinematics and evaluate.

Note the order of operations when setting up structure functions and phase space. The beams are first, they determine the `sqrts` value. We can also set up the chain of structure functions. We then configure the phase space. From this, we can obtain information about special configurations (resonances, etc.), which we need for allocating the possible structure-function channels (parameterizations and mappings). Finally, we match phase-space channels onto structure-function channels.

In the current example, this matching is trivial; we only have one structure-function channel.

```

<Processes: execute tests>+≡
  call test (processes_8, "processes_8", &
    "process evaluation with structure functions", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_8

<Processes: tests>+≡
  subroutine processes_8 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts

```

```

type(process_instance_t), allocatable, target :: process_instance
type(pdg_array_t) :: pdg_in
class(sf_data_t), allocatable, target :: data
type(sf_config_t), dimension(:), allocatable :: sf_config
type(sf_channel_t) :: sf_channel
type(particle_set_t) :: pset

write (u, "(A)")  "* Test output: processes_8"
write (u, "(A)")  "* Purpose: evaluate a process with &
                  &structure functions"
write (u, "(A)")

write (u, "(A)")  "* Build and initialize a process object"
write (u, "(A)")

libname = "processes8"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)

call reset_interaction_counter ()

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Set beam, structure functions, and mappings"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)

pdg_in = 25
allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (process%get_model_ptr (), pdg_in)
end select

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call process%init_sf_chain (sf_config)
deallocate (sf_config)

call process%configure_phs ()

call process%test_allocate_sf_channels (1)

```

```

call sf_channel%init (2)
call sf_channel%activate_mapping ([1,2])
call process%set_sf_channel (1, sf_channel)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_mci (dispatch_mci_empty)
call process%setup_terms ()

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")  "* Set up kinematics and evaluate"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%evaluate_sqme (1, &
    [0.8_default, 0.8_default, 0.1_default, 0.2_default])
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover process instance"
write (u, "(A)")

call reset_interaction_counter (2)

allocate (process_instance)
call process_instance%init (process)

call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover &
    (channel = 1, i_term = 1, update_sqme = .true., recover_phs = .true.)
call process_instance%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_8"

end subroutine processes_8

```

Multi-channel phase space and structure function

This is an extension of the previous example. This time, we have two distinct structure-function channels which are matched to the two distinct phase-space channels.

```

<Processes: execute tests>+≡
  call test (processes_9, "processes_9", &
    "multichannel kinematics and structure functions", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_9

<Processes: tests>+≡
  subroutine processes_9 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts
    type(process_instance_t), allocatable, target :: process_instance
    type(pdg_array_t) :: pdg_in
    class(sf_data_t), allocatable, target :: data
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_channel_t) :: sf_channel
    real(default), dimension(4) :: x_saved
    type(particle_set_t) :: pset

    write (u, "(A)")  "* Test output: processes_9"
    write (u, "(A)")  "* Purpose: evaluate a process with &

```

```

        &structure functions"
write (u, "(A)")  "*"           in a multi-channel configuration"
write (u, "(A)")

write (u, "(A)")  "* Build and initialize a process object"
write (u, "(A)")

libname = "processes9"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)

call reset_interaction_counter ()

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Set beam, structure functions, and mappings"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)

pdg_in = 25
allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (process%get_model_ptr (), pdg_in)
end select

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call process%init_sf_chain (sf_config)
deallocate (sf_config)

call process%configure_phs ()

call process%test_allocate_sf_channels (2)

call sf_channel%init (2)
call process%set_sf_channel (1, sf_channel)

call sf_channel%init (2)
call sf_channel%activate_mapping ([1,2])
call process%set_sf_channel (2, sf_channel)

```

```

call process%test_set_component_sf_channel ([1, 2])

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_mci (dispatch_mci_empty)
call process%setup_terms ()

call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")  "* Set up kinematics in channel 1 and evaluate"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%evaluate_sqme (1, &
    [0.8_default, 0.8_default, 0.1_default, 0.2_default])
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extract MC input parameters"
write (u, "(A)")

write (u, "(A)")  "Channel 1:"
call process_instance%get_mcpair (1, x_saved)
write (u, "(2x,9(1x,F7.5))") x_saved

write (u, "(A)")  "Channel 2:"
call process_instance%get_mcpair (2, x_saved)
write (u, "(2x,9(1x,F7.5))") x_saved

write (u, "(A)")
write (u, "(A)")  "* Set up kinematics in channel 2 and evaluate"
write (u, "(A)")

call process_instance%evaluate_sqme (2, x_saved)
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Recover process instance for channel 2"
write (u, "(A)")

call reset_interaction_counter (2)

```



```

allocate (process_instance)
call process_instance%init (process)

call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover &
    (channel = 2, i_term = 1, update_sqme = .true., recover_phs = .true.)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_9"

end subroutine processes_9

```

Event generation

Activate the MC integrator for the process object and use it to generate a single event. Note that the test integrator does not require integration in preparation for generating events.

```

<Processes: execute tests>+≡
    call test (processes_10, "processes_10", &
        "event generation", &
        u, results)

<Processes: test declarations>+≡
    public :: processes_10

<Processes: tests>+≡
    subroutine processes_10 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_t), allocatable, target :: process
        class(mci_t), pointer :: mci
        class(phs_config_t), allocatable :: phs_config_template
        real(default) :: sqrts
        type(process_instance_t), allocatable, target :: process_instance

```

```

write (u, "(A)")  "* Test output: processes_10"
write (u, "(A)")  "* Purpose: generate events for a process without &
    &structure functions"
write (u, "(A)")  "*           in a multi-channel configuration"
write (u, "(A)")

write (u, "(A)")  "* Build and initialize a process object"
write (u, "(A)")

libname = "processes10"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)

call reset_interaction_counter ()

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()

call process%setup_mci (dispatch_mci_test10)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write(.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")  "* Generate weighted event"
write (u, "(A)")

call process%test_get_mci_ptr (mci)
select type (mci)

```

```

type is (mci_test_t)
! This ensures that the next 'random' numbers are 0.3, 0.5, 0.7
call mci%rng%init (3)
! Include the constant PHS factor in the stored maximum of the integrand
call mci%set_max_factor (conv * twopi4 &
/ (2 * sqrt (lambda (sqrts **2, 125._default**2, 125._default**2))))
end select

call process_instance%generate_weighted_event (1)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate unweighted event"
write (u, "(A)")

call process_instance%generate_unweighted_event (1)
call process%test_get_mci_ptr (mci)
select type (mci)
type is (mci_test_t)
write (u, "(A,I0)")  " Success in try ", mci%tries
write (u, "(A)")
end select

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_10"

end subroutine processes_10

```

MCI record with some contents.

(Processes: test auxiliary)+≡

```

subroutine dispatch_mci_test10 (mci, var_list, process_id, is_nlo)
class(mci_t), allocatable, intent(out) :: mci
type(var_list_t), intent(in) :: var_list
type(string_t), intent(in) :: process_id
logical, intent(in), optional :: is_nlo
allocate (mci_test_t :: mci)
select type (mci)
type is (mci_test_t); call mci%set_divisions (100)
end select
end subroutine dispatch_mci_test10

```

Integration

Activate the MC integrator for the process object and use it to integrate over phase space.

```
<Processes: execute tests>+≡
    call test (processes_11, "processes_11", &
              "integration", &
              u, results)

<Processes: test declarations>+≡
    public :: processes_11

<Processes: tests>+≡
    subroutine processes_11 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_t), allocatable, target :: process
        class(mci_t), allocatable :: mci_template
        class(phs_config_t), allocatable :: phs_config_template
        real(default) :: sqrts
        type(process_instance_t), allocatable, target :: process_instance

        write (u, "(A)")  "* Test output: processes_11"
        write (u, "(A)")  "*   Purpose: integrate a process without &
                           &structure functions"
        write (u, "(A)")  "*                               in a multi-channel configuration"
        write (u, "(A)")

        write (u, "(A)")  "* Build and initialize a process object"
        write (u, "(A)")

        libname = "processes11"
        procname = libname

        call os_data%init ()
        call prc_test_create_library (libname, lib)

        call reset_interaction_counter ()

        call model%init_test ()

        allocate (process)
        call process%init (procname, lib, os_data, model)

        call process%setup_test_cores ()

        allocate (phs_test_config_t :: phs_config_template)
        call process%init_components (phs_config_template)
```

```

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()

call process%setup_mci (dispatch_mci_test10)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")  "* Integrate with default test parameters"
write (u, "(A)")

call process_instance%integrate (1, n_it=1, n_calls=10000)
call process%final_integration (1)

call process%write (.false., u)

write (u, "(A)")
write (u, "(A,ES13.7)")  " Integral divided by phs factor = ", &
    process%get_integral (1) &
    / process_instance%kin(1)%phs_factor

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_11"

end subroutine processes_11

```

Complete events

For the purpose of simplifying further tests, we implement a convenience routine that initializes a process and prepares a single event. This is a wrapup of the test `processes_10`.

The procedure is re-exported by the `processes_ut` module.

```
<Processes: public test auxiliary>≡
  public :: prepare_test_process
<Processes: test auxiliary>+≡
  subroutine prepare_test_process &
    (process, process_instance, model, var_list, run_id)
    type(process_t), intent(out), target :: process
    type(process_instance_t), intent(out), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(var_list_t), intent(inout), optional :: var_list
    type(string_t), intent(in), optional :: run_id
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), allocatable, target :: process_model
    class(mci_t), pointer :: mci
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts
    libname = "processes_test"
    procname = libname
    call os_data%init ()
    call prc_test_create_library (libname, lib)
    call reset_interaction_counter ()
    allocate (process_model)
    call process_model%init (model%get_name (), &
      model%get_n_real (), &
      model%get_n_complex (), &
      model%get_n_field (), &
      model%get_n_vtx ())
    call process_model%copy_from (model)
    call process%init (procname, lib, os_data, process_model, var_list)
    if (present (run_id)) call process%set_run_id (run_id)
    call process%setup_test_cores ()
    allocate (phs_test_config_t :: phs_config_template)
    call process%init_components (phs_config_template)
    sqrts = 1000
    call process%setup_beams_sqrts (sqrts, i_core = 1)
    call process%configure_phs ()
    call process%setup_mci (dispatch_mci_test10)
    call process%setup_terms ()
    call process_instance%init (process)
    call process%test_get_mci_ptr (mci)
    select type (mci)
    type is (mci_test_t)
      ! This ensures that the next 'random' numbers are 0.3, 0.5, 0.7
      call mci%rng%init (3)
      ! Include the constant PHS factor in the stored maximum of the integrand
      call mci%set_max_factor (conv * twopi4 &
```

```

/ (2 * sqrt (lambda (sqrt s **2, 125._default**2, 125._default**2)))
end select
call process%reset_library_ptr () ! avoid dangling pointer
call process_model%final ()
end subroutine prepare_test_process

```

Here we do the cleanup of the process and process instance emitted by the previous routine.

```

<Processes: public test auxiliary>+≡
public :: cleanup_test_process

<Processes: test auxiliary>+≡
subroutine cleanup_test_process (process, process_instance)
type(process_t), intent(inout) :: process
type(process_instance_t), intent(inout) :: process_instance
call process_instance%final ()
call process%final ()
end subroutine cleanup_test_process

```

This is the actual test. Prepare the test process and event, fill all evaluators, and display the results. Use a particle set as temporary storage, read kinematics and recalculate the event.

```

<Processes: execute tests>+≡
call test (processes_12, "processes_12", &
"event post-processing", &
u, results)

<Processes: test declarations>+≡
public :: processes_12

<Processes: tests>+≡
subroutine processes_12 (u)
integer, intent(in) :: u
type(process_t), allocatable, target :: process
type(process_instance_t), allocatable, target :: process_instance
type(particle_set_t) :: pset
type(model_data_t), target :: model

write (u, "(A)")  "* Test output: processes_12"
write (u, "(A)")  "* Purpose: generate a complete partonic event"
write (u, "(A)")

call model%init_test ()

write (u, "(A)")  "* Build and initialize process and process instance &
&and generate event"
write (u, "(A)")

allocate (process)
allocate (process_instance)
call prepare_test_process (process, process_instance, model, &
run_id = var_str ("run_12"))
call process_instance%setup_event_data (i_core = 1)

```

```

call process%prepare_simulation (1)
call process_instance%init_simulation (1)
call process_instance%generate_weighted_event (1)
call process_instance%evaluate_event_data ()

call process_instance%write (u)

call process_instance%get_trace (pset, 1)

call process_instance%final_simulation (1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Recover kinematics and recalculate"
write (u, "(A)")

call reset_interaction_counter (2)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()

call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover &
    (channel = 1, i_term = 1, update_sqme = .true., recover_phs = .true.)

call process_instance%recover_event ()
call process_instance%evaluate_event_data ()

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_12"

end subroutine processes_12

```

Colored interaction

This test specifically checks the transformation of process data (flavor, helicity, and color) into an interaction in a process term.

We use the `test_t` process core (which has no nontrivial particles), but call only the `is_allowed` method, which always returns true.

```

<Processes: execute tests>+≡
    call test (processes_13, "processes_13", &
              "colored interaction", &
              u, results)

<Processes: test declarations>+≡
    public :: processes_13

<Processes: tests>+≡
    subroutine processes_13 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_data_t), target :: model
        type(process_term_t) :: term
        class(prc_core_t), allocatable :: core

        write (u, "(A)")  "* Test output: processes_13"
        write (u, "(A)")  "* Purpose: initialized a colored interaction"
        write (u, "(A)")

        write (u, "(A)")  "* Set up a process constants block"
        write (u, "(A)")

        call os_data%init ()
        call model%init_sm_test ()

        allocate (test_t :: core)

        associate (data => term%data)
            data%n_in = 2
            data%n_out = 3
            data%n_flv = 2
            data%n_hel = 2
            data%n_col = 2
            data%n_cin = 2

            allocate (data%flv_state (5, 2))
            data%flv_state (:,1) = [ 1, 21, 1, 21, 21]
            data%flv_state (:,2) = [ 2, 21, 2, 21, 21]

            allocate (data%hel_state (5, 2))
            data%hel_state (:,1) = [1, 1, 1, 1, 0]
            data%hel_state (:,2) = [1,-1, 1,-1, 0]

            allocate (data%col_state (2, 5, 2))
            data%col_state (:,:,1) = &
                reshape ([[1, 0], [2,-1], [3, 0], [2,-3], [0,0]], [2,5])
            data%col_state (:,:,2) = &
                reshape ([[1, 0], [2,-3], [3, 0], [2,-1], [0,0]], [2,5])

            allocate (data%ghost_flag (5, 2))
            data%ghost_flag(1:4,:) = .false.
            data%ghost_flag(5,:) = .true.

```

```

end associate

write (u, "(A)")  "* Set up the interaction"
write (u, "(A)")

call reset_interaction_counter ()
call term%setup_interaction (core, model)
call term%int%basic_write (u)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_13"
end subroutine processes_13

```

MD5 sums

Configure a process with structure functions (multi-channel) and compute MD5 sums

```

<Processes: execute tests>+≡
    call test (processes_14, "processes_14", &
        "process configuration and MD5 sum", &
        u, results)

<Processes: test declarations>+≡
    public :: processes_14

<Processes: tests>+≡
    subroutine processes_14 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_t), allocatable, target :: process
        class(phs_config_t), allocatable :: phs_config_template
        real(default) :: sqrts
        type(pdg_array_t) :: pdg_in
        class(sf_data_t), allocatable, target :: data
        type(sf_config_t), dimension(:), allocatable :: sf_config
        type(sf_channel_t), dimension(3) :: sf_channel

        write (u, "(A)")  "* Test output: processes_14"
        write (u, "(A)")  "*   Purpose: initialize a process with &
            &structure functions"
        write (u, "(A)")  "*               and compute MD5 sum"
        write (u, "(A)")

        write (u, "(A)")  "* Build and initialize a process object"
        write (u, "(A)")
    end subroutine processes_14

```

```

libname = "processes7"
procname = libname

call os_data%init ()
call prc_test_create_library (libname, lib)
call lib%compute_md5sum ()

call model%init_test ()

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Set beam, structure functions, and mappings"
write (u, "(A)")

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()

pdg_in = 25
allocate (sf_test_data_t :: data)
select type (data)
type is (sf_test_data_t)
    call data%init (process%get_model_ptr (), pdg_in)
end select

call process%test_allocate_sf_channels (3)

allocate (sf_config (2))
call sf_config(1)%init ([1], data)
call sf_config(2)%init ([2], data)
call process%init_sf_chain (sf_config)
deallocate (sf_config)

call sf_channel(1)%init (2)
call process%set_sf_channel (1, sf_channel(1))

call sf_channel(2)%init (2)
call sf_channel(2)%activate_mapping ([1,2])
call process%set_sf_channel (2, sf_channel(2))

call sf_channel(3)%init (2)
call sf_channel(3)%set_s_mapping ([1,2])
call process%set_sf_channel (3, sf_channel(3))

call process%setup_mci (dispatch_mci_empty)

call process%compute_md5sum ()

call process%write (.false., u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_14"

end subroutine processes_14

```

Decay Process Evaluation

Initialize and evaluate a decay process.

```

<Processes: execute tests>+≡
  call test (processes_15, "processes_15", &
    "decay process", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_15

<Processes: tests>+≡
  subroutine processes_15 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    type(process_instance_t), allocatable, target :: process_instance
    type(particle_set_t) :: pset

    write (u, "(A)")  "* Test output: processes_15"
    write (u, "(A)")  "* Purpose: initialize a decay process object"
    write (u, "(A)")

    write (u, "(A)")  "* Build and load a test library with one process"
    write (u, "(A)")

    libname = "processes15"
    procname = libname

    call os_data%init ()
    call prc_test_create_library (libname, lib, scattering = .false., &
      decay = .true.)

    call model%init_test ()
    call model%set_par (var_str ("ff"), 0.4_default)

```

```

call model%set_par (var_str ("mf"), &
    model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))

write (u, "(A)")  "* Initialize a process object"
write (u, "(A)")

allocate (process)
call process%init (procname, lib, os_data, model)

call process%setup_test_cores ()
allocate (phs_single_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

call process%setup_beams_decay (i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

call reset_interaction_counter (3)

allocate (process_instance)
call process_instance%init (process)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Inject a set of random numbers"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%set_mcpair ([0._default, 0._default])
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Set up hard kinematics"
write (u, "(A)")

call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()

write (u, "(A)")  "* Evaluate matrix element and square"
write (u, "(A)")

```

```

call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()
call process_instance%evaluate_trace ()
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover process instance"
write (u, "(A)")

call reset_interaction_counter (3)

allocate (process_instance)
call process_instance%init (process)
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover (1, 1, .true., .true.)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()
call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_15"

end subroutine processes_15

```

Integration: decay

Activate the MC integrator for the decay object and use it to integrate over phase space.

```

<Processes: execute tests>+≡
    call test (processes_16, "processes_16", &
        "decay integration", &
        u, results)

<Processes: test declarations>+≡
    public :: processes_16

<Processes: tests>+≡
    subroutine processes_16 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(process_t), allocatable, target :: process
        class(phs_config_t), allocatable :: phs_config_template
        type(process_instance_t), allocatable, target :: process_instance

        write (u, "(A)")  "* Test output: processes_16"
        write (u, "(A)")  "*   Purpose: integrate a process without &
            &structure functions"
        write (u, "(A)")  "*               in a multi-channel configuration"
        write (u, "(A)")

        write (u, "(A)")  "* Build and initialize a process object"
        write (u, "(A)")

        libname = "processes16"
        procname = libname

        call os_data%init ()
        call prc_test_create_library (libname, lib, scattering = .false., &
            decay = .true.)

        call reset_interaction_counter ()

        call model%init_test ()
        call model%set_par (var_str ("ff"), 0.4_default)
        call model%set_par (var_str ("mf"), &
            model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))

        allocate (process)
        call process%init (procname, lib, os_data, model)

        call process%setup_test_cores ()
        allocate (phs_single_config_t :: phs_config_template)
        call process%init_components (phs_config_template)

        write (u, "(A)")  "* Prepare a trivial beam setup"
        write (u, "(A)")

        call process%setup_beams_decay (i_core = 1)
        call process%configure_phs ()

```

```

call process%setup_mci (dispatch_mci_test_midpoint)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")  "* Integrate with default test parameters"
write (u, "(A)")

call process_instance%integrate (1, n_it=1, n_calls=10000)
call process%final_integration (1)

call process%write (.false., u)

write (u, "(A)")
write (u, "(A,ES13.7)")  " Integral divided by phs factor = ", &
    process%get_integral (1) &
    / process_instance%kin(1)%phs_factor

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_16"

end subroutine processes_16

```

MCI record prepared for midpoint integrator.

(Processes: test auxiliary)+≡

```

subroutine dispatch_mci_test_midpoint (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
  allocate (mci_midpoint_t :: mci)

```



```
end subroutine dispatch_mci_test_midpoint
```

Decay Process Evaluation

Initialize and evaluate a decay process for a moving particle.

```
<Processes: execute tests>+≡
  call test (processes_17, "processes_17", &
    "decay of moving particle", &
    u, results)

<Processes: test declarations>+≡
  public :: processes_17

<Processes: tests>+≡
  subroutine processes_17 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(string_t) :: libname
    type(string_t) :: procname
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(process_t), allocatable, target :: process
    class(phs_config_t), allocatable :: phs_config_template
    type(process_instance_t), allocatable, target :: process_instance
    type(particle_set_t) :: pset
    type(flavor_t) :: flv_beam
    real(default) :: m, p, E

    write (u, "(A)")  "* Test output: processes_17"
    write (u, "(A)")  "* Purpose: initialize a decay process object"
    write (u, "(A)")

    write (u, "(A)")  "* Build and load a test library with one process"
    write (u, "(A)")

    libname = "processes17"
    procname = libname

    call os_data%init ()

    call prc_test_create_library (libname, lib, scattering = .false., &
      decay = .true.)

    write (u, "(A)")  "* Initialize a process object"
    write (u, "(A)")

    call model%init_test ()
    call model%set_par (var_str ("ff"), 0.4_default)
    call model%set_par (var_str ("mf"), &
      model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))

    allocate (process)
    call process%init (procname, lib, os_data, model)
```

```

call process%setup_test_cores ()
allocate (phs_single_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

call process%setup_beams_decay (rest_frame = .false., i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization"
write (u, "(A)")

call process%setup_terms ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

call reset_interaction_counter (3)

allocate (process_instance)
call process_instance%init (process)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Set parent momentum and random numbers"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%set_mcpair ([0._default, 0._default])

call flv_beam%init (25, process%get_model_ptr ())
m = flv_beam%get_mass ()
p = 3 * m / 4
E = sqrt (m**2 + p**2)
call process_instance%set_beam_momenta ([vector4_moving (E, p, 3)])

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Set up hard kinematics"
write (u, "(A)")

call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()

write (u, "(A)")  "* Evaluate matrix element and square"
write (u, "(A)")

call process_instance%compute_eff_kinematics ()

```

```

call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()
call process_instance%evaluate_trace ()
call process_instance%write (u)

call process_instance%get_trace (pset, 1)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Particle content:"
write (u, "(A)")

call write_separator (u)
call pset%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Recover process instance"
write (u, "(A)")

call reset_interaction_counter (3)

allocate (process_instance)
call process_instance%init (process)

call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1, check_match = .false.)
call process_instance%recover (1, 1, .true., .true.)
call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call pset%final ()
call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_17"

end subroutine processes_17

```

Resonances in Phase Space

This test demonstrates the extraction of the resonance-history set from the generated phase space. We need a nontrivial process, but no matrix element. This is provided by the `prc.template` method, using the SM model. We also

need the `phs_wood` method, otherwise we would not have resonances in the phase space configuration.

```

<Processes: execute tests>+≡
    call test (processes_18, "processes_18", &
               "extract resonance history set", &
               u, results)

<Processes: test declarations>+≡
    public :: processes_18

<Processes: tests>+≡
    subroutine processes_18 (u)
        integer, intent(in) :: u
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(string_t) :: model_name
        type(os_data_t) :: os_data
        class(model_data_t), pointer :: model
        class(vars_t), pointer :: vars
        type(process_t), pointer :: process
        type(resonance_history_set_t) :: res_set
        integer :: i

        write (u, "(A)")  "* Test output: processes_18"
        write (u, "(A)")  "* Purpose: extra resonance histories"
        write (u, "(A)")

        write (u, "(A)")  "* Build and load a test library with one process"
        write (u, "(A)")

        libname = "processes_18_lib"
        procname = "processes_18_p"

        call os_data%init ()

        call syntax_phs_forest_init ()

        model_name = "SM"
        model => null ()
        call prepare_model (model, model_name, vars)

        write (u, "(A)")  "* Initialize a process library with one process"
        write (u, "(A)")

        select type (model)
            class is (model_t)
                call prepare_resonance_test_library (lib, libname, procname, model, os_data, u)
            end select

        write (u, "(A)")
        write (u, "(A)")  "* Initialize a process object with phase space"

        allocate (process)
        select type (model)

```

```

class is (model_t)
    call prepare_resonance_test_process (process, lib, procname, model, os_data)
end select

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"
write (u, "(A)")

call process%extract_resonance_history_set (res_set)
call res_set%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process%final ()
deallocate (process)

call model%final ()
deallocate (model)

call syntax_phs_forest_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_18"

end subroutine processes_18

```

Auxiliary subroutine that constructs the process library for the above test.

(Processes: test auxiliary)+≡

```

subroutine prepare_resonance_test_library &
    (lib, libname, procname, model, os_data, u)
    type(process_library_t), target, intent(out) :: lib
    type(string_t), intent(in) :: libname
    type(string_t), intent(in) :: procname
    type(model_t), intent(in), target :: model
    type(os_data_t), intent(in) :: os_data
    integer, intent(in) :: u
    type(string_t), dimension(:), allocatable :: prt_in, prt_out
    class(prc_core_def_t), allocatable :: def
    type(process_def_entry_t), pointer :: entry

    call lib%init (libname)

    allocate (prt_in (2), prt_out (3))
    prt_in = [var_str ("e+"), var_str ("e-")]
    prt_out = [var_str ("d"), var_str ("ubar"), var_str ("W+")]

    allocate (template_me_def_t :: def)
    select type (def)
    type is (template_me_def_t)
        call def%init (model, prt_in, prt_out, unity = .false.)
    end select
    allocate (entry)

```

```

call entry%init (procname, &
    model_name = model%get_name (), &
    n_in = 2, n_components = 1)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("template"), &
    variant = def)
call entry%write (u)

call lib%append (entry)

call lib%configure (os_data)
call lib%write_makefile (os_data, force = .true., verbose = .false.)
call lib%clean (os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (os_data)

end subroutine prepare_resonance_test_library

```

We want a test process which has been initialized up to the point where we can evaluate the matrix element. This is in fact rather complicated. We copy the steps from `integration_setup_process` in the `integrate` module, which is not available at this point.

```

(Processes: test auxiliary) +=
subroutine prepare_resonance_test_process &
    (process, lib, procname, model, os_data)
    class(process_t), intent(out), target :: process
    type(process_library_t), intent(in), target :: lib
    type(string_t), intent(in) :: procname
    type(model_t), intent(in), target :: model
    type(os_data_t), intent(in) :: os_data
    class(phs_config_t), allocatable :: phs_config_template
    real(default) :: sqrts

    call process%init (procname, lib, os_data, model)

    allocate (phs_config_t :: phs_config_template)
    call process%init_components (phs_config_template)

    call process%setup_test_cores (type_string = var_str ("template"))

    sqrts = 1000
    call process%setup_beams_sqrts (sqrts, i_core = 1)
    call process%configure_phs ()
    call process%setup_mci (dispatch_mci_none)

    call process%setup_terms ()

end subroutine prepare_resonance_test_process

```

MCI record prepared for the none (dummy) integrator.

```

(Processes: test auxiliary) +=

```

```

subroutine dispatch_mci_none (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
  allocate (mci_none_t :: mci)
end subroutine dispatch_mci_none

```

Add after evaluate hook(s)

Initialize a process and process instance, add a trivial process hook, choose a sampling point and fill the process instance.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

(Processes: test types)≡

```

type, extends(process_instance_hook_t) :: process_instance_hook_test_t
  integer :: unit
  character(len=15) :: name
contains
  procedure :: init => process_instance_hook_test_init
  procedure :: final => process_instance_hook_test_final
  procedure :: evaluate => process_instance_hook_test_evaluate
end type process_instance_hook_test_t

```

(Processes: test auxiliary)+≡

```

subroutine process_instance_hook_test_init (hook, var_list, instance)
  class(process_instance_hook_test_t), intent(inout), target :: hook
  type(var_list_t), intent(in) :: var_list
  class(process_instance_t), intent(in), target :: instance
end subroutine process_instance_hook_test_init

subroutine process_instance_hook_test_final (hook)
  class(process_instance_hook_test_t), intent(inout) :: hook
end subroutine process_instance_hook_test_final

subroutine process_instance_hook_test_evaluate (hook, instance)
  class(process_instance_hook_test_t), intent(inout) :: hook
  class(process_instance_t), intent(in), target :: instance
  write (hook%unit, "(A)") "Execute hook:"
  write (hook%unit, "(2X,A,1X,A,I0,A)") hook%name, "(", len (trim (hook%name)), ")"
end subroutine process_instance_hook_test_evaluate

```

(Processes: execute tests)+≡

```

call test (processes_19, "processes_19", &
  "add trivial hooks to a process instance ", &
  u, results)

```

(Processes: test declarations)+≡

```

public :: processes_19

```

<Processes: tests>+≡

```

subroutine processes_19 (u)
  integer, intent(in) :: u
  type(process_library_t), target :: lib
  type(string_t) :: libname
  type(string_t) :: procname
  type(os_data_t) :: os_data
  class(model_data_t), pointer :: model
  type(process_t), allocatable, target :: process
  class(phs_config_t), allocatable :: phs_config_template
  real(default) :: sqrts
  type(process_instance_t) :: process_instance
  class(process_instance_hook_t), allocatable, target :: process_instance_hook, process_instance_hook2
  type(particle_set_t) :: pset

  write (u, "(A)")  "* Test output: processes_19"
  write (u, "(A)")  "*   Purpose: allocate process instance &
    &and add an after evaluate hook"
  write (u, "(A)")

  write (u, "(A)")
  write (u, "(A)")  "* Allocate a process instance"
  write (u, "(A)")

  call process_instance%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Allocate hook and add to process instance"
  write (u, "(A)")

  allocate (process_instance_hook_test_t :: process_instance_hook)
  call process_instance%append_after_hook (process_instance_hook)

  allocate (process_instance_hook_test_t :: process_instance_hook2)
  call process_instance%append_after_hook (process_instance_hook2)

  select type (process_instance_hook)
  type is (process_instance_hook_test_t)
    process_instance_hook%unit = u
    process_instance_hook%name = "Hook 1"
  end select
  select type (process_instance_hook2)
  type is (process_instance_hook_test_t)
    process_instance_hook2%unit = u
    process_instance_hook2%name = "Hook 2"
  end select

  write (u, "(A)")  "* Evaluate matrix element and square"
  write (u, "(A)")

  call process_instance%evaluate_after_hook ()

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

```



```

call process_instance_hook%final ()
deallocate (process_instance_hook)

write (u, "(A)")
write (u, "(A)")  "** Test output end: processes_19"

end subroutine processes_19

```

30.12 Process Stacks

For storing and handling multiple processes, we define process stacks. These are ordinary stacks where new process entries are pushed onto the top. We allow for multiple entries with identical process ID, but distinct run ID.

The implementation is essentially identical to the `prclib_stacks` module above. Unfortunately, Fortran supports no generic programming, so we do not make use of this fact.

When searching for a specific process ID, we will get (a pointer to) the top-most process entry with that ID on the stack, which was entered last. Usually, this is the best version of the process (in terms of integral, etc.) Thus the stack terminology makes sense.

```

<process_stacks.f90>≡
  <File header>

  module process_stacks

    <Use kinds>
    <Use strings>
    use io_units
    use format_utils, only: write_separator
    use diagnostics
    use os_interface
    use sm_qcd
    use model_data
    use rng_base
    use variables
    use observables
    use process_libraries
    use process

    <Standard module head>

    <Process stacks: public>

    <Process stacks: types>

    contains

    <Process stacks: procedures>

  end module process_stacks

```

30.12.1 The process entry type

A process entry is a process object, augmented by a pointer to the next entry. We do not need specific methods, all relevant methods are inherited.

On higher level, processes should be prepared as process entry objects.

```
<Process stacks: public>≡
    public :: process_entry_t

<Process stacks: types>≡
    type, extends (process_t) :: process_entry_t
        type(process_entry_t), pointer :: next => null ()
    end type process_entry_t
```

30.12.2 The process stack type

For easy conversion and lookup it is useful to store the filling number in the object. The content is stored as a linked list.

The `var_list` component stores process-specific results, so they can be retrieved as (pseudo) variables.

The process stack can be linked to another one. This allows us to work with stacks of local scope.

```
<Process stacks: public>+≡
    public :: process_stack_t

<Process stacks: types>+≡
    type :: process_stack_t
        integer :: n = 0
        type(process_entry_t), pointer :: first => null ()
        type(var_list_t), pointer :: var_list => null ()
        type(process_stack_t), pointer :: next => null ()
    contains
        <Process stacks: process stack: TBP>
    end type process_stack_t
```

Finalize partly: deallocate the process stack and variable list entries, but keep the variable list as an empty object. This way, the variable list links are kept.

```
<Process stacks: process stack: TBP>≡
    procedure :: clear => process_stack_clear

<Process stacks: procedures>≡
    subroutine process_stack_clear (stack)
        class(process_stack_t), intent(inout) :: stack
        type(process_entry_t), pointer :: process
        if (associated (stack%var_list)) then
            call stack%var_list%final ()
        end if
        do while (associated (stack%first))
            process => stack%first
            stack%first => process%next
            call process%final ()
            deallocate (process)
        end do
```

```

        stack%n = 0
    end subroutine process_stack_clear

```

Finalizer. Clear and deallocate the variable list.

```

<Process stacks: process stack: TBP>+≡
    procedure :: final => process_stack_final

<Process stacks: procedures>+≡
    subroutine process_stack_final (object)
        class(process_stack_t), intent(inout) :: object
        call object%clear ()
        if (associated (object%var_list)) then
            deallocate (object%var_list)
        end if
    end subroutine process_stack_final

```

Output. The processes on the stack will be ordered LIFO, i.e., backwards.

```

<Process stacks: process stack: TBP>+≡
    procedure :: write => process_stack_write

<Process stacks: procedures>+≡
    recursive subroutine process_stack_write (object, unit, pacify)
        class(process_stack_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: pacify
        type(process_entry_t), pointer :: process
        integer :: u
        u = given_output_unit (unit)
        call write_separator (u, 2)
        select case (object%n)
        case (0)
            write (u, "(1x,A)") "Process stack: [empty]"
            call write_separator (u, 2)
        case default
            write (u, "(1x,A)") "Process stack:"
            process => object%first
            do while (associated (process))
                call process%write (.false., u, pacify = pacify)
                process => process%next
            end do
        end select
        if (associated (object%next)) then
            write (u, "(1x,A)") "[Processes from context environment:]"
            call object%next%write (u, pacify)
        end if
    end subroutine process_stack_write

```

The variable list is printed by a separate routine, since it should be linked to the global variable list, anyway.

```

<Process stacks: process stack: TBP>+≡
    procedure :: write_var_list => process_stack_write_var_list

```

```

<Process stacks: procedures>+≡
  subroutine process_stack_write_var_list (object, unit)
    class(process_stack_t), intent(in) :: object
    integer, intent(in), optional :: unit
    if (associated (object%var_list)) then
      call var_list_write (object%var_list, unit)
    end if
  end subroutine process_stack_write_var_list

```

Short output.

Since this is a stack, the default output ordering for each stack will be last-in, first-out. To enable first-in, first-out, which is more likely to be requested, there is an optional `fifo` argument.

```

<Process stacks: process stack: TBP>+≡
  procedure :: show => process_stack_show

<Process stacks: procedures>+≡
  recursive subroutine process_stack_show (object, unit, fifo)
    class(process_stack_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: fifo
    type(process_entry_t), pointer :: process
    logical :: reverse
    integer :: u, i, j
    u = given_output_unit (unit)
    reverse = .false.; if (present (fifo)) reverse = fifo
    select case (object%n)
    case (0)
    case default
      if (.not. reverse) then
        process => object%first
        do while (associated (process))
          call process%show (u, verbose=.false.)
          process => process%next
        end do
      else
        do i = 1, object%n
          process => object%first
          do j = 1, object%n - i
            process => process%next
          end do
          call process%show (u, verbose=.false.)
        end do
      end if
    end select
    if (associated (object%next)) call object%next%show ()
  end subroutine process_stack_show

```

30.12.3 Link

Link the current process stack to a global one.

```

<Process stacks: process stack: TBP>+≡

```

```

    procedure :: link => process_stack_link
  <Process stacks: procedures>+≡
    subroutine process_stack_link (local_stack, global_stack)
      class(process_stack_t), intent(inout) :: local_stack
      type(process_stack_t), intent(in), target :: global_stack
      local_stack%next => global_stack
    end subroutine process_stack_link

```

Initialize the process variable list and link the main variable list to it.

```

  <Process stacks: process stack: TBP>+≡
    procedure :: init_var_list => process_stack_init_var_list
  <Process stacks: procedures>+≡
    subroutine process_stack_init_var_list (stack, var_list)
      class(process_stack_t), intent(inout) :: stack
      type(var_list_t), intent(inout), optional :: var_list
      allocate (stack%var_list)
      if (present (var_list)) call var_list%link (stack%var_list)
    end subroutine process_stack_init_var_list

```

Link the process variable list to a global variable list.

```

  <Process stacks: process stack: TBP>+≡
    procedure :: link_var_list => process_stack_link_var_list
  <Process stacks: procedures>+≡
    subroutine process_stack_link_var_list (stack, var_list)
      class(process_stack_t), intent(inout) :: stack
      type(var_list_t), intent(in), target :: var_list
      call stack%var_list%link (var_list)
    end subroutine process_stack_link_var_list

```

30.12.4 Push

We take a process pointer and push it onto the stack. The previous pointer is nullified. Subsequently, the process is ‘owned’ by the stack and will be finalized when the stack is deleted.

```

  <Process stacks: process stack: TBP>+≡
    procedure :: push => process_stack_push
  <Process stacks: procedures>+≡
    subroutine process_stack_push (stack, process)
      class(process_stack_t), intent(inout) :: stack
      type(process_entry_t), intent(inout), pointer :: process
      process%next => stack%first
      stack%first => process
      process => null ()
      stack%n = stack%n + 1
    end subroutine process_stack_push

```

Inverse: Remove the last process pointer in the list and return it.

```

  <Process stacks: process stack: TBP>+≡
    procedure :: pop_last => process_stack_pop_last

```

```

(Process stacks: procedures)+≡
subroutine process_stack_pop_last (stack, process)
  class(process_stack_t), intent(inout) :: stack
  type(process_entry_t), intent(inout), pointer :: process
  type(process_entry_t), pointer :: previous
  integer :: i
  select case (stack%n)
  case (:0)
    process => null ()
  case (1)
    process => stack%first
    stack%first => null ()
    stack%n = 0
  case (2:)
    process => stack%first
    do i = 2, stack%n
      previous => process
      process => process%next
    end do
    previous%next => null ()
    stack%n = stack%n - 1
  end select
end subroutine process_stack_pop_last

```

Initialize process variables for a given process ID, without setting values.

```

(Process stacks: process stack: TBP)+≡
procedure :: init_result_vars => process_stack_init_result_vars

(Process stacks: procedures)+≡
subroutine process_stack_init_result_vars (stack, id)
  class(process_stack_t), intent(inout) :: stack
  type(string_t), intent(in) :: id
  call var_list_init_num_id (stack%var_list, id)
  call var_list_init_process_results (stack%var_list, id)
end subroutine process_stack_init_result_vars

```

Fill process variables with values. This is executed after the integration pass.

Note: We set only integral and error. With multiple MCI records possible, the results for `n_calls`, `chi2` etc. are not necessarily unique. (We might set the efficiency, though.)

```

(Process stacks: process stack: TBP)+≡
procedure :: fill_result_vars => process_stack_fill_result_vars

(Process stacks: procedures)+≡
subroutine process_stack_fill_result_vars (stack, id)
  class(process_stack_t), intent(inout) :: stack
  type(string_t), intent(in) :: id
  type(process_t), pointer :: process
  process => stack%get_process_ptr (id)
  if (associated (process)) then
    call var_list_init_num_id (stack%var_list, id, process%get_num_id ())
    if (process%has_integral ()) then
      call var_list_init_process_results (stack%var_list, id, &
        integral = process%get_integral (), &

```

```

        error = process%get_error ()
    end if
else
    call msg_bug ("process_stack_fill_result_vars: unknown process ID")
end if
end subroutine process_stack_fill_result_vars

```

If one of the result variables has a local image in `var_list_local`, update the value there as well.

```

(Process stacks: process stack: TBP)+≡
    procedure :: update_result_vars => process_stack_update_result_vars

(Process stacks: procedures)+≡
    subroutine process_stack_update_result_vars (stack, id, var_list_local)
        class(process_stack_t), intent(inout) :: stack
        type(string_t), intent(in) :: id
        type(var_list_t), intent(inout) :: var_list_local
        call update ("integral(" // id // ")")
        call update ("error(" // id // ")")
    contains
        subroutine update (var_name)
            type(string_t), intent(in) :: var_name
            real(default) :: value
            if (var_list_local%contains (var_name, follow_link = .false.)) then
                value = stack%var_list%get_rval (var_name)
                call var_list_local%set_real (var_name, value, is_known = .true.)
            end if
        end subroutine update
    end subroutine process_stack_update_result_vars

```

30.12.5 Data Access

Tell if a process exists.

```

(Process stacks: process stack: TBP)+≡
    procedure :: exists => process_stack_exists

(Process stacks: procedures)+≡
    function process_stack_exists (stack, id) result (flag)
        class(process_stack_t), intent(in) :: stack
        type(string_t), intent(in) :: id
        logical :: flag
        type(process_t), pointer :: process
        process => stack%get_process_ptr (id)
        flag = associated (process)
    end function process_stack_exists

```

Return a pointer to a process with specific ID. Look also at a linked stack, if necessary.

```

(Process stacks: process stack: TBP)+≡
    procedure :: get_process_ptr => process_stack_get_process_ptr

```

```

<Process stacks: procedures>+≡
  recursive function process_stack_get_process_ptr (stack, id) result (ptr)
    class(process_stack_t), intent(in) :: stack
    type(string_t), intent(in) :: id
    type(process_t), pointer :: ptr
    type(process_entry_t), pointer :: entry
    ptr => null ()
    entry => stack%first
    do while (associated (entry))
      if (entry%get_id () == id) then
        ptr => entry%process_t
        return
      end if
      entry => entry%next
    end do
    if (associated (stack%next)) ptr => stack%next%get_process_ptr (id)
  end function process_stack_get_process_ptr

```

30.12.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<process_stacks_ut.f90>≡
  <File header>

  module process_stacks_ut
    use unit_tests
    use process_stacks_uti

    <Standard module head>

    <Process stacks: public test>

    contains

    <Process stacks: test driver>

  end module process_stacks_ut

<process_stacks_uti.f90>≡
  <File header>

  module process_stacks_uti

    <Use strings>
    use os_interface
    use sm_qcd
    use models
    use model_data
    use variables, only: var_list_t
    use process_libraries
    use rng_base
    use prc_test, only: prc_test_create_library
    use process, only: process_t

```



```

    use instances, only: process_instance_t
    use processes_ut, only: prepare_test_process

    use process_stacks

    use rng_base_ut, only: rng_test_factory_t

    <Standard module head>

    <Process stacks: test declarations>

contains

    <Process stacks: tests>

end module process_stacks_ut

API: driver for the unit tests below.
<Process stacks: public test>≡
    public :: process_stacks_test
<Process stacks: test driver>≡
    subroutine process_stacks_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Process stacks: execute tests>
    end subroutine process_stacks_test

```

Write an empty process stack

The most trivial test is to write an uninitialized process stack.

```

<Process stacks: execute tests>≡
    call test (process_stacks_1, "process_stacks_1", &
        "write an empty process stack", &
        u, results)
<Process stacks: test declarations>≡
    public :: process_stacks_1
<Process stacks: tests>≡
    subroutine process_stacks_1 (u)
        integer, intent(in) :: u
        type(process_stack_t) :: stack

        write (u, "(A)")  "* Test output: process_stacks_1"
        write (u, "(A)")  "* Purpose: display an empty process stack"
        write (u, "(A)")

        call stack%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: process_stacks_1"

    end subroutine process_stacks_1

```

Fill a process stack

Fill a process stack with two (identical) processes.

```
<Process stacks: execute tests>+≡
    call test (process_stacks_2, "process_stacks_2", &
              "fill a process stack", &
              u, results)

<Process stacks: test declarations>+≡
    public :: process_stacks_2

<Process stacks: tests>+≡
    subroutine process_stacks_2 (u)
        integer, intent(in) :: u
        type(process_stack_t) :: stack
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), target :: model
        type(var_list_t) :: var_list
        type(process_entry_t), pointer :: process => null ()

        write (u, "(A)")  "* Test output: process_stacks_2"
        write (u, "(A)")  "* Purpose: fill a process stack"
        write (u, "(A)")

        write (u, "(A)")  "* Build, initialize and store two test processes"
        write (u, "(A)")

        libname = "process_stacks2"
        procname = libname

        call os_data%init ()
        call prc_test_create_library (libname, lib)

        call model%init_test ()
        call var_list%append_string (var_str ("$run_id"))
        call var_list%append_log (var_str ("?alphas_is_fixed"), .true.)
        call var_list%append_int (var_str ("seed"), 0)

        allocate (process)

        call var_list%set_string &
            (var_str ("$run_id"), var_str ("run1"), is_known=.true.)
        call process%init (procname, lib, os_data, model, var_list)
        call stack%push (process)

        allocate (process)

        call var_list%set_string &
            (var_str ("$run_id"), var_str ("run2"), is_known=.true.)
        call process%init (procname, lib, os_data, model, var_list)
```

```

call stack%push (process)

call stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call stack%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_stacks_2"

end subroutine process_stacks_2

```

Fill a process stack

Fill a process stack with two (identical) processes.

```

<Process stacks: execute tests>+≡
  call test (process_stacks_3, "process_stacks_3", &
    "process variables", &
    u, results)

<Process stacks: test declarations>+≡
  public :: process_stacks_3

<Process stacks: tests>+≡
  subroutine process_stacks_3 (u)
    integer, intent(in) :: u
    type(process_stack_t) :: stack
    type(model_t), target :: model
    type(string_t) :: procname
    type(process_entry_t), pointer :: process => null ()
    type(process_instance_t), target :: process_instance

    write (u, "(A)")  "* Test output: process_stacks_3"
    write (u, "(A)")  "* Purpose: setup process variables"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process variables"
    write (u, "(A)")

    procname = "processes_test"
    call model%init_test ()

    write (u, "(A)")  "* Initialize process variables"
    write (u, "(A)")

    call stack%init_var_list ()
    call stack%init_result_vars (procname)
    call stack%write_var_list (u)

    write (u, "(A)")
    write (u, "(A)")  "* Build and integrate a test process"

```

```

write (u, "(A)")

allocate (process)
call prepare_test_process (process%process_t, process_instance, model)
call process_instance%integrate (1, 1, 1000)
call process_instance%final ()
call process%final_integration (1)
call stack%push (process)

write (u, "(A)")  "* Fill process variables"
write (u, "(A)")

call stack%fill_result_vars (procname)
call stack%write_var_list (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call stack%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_stacks_3"

end subroutine process_stacks_3

```

Linked a process stack

Fill two process stack, linked to each other.

```

<Process stacks: execute tests>+≡
  call test (process_stacks_4, "process_stacks_4", &
    "linked stacks", &
    u, results)

<Process stacks: test declarations>+≡
  public :: process_stacks_4

<Process stacks: tests>+≡
  subroutine process_stacks_4 (u)
    integer, intent(in) :: u
    type(process_library_t), target :: lib
    type(process_stack_t), target :: stack1, stack2
    type(model_t), target :: model
    type(string_t) :: libname
    type(string_t) :: procname1, procname2
    type(os_data_t) :: os_data
    type(process_entry_t), pointer :: process => null ()

    write (u, "(A)")  "* Test output: process_stacks_4"
    write (u, "(A)")  "* Purpose: link process stacks"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process variables"
    write (u, "(A)")

```

```

libname = "process_stacks_4_lib"
procname1 = "process_stacks_4a"
procname2 = "process_stacks_4b"

call os_data%init ()

write (u, "(A)")  "* Initialize first process"
write (u, "(A)")

call prc_test_create_library (procname1, lib)

call model%init_test ()

allocate (process)
call process%init (procname1, lib, os_data, model)
call stack1%push (process)

write (u, "(A)")  "* Initialize second process"
write (u, "(A)")

call stack2%link (stack1)

call prc_test_create_library (procname2, lib)

allocate (process)

call process%init (procname2, lib, os_data, model)
call stack2%push (process)

write (u, "(A)")  "* Show linked stacks"
write (u, "(A)")

call stack2%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call stack2%final ()
call stack1%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_stacks_4"

end subroutine process_stacks_4

```

Chapter 31

Matching

```
<matching_base.f90>≡  
  <File header>  
  
  module matching_base  
  
    <Use strings>  
    <Use debug>  
    use diagnostics  
    use sm_qcd  
    use model_data  
    use particles  
    use variables  
    use shower_base  
    use instances, only: process_instance_t  
    use rng_base  
  
    <Standard module head>  
  
    <Matching base: public>
```

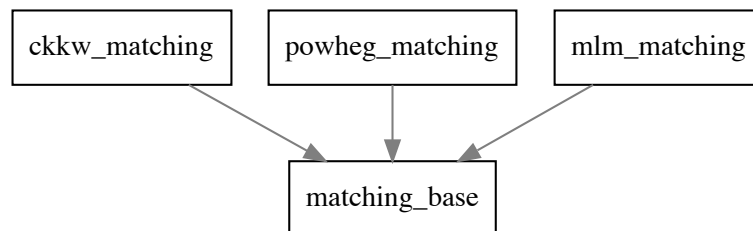


Figure 31.1: Module dependencies in `src/matching`.

<Matching base: parameters>

<Matching base: types>

<Matching base: interfaces>

contains

<Matching base: procedures>

end module matching_base

31.1 Abstract Matching Type

A matching will need access to the `shower` as well as matrix elements that we currently get over `process_instace`. The `model` is intended for the backup `model_hadrons`.

<Matching base: public>≡

public :: matching_t

<Matching base: types>≡

type, abstract :: matching_t

logical :: is_hadron_collision = .false.

type(qcd_t) :: qcd

class(shower_base_t), pointer :: shower => null ()

type(process_instance_t), pointer :: process_instance => null ()

class(model_data_t), pointer :: model => null ()

class(rng_t), allocatable :: rng

type(string_t) :: process_name

contains

<Matching base: matching: TBP>

end type matching_t

<Matching base: matching: TBP>≡

procedure (matching_init), deferred :: init

<Matching base: interfaces>≡

abstract interface

subroutine matching_init (matching, var_list, process_name)

import

class(matching_t), intent(out) :: matching

type(var_list_t), intent(in) :: var_list

type(string_t), intent(in) :: process_name

end subroutine matching_init

end interface

If we use a polymorphic settings type, this boilerplate wouldn't be necessary but then we introduce `select type` statements all over the place.

<default matching init>≡

type(var_list_t), intent(in) :: var_list

type(string_t), intent(in) :: process_name

if (debug_on) call msg_debug (D_MATCHING, "matching_init")

```

    call matching%settings%init (var_list)
    matching%process_name = process_name

<Matching base: matching: TBP>+≡
    procedure (matching_write), deferred :: write

<Matching base: interfaces>+≡
    abstract interface
        subroutine matching_write (matching, unit)
            import
            class(matching_t), intent(in) :: matching
            integer, intent(in), optional :: unit
        end subroutine matching_write
    end interface

<Matching base: matching: TBP>+≡
    procedure :: import_rng => matching_import_rng

<Matching base: procedures>≡
    pure subroutine matching_import_rng (matching, rng)
        class(matching_t), intent(inout) :: matching
        class(rng_t), allocatable, intent(inout) :: rng
        call move_alloc (from = rng, to = matching%rng)
    end subroutine matching_import_rng

<Matching base: matching: TBP>+≡
    procedure :: connect => matching_connect
    procedure :: base_connect => matching_connect

<Matching base: procedures>+≡
    subroutine matching_connect (matching, process_instance, model, shower)
        class(matching_t), intent(inout) :: matching
        type(process_instance_t), intent(in), target :: process_instance
        class(model_data_t), intent(in), target, optional :: model
        class(shower_base_t), intent(in), target, optional :: shower
        if (debug_on) call msg_debug (D_MATCHING, "matching_connect")
        matching%process_instance => process_instance
        if (present (model)) matching%model => model
        if (present (shower)) matching%shower => shower
    end subroutine matching_connect

<Matching base: matching: TBP>+≡
    procedure (matching_before_shower), deferred :: before_shower

<Matching base: interfaces>+≡
    abstract interface
        subroutine matching_before_shower (matching, particle_set, vetoed)
            import
            class(matching_t), intent(inout) :: matching
            type(particle_set_t), intent(inout) :: particle_set
            logical, intent(out) :: vetoed
        end subroutine matching_before_shower
    end interface

```



```

<Matching base: matching: TBP>+≡
  procedure (matching_after_shower), deferred :: after_shower

<Matching base: interfaces>+≡
  abstract interface
    subroutine matching_after_shower (matching, particle_set, vetoed)
      import
      class(matching_t), intent(inout) :: matching
      type(particle_set_t), intent(inout) :: particle_set
      logical, intent(out) :: vetoed
    end subroutine matching_after_shower
  end interface

```

Per default, do nothing here.

```

<Matching base: matching: TBP>+≡
  procedure :: prepare_for_events => matching_prepare_for_events

<Matching base: procedures>+≡
  subroutine matching_prepare_for_events (matching)
    class(matching_t), intent(inout), target :: matching
  end subroutine matching_prepare_for_events

```

```

<Matching base: matching: TBP>+≡
  procedure :: first_event => matching_first_event

<Matching base: procedures>+≡
  subroutine matching_first_event (matching)
    class(matching_t), intent(inout), target :: matching
  end subroutine matching_first_event

```

```

<Matching base: matching: TBP>+≡
  procedure (matching_get_method), deferred :: get_method

<Matching base: interfaces>+≡
  abstract interface
    function matching_get_method (matching) result (method)
      import
      type(string_t) :: method
      class(matching_t), intent(in) :: matching
    end function matching_get_method
  end interface

```

```

<Matching base: matching: TBP>+≡
  procedure :: final => matching_final

<Matching base: procedures>+≡
  subroutine matching_final (matching)
    class(matching_t), intent(in) :: matching
  end subroutine matching_final

```

31.1.1 Matching implementations

```

<Matching base: public>+≡
  public :: MATCH_MLM, MATCH_CKKW, MATCH_POWHEG

```

```

<Matching base: parameters>≡
    integer, parameter :: MATCH_MLM = 1
    integer, parameter :: MATCH_CKKW = 2
    integer, parameter :: MATCH_POWHEG = 3
    integer, parameter :: MATCH_UNDEFINED = 17

A dictionary
<Matching base: public>+≡
    public :: matching_method

<Matching base: interfaces>+≡
    interface matching_method
        module procedure matching_method_of_string
        module procedure matching_method_to_string
    end interface

<Matching base: procedures>+≡
    elemental function matching_method_of_string (string) result (i)
        integer :: i
        type(string_t), intent(in) :: string
        select case (char (string))
        case ("MLM")
            i = MATCH_MLM
        case ("CKKW")
            i = MATCH_CKKW
        case ("POWHEG")
            i = MATCH_POWHEG
        case default
            i = MATCH_UNDEFINED
        end select
    end function matching_method_of_string

    elemental function matching_method_to_string (i) result (string)
        type(string_t) :: string
        integer, intent(in) :: i
        select case (i)
        case (MATCH_MLM)
            string = "MLM"
        case (MATCH_CKKW)
            string = "CKKW"
        case (MATCH_POWHEG)
            string = "POWHEG"
        case default
            string = "UNDEFINED"
        end select
    end function matching_method_to_string

```

31.2 MLM Matching

```

<mlm_matching.f90>≡
    <File header>

    module mlm_matching

```

```

    <Use kinds with double>
    <Use strings>
    <Use debug>
    use io_units
    use constants
    use format_utils, only: write_separator
    use diagnostics
    use file_utils
    use lorentz
    use subevents, only: PRT_OUTGOING
    use particles
    use variables
    use shower_base
    use ktclus
    use matching_base

    <Standard module head>

    <MLM matching: public>

    <MLM matching: types>

contains

    <MLM matching: procedures>

end module mlm_matching

<MLM matching: public>≡
    public :: mlm_matching_settings_t

<MLM matching: types>≡
    type :: mlm_matching_settings_t
        real(default) :: mlm_Qcut_ME = one
        real(default) :: mlm_Qcut_PS = one
        real(default) :: mlm_ptmin, mlm_etamax, mlm_Rmin, mlm_Emin
        real(default) :: mlm_ETclusfactor = 0.2_default
        real(default) :: mlm_ETclusminE = five
        real(default) :: mlm_etaclusfactor = one
        real(default) :: mlm_Rclusfactor = one
        real(default) :: mlm_Eclusfactor = one
        integer :: kt_imode_hadronic = 4313
        integer :: kt_imode_leptonic = 1111
        integer :: mlm_nmaxMEjets = 0
    contains
        <MLM matching: mlm matching settings: TBP>
end type mlm_matching_settings_t

<MLM matching: mlm matching settings: TBP>≡
    procedure :: init => mlm_matching_settings_init

<MLM matching: procedures>≡
    subroutine mlm_matching_settings_init (settings, var_list)
        class(mlm_matching_settings_t), intent(out) :: settings

```

```

type(var_list_t), intent(in) :: var_list
settings%mlm_Qcut_ME = &
    var_list%get_rval (var_str ("mlm_Qcut_ME"))
settings%mlm_Qcut_PS = &
    var_list%get_rval (var_str ("mlm_Qcut_PS"))
settings%mlm_ptmin = &
    var_list%get_rval (var_str ("mlm_ptmin"))
settings%mlm_etamax = &
    var_list%get_rval (var_str ("mlm_etamax"))
settings%mlm_Rmin = &
    var_list%get_rval (var_str ("mlm_Rmin"))
settings%mlm_Emin = &
    var_list%get_rval (var_str ("mlm_Emin"))
settings%mlm_nmaxMEjets = &
    var_list%get_ival (var_str ("mlm_nmaxMEjets"))

settings%mlm_ETclusfactor = &
    var_list%get_rval (var_str ("mlm_ETclusfactor"))
settings%mlm_ETclusminE = &
    var_list%get_rval (var_str ("mlm_ETclusminE"))
settings%mlm_etaclusfactor = &
    var_list%get_rval (var_str ("mlm_etaclusfactor"))
settings%mlm_Rclusfactor = &
    var_list%get_rval (var_str ("mlm_Rclusfactor"))
settings%mlm_Eclusfactor = &
    var_list%get_rval (var_str ("mlm_Eclusfactor"))
end subroutine mlm_matching_settings_init

```

(MLM matching: mlm matching settings: TBP)+≡

```

procedure :: write => mlm_matching_settings_write

```

(MLM matching: procedures)+≡

```

subroutine mlm_matching_settings_write (settings, unit)
class(mlm_matching_settings_t), intent(in) :: settings
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit); if (u < 0) return
write (u, "(3x,A,ES19.12)") &
    "mlm_Qcut_ME" = ", settings%mlm_Qcut_ME
write (u, "(3x,A,ES19.12)") &
    "mlm_Qcut_PS" = ", settings%mlm_Qcut_PS
write (u, "(3x,A,ES19.12)") &
    "mlm_ptmin" = ", settings%mlm_ptmin
write (u, "(3x,A,ES19.12)") &
    "mlm_etamax" = ", settings%mlm_etamax
write (u, "(3x,A,ES19.12)") &
    "mlm_Rmin" = ", settings%mlm_Rmin
write (u, "(3x,A,ES19.12)") &
    "mlm_Emin" = ", settings%mlm_Emin
write (u, "(3x,A,1x,I0)") &
    "mlm_nmaxMEjets" = ", settings%mlm_nmaxMEjets
write (u, "(3x,A,ES19.12)") &
    "mlm_ETclusfactor (D=0.2)" = ", settings%mlm_ETclusfactor
write (u, "(3x,A,ES19.12)") &

```

```

      "mlm_ETclusminE      (D=5.0)      = ", settings%mlm_ETclusminE
write (u, "(3x,A,ES19.12)") &
      "mlm_etaclusfactor (D=1.0)      = ", settings%mlm_etaClusfactor
write (u, "(3x,A,ES19.12)") &
      "mlm_Rclusfactor   (D=1.0)      = ", settings%mlm_RClusfactor
write (u, "(3x,A,ES19.12)") &
      "mlm_Eclusfactor   (D=1.0)      = ", settings%mlm_EClusfactor
end subroutine mlm_matching_settings_write

```

This is a container for the (colored) parton momenta as well as the jet momenta.

```

<MLM matching: public>+≡
  public :: mlm_matching_t

<MLM matching: types>+≡
  type, extends (matching_t) :: mlm_matching_t
    type(vector4_t), dimension(:), allocatable, public :: P_ME
    type(vector4_t), dimension(:), allocatable, public :: P_PS
    type(vector4_t), dimension(:), allocatable, private :: JETS_ME
    type(vector4_t), dimension(:), allocatable, private :: JETS_PS
    type(mlm_matching_settings_t) :: settings
  contains
    <MLM matching: mlm matching: TBP>
  end type mlm_matching_t

<MLM matching: mlm matching: TBP>≡
  procedure :: init => mlm_matching_init

<MLM matching: procedures>+≡
  subroutine mlm_matching_init (matching, var_list, process_name)
    class(mlm_matching_t), intent(out) :: matching
    <default matching init>
  end subroutine mlm_matching_init

<MLM matching: mlm matching: TBP>+≡
  procedure :: write => mlm_matching_write

<MLM matching: procedures>+≡
  subroutine mlm_matching_write (matching, unit)
    class(mlm_matching_t), intent(in) :: matching
    integer, intent(in), optional :: unit
    integer :: i, u
    u = given_output_unit (unit); if (u < 0) return

    write (u, "(1x,A)") "MLM matching:"
    call matching%settings%write (u)
    write (u, "(3x,A)") "Momenta of ME partons:"
    if (allocated (matching%P_ME)) then
      do i = 1, size (matching%P_ME)
        write (u, "(4x)", advance = "no")
        call vector4_write (matching%P_ME(i), unit = u)
      end do
    else
      write (u, "(5x,A)") "[empty]"
    end if
  end subroutine mlm_matching_write

```

```

call write_separator (u)
write (u, "(3x,A)") "Momenta of ME jets:"
if (allocated (matching%JETS_ME)) then
  do i = 1, size (matching%JETS_ME)
    write (u, "(4x)", advance = "no")
    call vector4_write (matching%JETS_ME(i), unit = u)
  end do
else
  write (u, "(5x,A)") "[empty]"
end if
call write_separator (u)
write(u, "(3x,A)") "Momenta of shower partons:"
if (allocated (matching%P_PS)) then
  do i = 1, size (matching%P_PS)
    write (u, "(4x)", advance = "no")
    call vector4_write (matching%P_PS(i), unit = u)
  end do
else
  write (u, "(5x,A)") "[empty]"
end if
call write_separator (u)
write (u, "(3x,A)") "Momenta of shower jets:"
if (allocated (matching%JETS_PS)) then
  do i = 1, size (matching%JETS_PS)
    write (u, "(4x)", advance = "no")
    call vector4_write (matching%JETS_PS(i), unit = u)
  end do
else
  write (u, "(5x,A)") "[empty]"
end if
call write_separator (u)
end subroutine mlm_matching_write

```

```

<MLM matching: mlm matching: TBP>+≡
  procedure :: get_method => mlm_matching_get_method

<MLM matching: procedures>+≡
  function mlm_matching_get_method (matching) result (method)
    type(string_t) :: method
    class(mlm_matching_t), intent(in) :: matching
    method = matching_method (MATCH_MLM)
  end function mlm_matching_get_method

<MLM matching: mlm matching: TBP>+≡
  procedure :: before_shower => mlm_matching_before_shower

<MLM matching: procedures>+≡
  subroutine mlm_matching_before_shower &
    (matching, particle_set, vetoed)
    class(mlm_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(inout) :: particle_set
    logical, intent(out) :: vetoed
    vetoed = .false.
  end subroutine mlm_matching_before_shower

```

```

<MLM matching: mlm matching: TBP>+≡
  procedure :: after_shower => mlm_matching_after_shower

<MLM matching: procedures>+≡
  subroutine mlm_matching_after_shower (matching, particle_set, vetoed)
    class(mlm_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(inout) :: particle_set
    logical, intent(out) :: vetoed
    if (debug_on) call msg_debug (D_MATCHING, "mlm_matching_after_shower")
    call matching%shower%get_final_colored_ME_momenta (matching%P_ME)
    call matching%fill_P_PS (particle_set)
    !!! MLM stage 3 -> reconstruct and possibly reject
    call matching%apply (vetoed)
    if (debug_active (D_MATCHING)) call matching%write ()
    if (allocated (matching%P_ME)) deallocate (matching%P_ME)
    if (allocated (matching%P_PS)) deallocate (matching%P_PS)
    if (allocated (matching%JETS_ME)) deallocate (matching%JETS_ME)
    if (allocated (matching%JETS_PS)) deallocate (matching%JETS_PS)
  end subroutine mlm_matching_after_shower

Transfer partons after parton shower to matching%P_PS
<MLM matching: mlm matching: TBP>+≡
  procedure :: fill_P_PS => mlm_matching_fill_P_PS

<MLM matching: procedures>+≡
  subroutine mlm_matching_fill_P_PS (matching, particle_set)
    class(mlm_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(in) :: particle_set
    integer :: i, j, n_jets_PS
    integer, dimension(2) :: col
    type(particle_t) :: tempprt
    real(double) :: eta
    type(vector4_t) :: p_tmp

    !!! loop over particles and extract final colored ones with eta<etamax
    n_jets_PS = 0
    do i = 1, particle_set%get_n_tot ()
      if (signal_is_pending ()) return
      tempprt = particle_set%get_particle (i)
      if (tempprt%get_status () /= PRT_OUTGOING) cycle
      col = tempprt%get_color ()
      if (all (col == 0)) cycle
! TODO: (bcn 2015-04-28) where is the corresponding part for lepton colliders?
      if (matching%is_hadron_collision) then
        p_tmp = tempprt%get_momentum ()
        if (energy (p_tmp) - longitudinal_part (p_tmp) < 1.E-10_default .or. &
            energy (p_tmp) + longitudinal_part (p_tmp) < 1.E-10_default) then
          eta = pseudorapidity (p_tmp)
        else
          eta = rapidity (p_tmp)
        end if
        if (eta > matching%settings%mlm_etaClusfactor * &
            matching%settings%mlm_etamax) then
          if (debug_active (D_MATCHING)) then
            call msg_debug (D_MATCHING, "Rejecting this particle")
          end if
        end if
      end if
    end do
  end subroutine mlm_matching_fill_P_PS

```

```

        call tempprt%write ()
    end if
    cycle
end if
end if
n_jets_PS = n_jets_PS + 1
end do

allocate (matching%P_PS(1:n_jets_PS))
if (debug_on) call msg_debug (D_MATCHING, "n_jets_ps", n_jets_ps)

j = 1
do i = 1, particle_set%get_n_tot ()
    tempprt = particle_set%get_particle (i)
    if (tempprt%get_status () /= PRT_OUTGOING) cycle
    col = tempprt%get_color ()
    if (all(col == 0)) cycle
! TODO: (bcn 2015-04-28) where is the corresponding part for lepton colliders?
    if (matching%is_hadron_collision) then
        p_tmp = tempprt%get_momentum ()
        if (energy (p_tmp) - longitudinal_part (p_tmp) < 1.E-10_default .or. &
            energy (p_tmp) + longitudinal_part (p_tmp) < 1.E-10_default) then
            eta = pseudorapidity (p_tmp)
        else
            eta = rapidity (p_tmp)
        end if
        if (eta > matching%settings%mlm_etaClusfactor * &
            matching%settings%mlm_etamax) cycle
    end if
    matching%P_PS(j) = tempprt%get_momentum ()
    j = j + 1
end do
end subroutine mlm_matching_fill_P_PS

```

<MLM matching: mlm matching: TBP>+≡

```
procedure :: apply => mlm_matching_apply
```

<MLM matching: procedures>+≡

```

subroutine mlm_matching_apply (matching, vetoed)
    class(mlm_matching_t), intent(inout) :: matching
    logical, intent(out) :: vetoed
    integer :: i, j
    integer :: n_jets_ME, n_jets_PS, n_jets_PS_atycut
    real(double) :: ycut
    real(double), dimension(:, :), allocatable :: PP
    real(double), dimension(:), allocatable :: Y
    real(double), dimension(:, :), allocatable :: P_JETS
    real(double), dimension(:, :), allocatable :: P_ME
    integer, dimension(:), allocatable :: JET
    integer :: NJET, NSUB
    integer :: imode
!!! TODO: (bcn 2014-03-26) Why is ECUT hard coded to 1?
!!! It is the denominator of the KT measure. Candidate for removal
    real(double) :: ECUT = 1._double

```



```

integer :: ip1,ip2

! KTCLUS COMMON BLOCK
INTEGER NMAX,NUM,HIST
PARAMETER (NMAX=512)
DOUBLE PRECISION P,KT,KTP,KTS,ETOT,RSQ,KTLAST
COMMON /KTCOMM/ETOT,RSQ,P(9,NMAX),KTP(NMAX,NMAX),KTS(NMAX), &
      KT(NMAX),KTLAST(NMAX),HIST(NMAX),NUM

vetoed = .true.
if (signal_is_pending ()) return

<Set n_jets_ME/PS from matching (or equal zero)>

<Jet clustering for partons after matrix element>

<Jet clustering for partons after shower>

<Veto: too many or not enough jets after PS>

<Cluster ME jets with PS jets one at a time>

vetoed = .false.
999 continue
end subroutine mlm_matching_apply

<Set n_jets_ME/PS from matching (or equal zero)>≡
if (allocated (matching%P_ME)) then
  ! print *, "number of partons after ME: ", size(matching%P_ME)
  n_jets_ME = size (matching%P_ME)
else
  n_jets_ME = 0
end if
if (allocated (matching%p_PS)) then
  ! print *, "number of partons after PS: ", size(matching%p_PS)
  n_jets_PS = size (matching%p_PS)
else
  n_jets_PS = 0
end if

<Jet clustering for partons after matrix element>≡
if (n_jets_ME > 0) then
  ycut = (matching%settings%mlm_ptmin)**2
  allocate (PP(1:4, 1:n_jets_ME))
  do i = 1, n_jets_ME
    PP(1:3,i) = matching%p_ME(i)%p(1:3)
    PP(4,i) = matching%p_ME(i)%p(0)
  end do

  <Set imode for lepton or hadron collisions>

  allocate (P_ME(1:4,1:n_jets_ME))
  allocate (JET(1:n_jets_ME))
  allocate (Y(1:n_jets_ME))

```

```

if (signal_is_pending ()) return
call KTCLUR (imode, PP, n_jets_ME, &
             dble (matching%settings%mlm_Rclusfactor * matching%settings%mlm_Rmin), ECUT, y, *999)
call KTRECO (1, PP, n_jets_ME, ECUT, ycut, ycut, P_ME, JET, &
             NJET, NSUB, *999)

n_jets_ME = NJET
if (NJET > 0) then
  allocate (matching%JETS_ME (1:NJET))
  do i = 1, NJET
    matching%JETS_ME(i) = vector4_moving (REAL(P_ME(4,i), default), &
      vector3_moving([REAL(P_ME(1,i), default), &
        REAL(P_ME(2,i), default), REAL(P_ME(3,i), default)]))
  end do
end if
deallocate (P_ME)
deallocate (JET)
deallocate (Y)
deallocate (PP)
end if

<Jet clustering for partons after shower>≡
if (n_jets_PS > 0) then
  ycut = (matching%settings%mlm_ptmin + max (matching%settings%mlm_ETclusminE, &
    matching%settings%mlm_ETclusfactor * matching%settings%mlm_ptmin))*2
  allocate (PP(1:4, 1:n_jets_PS))
  do i = 1, n_jets_PS
    PP(1:3,i) = matching%p_PS(i)%p(1:3)
    PP(4,i) = matching%p_PS(i)%p(0)
  end do

  <Set imode for lepton or hadron collisions>

  allocate (P_JETS(1:4,1:n_jets_PS))
  allocate (JET(1:n_jets_PS))
  allocate (Y(1:n_jets_PS))

  if (signal_is_pending ()) return
  call KTCLUR (imode, PP, n_jets_PS, &
               dble (matching%settings%mlm_Rclusfactor * matching%settings%mlm_Rmin), &
               ECUT, y, *999)
  call KTRECO (1, PP, n_jets_PS, ECUT, ycut, ycut, P_JETS, JET, &
               NJET, NSUB, *999)
  n_jets_PS_atycut = NJET
  if (n_jets_ME == matching%settings%mlm_nmaxMEjets .and. NJET > 0) then
    ! print *, " resetting ycut to ", Y(matching%settings%mlm_nmaxMEjets)
    ycut = y(matching%settings%mlm_nmaxMEjets)
    call KTRECO (1, PP, n_jets_PS, ECUT, ycut, ycut, P_JETS, JET, &
                 NJET, NSUB, *999)
  end if

  ! !Sample of code for a FastJet interface
  ! palg = 1d0           ! 1.0d0 = kt, 0.0d0 = Cam/Aachen, -1.0d0 = anti-kt
  ! R = 0.7_double      ! radius parameter

```

```

! f = 0.75_double      ! overlap threshold
! !call fastjetppgenkt(PP,n,R,palg,P_JETS,NJET)      ! KT-Algorithm
! !call fastjetsiscone(PP,n,R,f,P_JETS,NJET)         ! SiSCone-Algorithm

if (NJET > 0) then
  allocate (matching%JETS_PS(1:NJET))
  do i = 1, NJET
    matching%JETS_PS(i) = vector4_moving (REAL(P_JETS(4,i), default), &
      vector3_moving([REAL(P_JETS(1,i), default), &
        REAL(P_JETS(2,i), default), REAL(P_JETS(3,i), default)]))
  end do
end if

deallocate (P_JETS)
deallocate (JET)
deallocate (Y)
else
  n_jets_PS_atycut = 0
end if

<Set imode for lepton or hadron collisions>≡
if (matching%is_hadron_collision) then
  imode = matching%settings%kt_imode_hadronic
else
  imode = matching%settings%kt_imode_leptonic
end if

<Veto: too many or not enough jets after PS>≡
if (n_jets_PS_atycut < n_jets_ME) then
  ! print *, "DISCARDING: Not enough PS jets: ", n_jets_PS_atycut
  return
end if
if (n_jets_PS_atycut > n_jets_ME .and. n_jets_ME /= matching%settings%mlm_nmaxMEjets) then
  ! print *, "DISCARDING: Too many PS jets: ", n_jets_PS_atycut
  return
end if

<Cluster ME jets with PS jets one at a time>≡
if (allocated(matching%JETS_PS)) then
  ! print *, "number of jets after PS: ", size(matching%JETS_PS)
  n_jets_PS = size (matching%JETS_PS)
else
  n_jets_PS = 0
end if
if (n_jets_ME > 0 .and. n_jets_PS > 0) then
  n_jets_PS = size (matching%JETS_PS)
  if (allocated (PP)) deallocate(PP)
  allocate (PP(1:4, 1:n_jets_PS + 1))
  do i = 1, n_jets_PS
    if (signal_is_pending ()) return
    PP(1:3,i) = matching%JETS_PS(i)%p(1:3)
    PP(4,i) = matching%JETS_PS(i)%p(0)
  end do
  if (allocated (Y)) deallocate(Y)
  allocate (Y(1:n_jets_PS + 1))
  y = zero

```

```

do i = 1, n_jets_ME
  PP(1:3,n_jets_PS + 2 - i) = matching%JETS_ME(i)%p(1:3)
  PP(4,n_jets_PS + 2 - i) = matching%JETS_ME(i)%p(0)
  !!! This makes more sense than hardcoding
  ! call KTCLUS (4313, PP, (n_jets_PS + 2 - i), 1.0_double, Y, *999)
  call KTCLUR (imode, PP, (n_jets_PS + 2 - i), &
    dble (matching%settings%mlm_Rclusfactor * matching%settings%mlm_Rmin), &
    ECUT, y, *999)
  if (0.99 * y(n_jets_PS + 1 - (i - 1)).gt.ycut) then
    ! print *, "DISCARDING: Jet ", i, " not clusterd"
    return
  end if
  !!! search for and remove PS jet clustered with ME Jet
  ip1 = HIST(n_jets_PS + 2 - i) / NMAX
  ip2 = mod(hist(n_jets_PS + 2 - i), NMAX)
  if ((ip2 /= n_jets_PS + 2 - i) .or. (ip1 <= 0)) then
    ! print *, "DISCARDING: Jet ", i, " not clustered ", ip1, ip2, &
    !       hist(n_jets_PS + 2 - i)
    return
  else
    ! print *, "PARTON clustered", ip1, ip2, hist(n_jets_PS + 2 - i)
    PP(:,IP1) = zero
    do j = IP1, n_jets_PS - i
      PP(:, j) = PP(:,j + 1)
    end do
  end if
end do
end if

```

31.3 CKKW matching

This module contains the CKKW matching.

The type `ckkw_pseudo_shower_weights_t` gives the (relative) weights for different clusterings of the final particles, as given in Eq. (2.7) of hep-ph/0503281v1. Each particle has a binary labelling (power of 2) (first particle = 1, second particle = 2, third particle = 4, ...). Each recombination therefore corresponds to an integer, that is not a power of 2. For multiple subsequent recombinations, no different weights for different sequences of clustering are stored. It is assumed that the weight of a multiply recombined state is a combination of the states with one fewer recombination and that these states' contributions are proportional to their weights. For a $2 - > n$ event, the weights array thus has the size $2^{(2+n)-1}$. The `weights_by_type` array gives the weights depending on the type of the particle, the first index is the same as for weights, the second index gives the type of the new mother particle:

- 0: uncolored (γ , Z , W , Higgs)
- 1: colored (quark)
- 2: gluon
- 3: squark

4: gluino

`alphaS` gives the value for α_s used in the generation of the matrix element. This is needed for the reweighting using the values for a running α_s at the scales of the clusterings.

```

<ckkw_matching.f90>≡
  <File header>

  module ckkw_matching

    <Use kinds with double>
    <Use strings>
    <Use debug>
    use io_units
    use constants
    use format_utils, only: write_separator
    use diagnostics
    use physics_defs
    use lorentz
    use particles
    use rng_base
    use shower_base
    use shower_partons
    use shower_core
    use variables
    use matching_base

    <Standard module head>

    <CKKW matching: public>

    <CKKW matching: types>

    contains

    <CKKW matching: procedures>

  end module ckkw_matching

```

The fundamental CKKW matching parameter are defined here:

```

<CKKW matching: public>≡
  public :: ckkw_matching_settings_t
<CKKW matching: types>≡
  type :: ckkw_matching_settings_t
    real(default) :: alphaS = 0.118_default
    real(default) :: Qmin = one
    integer :: n_max_jets = 0
  contains
    <CKKW matching: ckkw matching settings: TBP>
  end type ckkw_matching_settings_t

```

This is empty for the moment.

```

<CKKW matching: ckkw matching settings: TBP>≡
  procedure :: init => ckkw_matching_settings_init

```

```

<CKKW matching: procedures>≡
  subroutine ckkw_matching_settings_init (settings, var_list)
    class(ckkw_matching_settings_t), intent(out) :: settings
    type(var_list_t), intent(in) :: var_list
    settings%alphaS = 1.0_default
    settings%Qmin = 1.0_default
    settings%n_max_jets = 3
  end subroutine ckkw_matching_settings_init

<CKKW matching: ckkw matching settings: TBP>+≡
  procedure :: write => ckkw_matching_settings_write

<CKKW matching: procedures>+≡
  subroutine ckkw_matching_settings_write (settings, unit)
    class(ckkw_matching_settings_t), intent(in) :: settings
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1x,A)") "CKKW matching settings:"
    call write_separator (u)
    write (u, "(3x,A,1x,ES19.12)") &
      "alphaS      = ", settings%alphaS
    write (u, "(3x,A,1x,ES19.12)") &
      "Qmin        = ", settings%Qmin
    write (u, "(3x,A,1x,I0)") &
      "n_max_jets  = ", settings%n_max_jets
  end subroutine ckkw_matching_settings_write

<CKKW matching: public>+≡
  public :: ckkw_pseudo_shower_weights_t

<CKKW matching: types>+≡
  type :: ckkw_pseudo_shower_weights_t
    real(default) :: alphaS
    real(default), dimension(:), allocatable :: weights
    real(default), dimension(:,:), allocatable :: weights_by_type
  contains
    <CKKW matching: ckkw pseudo shower weights: TBP>
  end type ckkw_pseudo_shower_weights_t

<CKKW matching: ckkw pseudo shower weights: TBP>≡
  procedure :: init => ckkw_pseudo_shower_weights_init

<CKKW matching: procedures>+≡
  subroutine ckkw_pseudo_shower_weights_init (weights)
    class(ckkw_pseudo_shower_weights_t), intent(out) :: weights
    weights%alphaS = zero
  end subroutine ckkw_pseudo_shower_weights_init

<CKKW matching: ckkw pseudo shower weights: TBP>+≡
  procedure :: write => ckkw_pseudo_shower_weights_write

```

```

<CKKW matching: procedures>+≡
subroutine ckkw_pseudo_shower_weights_write (weights, unit)
  class(ckkw_pseudo_shower_weights_t), intent(in) :: weights
  integer, intent(in), optional :: unit
  integer :: s, i, u
  u = given_output_unit (unit); if (u < 0) return
  s = size (weights%weights)
  write (u, "(1x,A)") "CKKW (pseudo) shower weights: "
  do i = 1, s
    write (u, "(3x,I0,2(ES19.12))") i, weights%weights(i), &
      weights%weights_by_type(i,:)
  end do
  write (u, "(3x,A,1x,I0)") "alphaS =", weights%alphaS
end subroutine ckkw_pseudo_shower_weights_write

```

Generate fake ckkw weights. This can be dropped, once information from the matrix element generation is available.

```

<CKKW matching: ckkw pseudo shower weights: TBP>+≡
procedure :: fake => ckkw_pseudo_shower_weights_fake

<CKKW matching: procedures>+≡
pure subroutine ckkw_pseudo_shower_weights_fake (weights, particle_set)
  class(ckkw_pseudo_shower_weights_t), intent(inout) :: weights
  type(particle_set_t), intent(in) :: particle_set
  integer :: i, j, n
  type(vector4_t) :: momentum
  n = 2**particle_set%n_tot
  if (allocated (weights%weights)) then
    deallocate (weights%weights)
  end if
  allocate (weights%weights (1:n))
  do i = 1, n
    momentum = vector4_null
    do j = 1, particle_set%n_tot
      if (btest (i,j-1)) then
        momentum = momentum + particle_set%prt(j)%p
      end if
    end do
    if (momentum**1 > 0.0) then
      weights%weights(i) = 1.0 / (momentum**2)
    end if
  end do
  ! equally distribute the weights by type
  if (allocated (weights%weights_by_type)) then
    deallocate (weights%weights_by_type)
  end if
  allocate (weights%weights_by_type (1:n, 0:4))
  do i = 1, n
    do j = 0, 4
      weights%weights_by_type(i,j) = 0.2 * weights%weights(i)
    end do
  end do
end subroutine ckkw_pseudo_shower_weights_fake

```

```

<CKKW matching: public>+≡
  public :: ckkw_matching_t

<CKKW matching: types>+≡
  type, extends (matching_t) :: ckkw_matching_t
  type(ckkw_matching_settings_t) :: settings
  type(ckkw_pseudo_shower_weights_t) :: weights
  contains
    <CKKW matching: ckkw matching: TBP>
  end type ckkw_matching_t

<CKKW matching: ckkw matching: TBP>≡
  procedure :: init => ckkw_matching_init

<CKKW matching: procedures>+≡
  subroutine ckkw_matching_init (matching, var_list, process_name)
    class(ckkw_matching_t), intent(out) :: matching
    <default matching init>
  end subroutine ckkw_matching_init

<CKKW matching: ckkw matching: TBP>+≡
  procedure :: write => ckkw_matching_write

<CKKW matching: procedures>+≡
  subroutine ckkw_matching_write (matching, unit)
    class(ckkw_matching_t), intent(in) :: matching
    integer, intent(in), optional :: unit
    call matching%settings%write (unit)
    call matching%weights%write (unit)
  end subroutine ckkw_matching_write

<CKKW matching: ckkw matching: TBP>+≡
  procedure :: get_method => ckkw_matching_get_method

<CKKW matching: procedures>+≡
  function ckkw_matching_get_method (matching) result (method)
    type(string_t) :: method
    class(ckkw_matching_t), intent(in) :: matching
    method = matching_method (MATCH_CKKW)
  end function ckkw_matching_get_method

<CKKW matching: ckkw matching: TBP>+≡
  procedure :: before_shower => ckkw_matching_before_shower

<CKKW matching: procedures>+≡
  subroutine ckkw_matching_before_shower &
    (matching, particle_set, vetoed)
    class(ckkw_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(inout) :: particle_set
    logical, intent(out) :: vetoed
    call matching%weights%init ()
    call matching%weights%fake (particle_set)
    select type (shower => matching%shower)
    type is (shower_t)

```



```

        call ckkw_matching_apply (shower%partons, &
            matching%settings, &
            matching%weights, matching%rng, vetoed)
    class default
        call msg_bug ("CKKW matching only works with WHIZARD shower.")
    end select
end subroutine ckkw_matching_before_shower

```

<CKKW matching: public>+≡

```
public :: ckkw_matching_apply
```

<CKKW matching: procedures>+≡

```

subroutine ckkw_matching_apply (partons, settings, weights, rng, vetoed)
    type(parton_pointer_t), dimension(:), intent(inout), allocatable :: &
        partons
    type(ckkw_matching_settings_t), intent(in) :: settings
    type(ckkw_pseudo_shower_weights_t), intent(in) :: weights
    class(rng_t), intent(inout), allocatable :: rng
    logical, intent(out) :: vetoed

    real(default), dimension(:), allocatable :: scales
    real(double) :: weight, sf
    real(default) :: rand
    integer :: i, n_partons

    if (signal_is_pending ()) return
    weight = one

    n_partons = size (partons)

    do i = 1, n_partons
        call partons(i)%p%write ()
    end do

    !!! the pseudo parton shower is already simulated by shower_add_interaction
    !!! get the respective clustering scales
    allocate (scales (1:n_partons))
    do i = 1, n_partons
        if (.not. associated (partons(i)%p)) cycle
        if (partons(i)%p%type == INTERNAL) then
            scales(i) = two * min (partons(i)%p%child1%momentum%p(0), &
                partons(i)%p%child2%momentum%p(0))**2 * &
                (1.0 - (space_part (partons(i)%p%child1%momentum) * &
                    space_part (partons(i)%p%child2%momentum)) / &
                (space_part (partons(i)%p%child1%momentum)**1 * &
                    space_part (partons(i)%p%child2%momentum)**1))
            scales(i) = sqrt (scales(i))
            partons(i)%p%ckkwscale = scales(i)
            print *, scales(i)
        end if
    end do

    print *, " scales finished"
    !!! if (highest multiplicity) -> reweight with PDF(mu_F) / PDF(mu_cut)

```

```

do i = 1, n_partons
  call partons(i)%p%write ()
end do

!!! Reweight and possibly veto the whole event

!!! calculate the relative alpha_S weight

!! calculate the Sudakov weights for internal lines
!! calculate the Sudakov weights for external lines
do i = 1, n_partons
  if (signal_is_pending ()) return
  if (.not. associated (partons(i)%p)) cycle
  if (partons(i)%p%type == INTERNAL) then
    !!! get type
    !!! check that all particles involved are colored
    if ((partons(i)%p%is_colored () .or. &
      partons(i)%p%ckkwtype > 0) .and. &
      (partons(i)%p%child1%is_colored () .or. &
      partons(i)%p%child1%ckkwtype > 0) .and. &
      (partons(i)%p%child1%is_colored () .or. &
      partons(i)%p%child1%ckkwtype > 0)) then
      print *, "reweight with alphaS(" , partons(i)%p%ckkwscale, &
        ") for particle ", partons(i)%p%nr
      if (partons(i)%p%belongstoFSR) then
        print *, "FSR"
        weight = weight * D_alpha_s_fsr (partons(i)%p%ckkwscale**2, &
          partons(i)%p%settings) / settings%alphas
      else
        print *, "ISR"
        weight = weight * &
          D_alpha_s_isr (partons(i)%p%ckkwscale**2, &
          partons(i)%p%settings) / settings%alphas
      end if
    else
      print *, "no reweight with alphaS for ", partons(i)%p%nr
    end if
  if (partons(i)%p%child1%type == INTERNAL) then
    print *, "internal line from ", &
      partons(i)%p%child1%ckkwscale, &
      " to ", partons(i)%p%ckkwscale, &
      " for type ", partons(i)%p%child1%ckkwtype
    if (partons(i)%p%child1%ckkwtype == 0) then
      sf = 1.0
    else if (partons(i)%p%child1%ckkwtype == 1) then
      sf = SudakovQ (partons(i)%p%child1%ckkwscale, &
        partons(i)%p%ckkwscale, &
        partons(i)%p%settings, .true., rng)
      print *, "SFQ = ", sf
    else if (partons(i)%p%child1%ckkwtype == 2) then
      sf = SudakovG (partons(i)%p%child1%ckkwscale, &
        partons(i)%p%ckkwscale, &
        partons(i)%p%settings, .true., rng)
      print *, "SFG = ", sf
    end if
  end if
end do

```

```

else
  print *, "SUSY not yet implemented"
end if
weight = weight * min (one, sf)
else
  print *, "external line from ", settings%Qmin, &
    partons(i)%p%ckkwscale
  if (partons(i)%p%child1%is_quark ()) then
    sf = SudakovQ (settings%Qmin, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFQ = ", sf
  else if (partons(i)%p%child1%is_gluon ()) then
    sf = SudakovG (settings%Qmin, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFG = ", sf
  else
    print *, "not yet implemented (", &
      partons(i)%p%child2%type, ")"
    sf = one
  end if
  weight = weight * min (one, sf)
end if
if (partons(i)%p%child2%type == INTERNAL) then
  print *, "internal line from ", partons(i)%p%child2%ckkwscale, &
    " to ", partons(i)%p%ckkwscale, &
    " for type ", partons(i)%p%child2%ckkwtype
  if (partons(i)%p%child2%ckkwtype == 0) then
    sf = 1.0
  else if (partons(i)%p%child2%ckkwtype == 1) then
    sf = SudakovQ (partons(i)%p%child2%ckkwscale, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFQ = ", sf
  else if (partons(i)%p%child2%ckkwtype == 2) then
    sf = SudakovG (partons(i)%p%child2%ckkwscale, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFG = ", sf
  else
    print *, "SUSY not yet implemented"
  end if
  weight = weight * min (one, sf)
else
  print *, "external line from ", settings%Qmin, &
    partons(i)%p%ckkwscale
  if (partons(i)%p%child2%is_quark ()) then
    sf = SudakovQ (settings%Qmin, &
      partons(i)%p%ckkwscale, &
      partons(i)%p%settings, .true., rng)
    print *, "SFQ = ", sf
  else if (partons(i)%p%child2%is_gluon ()) then
    sf = SudakovG (settings%Qmin, &

```

```

        partons(i)%p%ckkwscale, &
        partons(i)%p%settings, .true., rng)
    print *, "SFG = ", sf
else
    print *, "not yet implemented (", &
        partons(i)%p%child2%type, ")"
    sf = one
end if
weight = weight * min (one, sf)
end if
end if
end do

call rng%generate (rand)

print *, "final weight: ", weight

!!!!!!! WRONG
vetoed = .false.
! vetoed = (rand > weight)
if (vetoed) then
    return
end if

!!! finally perform the parton shower
!!! veto emissions that are too hard

deallocate (scales)
end subroutine ckkw_matching_apply

<CKKW matching: ckkw matching: TBP>+≡
    procedure :: after_shower => ckkw_matching_after_shower

<CKKW matching: procedures>+≡
    subroutine ckkw_matching_after_shower (matching, particle_set, vetoed)
        class(ckkw_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
        vetoed = .false.
    end subroutine ckkw_matching_after_shower

<CKKW matching: procedures>+≡
    function GammaQ (smallq, largeq, settings, fsr) result (gamma)
        real(default), intent(in) :: smallq, largeq
        type(shower_settings_t), intent(in) :: settings
        logical, intent(in) :: fsr
        real(default) :: gamma
        gamma = (8._default / three) / (pi * smallq)
        gamma = gamma * (log(largeq / smallq) - 0.75)
        if (fsr) then
            gamma = gamma * D_alpha_s_fsr (smallq**2, settings)
        else
            gamma = gamma * D_alpha_s_isr (smallq**2, settings)
        end if
    end function

```

```
end function GammaQ
```

<CKKW matching: procedures>+≡

```
function GammaG (smallq, largeq, settings, fsr) result (gamma)
  real(default), intent(in) :: smallq, largeq
  type(shower_settings_t), intent(in) :: settings
  logical, intent(in) :: fsr
  real(default) :: gamma
  gamma = 6._default / (pi * smallq)
  gamma = gamma * ( log(largeq / smallq) - 11.0 / 12.0)
  if (fsr) then
    gamma = gamma * D_alpha_s_fsr (smallq**2, settings)
  else
    gamma = gamma * D_alpha_s_isr (smallq**2, settings)
  end if
end function GammaG
```

<CKKW matching: procedures>+≡

```
function GammaF (smallq, settings, fsr) result (gamma)
  real(default), intent(in) :: smallq
  type(shower_settings_t), intent(in) :: settings
  logical, intent(in) :: fsr
  real(default) :: gamma
  gamma = number_of_flavors (smallq, settings%max_n_flavors, &
    settings%min_virtuality) / (three * pi * smallq)
  if (fsr) then
    gamma = gamma * D_alpha_s_fsr (smallq**2, settings)
  else
    gamma = gamma * D_alpha_s_isr (smallq**2, settings)
  end if
end function GammaF
```

<CKKW matching: procedures>+≡

```
function SudakovQ (Q1, Q, settings, fsr, rng) result (sf)
  real(default), intent(in) :: Q1, Q
  type(shower_settings_t), intent(in) :: settings
  class(rng_t), intent(inout), allocatable :: rng
  logical, intent(in) :: fsr
  real(default) :: sf
  real(default) :: integral
  integer, parameter :: NTRIES = 100
  integer :: i
  real(default) :: rand
  integral = zero
  do i = 1, NTRIES
    call rng%generate (rand)
    integral = integral + GammaQ (Q1 + rand * (Q - Q1), Q, settings, fsr)
  end do
  integral = integral / NTRIES
  sf = exp (-integral)
end function SudakovQ
```

```

⟨CKKW matching: procedures⟩+≡
function SudakovG (Q1, Q, settings, fsr, rng) result (sf)
  real(default), intent(in) :: Q1, Q
  type(shower_settings_t), intent(in) :: settings
  logical, intent(in) :: fsr
  real(default) :: sf
  real(default) :: integral
  class(rng_t), intent(inout), allocatable :: rng
  integer, parameter :: NTRIES = 100
  integer :: i
  real(default) :: rand
  integral = zero
  do i = 1, NTRIES
    call rng%generate (rand)
    integral = integral + &
      GammaG (Q1 + rand * (Q - Q1), Q, settings, fsr) + &
      GammaF (Q1 + rand * (Q - Q1), settings, fsr)
  end do
  integral = integral / NTRIES
  sf = exp (-integral)
end function SudakovG

```

31.4 POWHEG

This module generates radiation according to the POWHEG Sudakov form factor

$$\Delta^{f_b}(\Phi_n, p_T) = \prod_{\alpha_r \in \{\alpha_r | f_b\}} \Delta_{\alpha_r}^{f_b}(\Phi_n, p_T), \quad (31.1)$$

with

$$\Delta_{\alpha_r}^{f_b}(\Phi_n, p_T) = \exp \left\{ - \left[\int d\Phi_{\text{rad}} \frac{R(\Phi_{n+1})}{B^{f_b}(\Phi_n)} \theta(k_T(\Phi_{n+1}) - p_T) \right]_{\alpha_r}^{\tilde{\Phi}_n^{\alpha_r} = \Phi_n} \right\} \quad (31.2)$$

We expect that an underlying Born flavor structure f_b has been generated with a probability proportional to its contribution to the \tilde{B} at the given kinematic point.

```

⟨powheg_matching.f90⟩≡
⟨File header⟩

module powheg_matching

  use, intrinsic :: iso_fortran_env

  ⟨Use kinds⟩
  ⟨Use strings⟩
  ⟨Use debug⟩
  use diagnostics
  use constants, only: ZERO, ONE, TWO, THREE, FOUR, FIVE, TINY_07, PI, TWOPI
  use numeric_utils
  use io_units, only: given_output_unit, free_unit

```

```

use format_utils, only: write_separator
use format_defs, only: FMT_16, FMT_19
use string_utils, only: str
use os_interface, only: os_file_exist
use physics_defs, only: CA, BORN, NLO_REAL
use lorentz
use phs_points, only: assignment(=), operator(*)
use sm_qcd, only: qcd_t, alpha_qcd_from_scale_t, alpha_qcd_from_lambda_t
use sm_physics, only: Li2
use subevents, only: PRT_INCOMING, PRT_OUTGOING
use colors
use particles
use grids
use solver
use rng_base
use variables
use process_config, only: COMP_REAL_FIN

use phs_fks, only: phs_fks_generator_t, compute_dalitz_bounds, beta_emitter
use phs_fks, only: phs_point_set_t, phs_identifier_t, phs_fks_t
use phs_fks, only: I_XI, I_Y, UBF_FSR_SIMPLE, UBF_FSR_MASSIVE, UBF_FSR_MASSLESS_RECOIL
use matching_base
use instances, only: process_instance_t, process_instance_hook_t
use pcm, only: pcm_nlo_t, pcm_nlo_workspace_t
<Use mpi f08>

<Standard module head>

<POWHEG matching: public>

<POWHEG matching: parameters>

<POWHEG matching: types>

<POWHEG matching: interfaces>

contains

<POWHEG matching: procedures>

end module powheg_matching

```

31.4.1 Base types for settings and data

λ enters for now as the lowest scale $2\Lambda^{(5)}_{\text{MS}}$ where the radiation α_s^{rad} is still larger than the true α_s .

```

<POWHEG matching: public>≡
    public :: powheg_settings_t

<POWHEG matching: types>≡
    type :: powheg_settings_t
        real(default) :: pt2_min = zero
        real(default) :: lambda = zero
        integer :: size_grid_xi = 0

```

```

        integer :: size_grid_y = 0
        integer :: upper_bound_func_type = UBF_FSR_SIMPLE
        logical :: test_sudakov = .false.
        logical :: disable_sudakov = .false.
        logical :: singular_jacobian = .false.
contains
    <POWHEG matching: powheg settings: TBP>
end type powheg_settings_t

<POWHEG matching: powheg settings: TBP>≡
    procedure :: init => powheg_settings_init

<POWHEG matching: procedures>≡
    subroutine powheg_settings_init (settings, var_list)
        class(powheg_settings_t), intent(out) :: settings
        type(var_list_t), intent(in) :: var_list
        settings%pt2_min = &
            var_list%get_rval (var_str ("powheg_pt_min"))**2
        settings%size_grid_xi = &
            var_list%get_ival (var_str ("powheg_grid_size_xi"))
        settings%size_grid_y = &
            var_list%get_ival (var_str ("powheg_grid_size_y"))
        settings%lambda = var_list%get_rval (var_str ("powheg_lambda"))
        settings%singular_jacobian = &
            var_list%get_lval (var_str ("?powheg_use_singular_jacobian"))
        settings%test_sudakov = &
            var_list%get_lval (var_str ("?powheg_test_sudakov"))
        settings%disable_sudakov = &
            var_list%get_lval (var_str ("?powheg_disable_sudakov"))
    end subroutine powheg_settings_init

<POWHEG matching: powheg settings: TBP>+≡
    procedure :: write => powheg_settings_write

<POWHEG matching: procedures>+≡
    subroutine powheg_settings_write (powheg_settings, unit)
        class(powheg_settings_t), intent(in) :: powheg_settings
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1X,A)") "POWHEG settings:"
        write (u, "(3X,A," // FMT_16 //)") "pt2_min = ", powheg_settings%pt2_min
        write (u, "(3X,A," // FMT_16 //)") "lambda = ", powheg_settings%lambda
        write (u, "(3X,A,I12)") "size_grid_xi = ", powheg_settings%size_grid_xi
        write (u, "(3X,A,I12)") "size_grid_y = ", powheg_settings%size_grid_y
        write (u, "(3X,A,I12)") "upper_bound_func_type = ", powheg_settings%upper_bound_func_type
    end subroutine powheg_settings_write

<POWHEG matching: public>+≡
    public :: radiation_t

<POWHEG matching: types>+≡
    type :: radiation_t
        real(default) :: xi, y, phi, pt2

```



```

        integer :: alr
        logical :: valid = .false.
contains
<POWHEG matching: radiation: TBP>
end type radiation_t

<POWHEG matching: radiation: TBP>≡
    procedure :: write => radiation_write
<POWHEG matching: procedures>+≡
    subroutine radiation_write (radiation, unit)
        class(radiation_t), intent(in) :: radiation
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1X, A)") "Radiation:"
        write (u, "(3X, A," // FMT_16 // ")") "xi = ", radiation%xi
        write (u, "(3X, A," // FMT_16 // ")") "y = ", radiation%y
        write (u, "(3X, A," // FMT_16 // ")") "phi = ", radiation%phi
        write (u, "(3X, A," // FMT_16 // ")") "pt2 = ", radiation%pt2
        write (u, "(3X, A, I12)") "alr = ", radiation%alr
    end subroutine radiation_write

lambda2_gen is the scale used in the (log integrated) upper bounding functions.
It is not equivalent to lambda which is the reference scale for the  $\alpha_s$  evolution.

<POWHEG matching: public>+≡
    public :: process_deps_t
<POWHEG matching: types>+≡
    type :: process_deps_t
        real(default) :: lambda2_gen, sqrts
        integer :: n_alr
        logical :: lab_is_cm = .true.
        type(phs_identifier_t), dimension(:), allocatable :: phs_identifiers
        integer, dimension(:), allocatable :: alr_to_i_phs
        integer :: i_born
        integer, dimension(:), allocatable :: i_real
contains
    <POWHEG matching: process deps: TBP>
end type process_deps_t

<POWHEG matching: process deps: TBP>≡
    procedure :: write => process_deps_write
<POWHEG matching: procedures>+≡
    subroutine process_deps_write (process_deps, unit)
        class(process_deps_t), intent(in) :: process_deps
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        write (u, "(1X,A)") "Process dependencies:"
        write (u, "(3X,A," // FMT_19 // ")") "lambda2_gen = ", process_deps%lambda2_gen
        write (u, "(3X,A, I12)") "n_alr = ", process_deps%n_alr
    end subroutine process_deps_write

```

```

<POWHEG matching: public>+≡
  public :: event_deps_t
<POWHEG matching: types>+≡
  type :: event_deps_t
    real(default) :: s_hat
    type(phs_point_set_t) :: p_born_cms
    type(phs_point_set_t) :: p_born_lab
    type(phs_point_set_t) :: p_real_cms
    type(phs_point_set_t) :: p_real_lab
    real(default) :: sqme_born
  contains
    <POWHEG matching: event deps: TBP>
  end type event_deps_t

<POWHEG matching: event deps: TBP>≡
  procedure :: write => event_deps_write
<POWHEG matching: procedures>+≡
  subroutine event_deps_write (event_deps, unit)
    class(event_deps_t), intent(in) :: event_deps
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(1X,A)") "Event dependencies:"
    write (u, "(3X,A," // FMT_19 // ")") "s_hat = ", event_deps%s_hat
    write (u, "(3X,A," // FMT_19 // ")") "sqme_born = ", event_deps%sqme_born
  end subroutine event_deps_write

<POWHEG matching: event deps: TBP>+≡
  procedure :: update => event_deps_update
<POWHEG matching: procedures>+≡
  subroutine event_deps_update (event_deps, sqme_born, p_born, lt_lab_to_cms)
    class(event_deps_t), intent(inout) :: event_deps
    real(default), intent(in) :: sqme_born
    type(vector4_t), dimension(:), intent(in) :: p_born
    type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
    integer :: n_born
    event_deps%sqme_born = sqme_born
    n_born = size (p_born)
    if (debug_active (D_MATCHING)) then
      if (n_born /= event_deps%p_born_lab%get_n_particles (1)) then
        call msg_fatal &
          ("event_deps_update: number of born momenta has changed")
      end if
    end if
    call event_deps%p_born_lab%set_momenta (1, p_born)
    call event_deps%set_cms (lt_lab_to_cms)
  end subroutine event_deps_update

```

This has to be changed when we have sorted out the handling of ISR, partonic vs hadronic cms as well as decays in POWHEG:

```

<POWHEG matching: event deps: TBP>+≡
  procedure :: set_cms => event_deps_set_cms

```

```

<POWHEG matching: procedures>+≡
subroutine event_deps_set_cms (event_deps, lt_lab_to_cms)
  class(event_deps_t), intent(inout) :: event_deps
  type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
  associate (pp => event_deps%p_born_lab%phs_point(1))
    event_deps%s_hat = pp%get_msq ([1,2])
    if (present (lt_lab_to_cms)) then
      event_deps%p_born_cms%phs_point(1) = lt_lab_to_cms * pp
    else
      event_deps%p_born_cms%phs_point(1) = pp
    end if
  end associate
end subroutine event_deps_set_cms

```

```

<POWHEG matching: types>+≡
type :: veto_counter_t
  integer :: n_ubf = 0
  integer :: n_first_fail = 0
  integer :: n_alpha_s = 0
  integer :: n_xi_max = 0
  integer :: n_norm = 0
  integer :: n_sqme = 0
  integer :: n_veto_ubf = 0
  integer :: n_veto_alpha_s = 0
  integer :: n_veto_xi_max = 0
  integer :: n_veto_norm = 0
  integer :: n_veto_sqme = 0
  integer :: n_fail_ubf = 0
contains
  <POWHEG matching: veto counter: TBP>
end type veto_counter_t

```

```

<POWHEG matching: veto counter: TBP>≡
procedure :: record_ubf => veto_counter_record_ubf

```

```

<POWHEG matching: procedures>+≡
pure subroutine veto_counter_record_ubf (counter, vetoed)
  class(veto_counter_t), intent(inout) :: counter
  logical, intent(in) :: vetoed
  counter%n_ubf = counter%n_ubf + 1
  if (vetoed) counter%n_veto_ubf = counter%n_veto_ubf + 1
end subroutine veto_counter_record_ubf

```

```

<POWHEG matching: veto counter: TBP>+≡
procedure :: record_first_fail => veto_counter_record_first_fail

```

```

<POWHEG matching: procedures>+≡
subroutine veto_counter_record_first_fail (counter)
  class(veto_counter_t), intent(inout) :: counter
  counter%n_first_fail = counter%n_first_fail + 1
end subroutine veto_counter_record_first_fail

```

```

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_alpha_s => veto_counter_record_alpha_s

<POWHEG matching: procedures>+≡
  subroutine veto_counter_record_alpha_s (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
    counter%n_alpha_s = counter%n_alpha_s + 1
    if (vetoed) counter%n_veto_alpha_s = counter%n_veto_alpha_s + 1
  end subroutine veto_counter_record_alpha_s

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_xi_max => veto_counter_record_xi_max

<POWHEG matching: procedures>+≡
  subroutine veto_counter_record_xi_max (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
    counter%n_xi_max = counter%n_xi_max + 1
    if (vetoed) counter%n_veto_xi_max = counter%n_veto_xi_max + 1
  end subroutine veto_counter_record_xi_max

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_norm => veto_counter_record_norm

<POWHEG matching: procedures>+≡
  subroutine veto_counter_record_norm (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
    counter%n_norm = counter%n_norm + 1
    if (vetoed) counter%n_veto_norm = counter%n_veto_norm + 1
  end subroutine veto_counter_record_norm

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_sqme => veto_counter_record_sqme

<POWHEG matching: procedures>+≡
  subroutine veto_counter_record_sqme (counter, vetoed)
    class(veto_counter_t), intent(inout) :: counter
    logical, intent(in) :: vetoed
    counter%n_sqme = counter%n_sqme + 1
    if (vetoed) counter%n_veto_sqme = counter%n_veto_sqme + 1
  end subroutine veto_counter_record_sqme

<POWHEG matching: veto counter: TBP>+≡
  procedure :: record_ubf_fail => veto_counter_record_ubf_fail

<POWHEG matching: procedures>+≡
  subroutine veto_counter_record_ubf_fail (counter)
    class(veto_counter_t), intent(inout) :: counter
    counter%n_fail_ubf = counter%n_fail_ubf + 1
  end subroutine veto_counter_record_ubf_fail

```

This routine fills the POWHEG veto log file with content showing how many events have been vetoed in which step of the sudakov veto algorithm.

```

<POWHEG matching: veto counter: TBP>+≡
  procedure :: write => veto_counter_write

<POWHEG matching: procedures>+≡
  subroutine veto_counter_write (counter, unit)
    class(veto_counter_t), intent(in) :: counter
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(A29,I10)") "Nr. of ubf-veto calls: ", counter%n_ubf
    write (u, "(A29,I10)") "Nr. of ubf-vetos: ", counter%n_veto_ubf
    if (counter%n_ubf > 0) &
      write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
        one * counter%n_veto_ubf / counter%n_ubf * 100, "%"
    call write_separator (u)

    write (u, "(A29,I10)") "Nr. of alpha_s-veto calls: ", counter%n_alpha_s
    write (u, "(A29,I10)") "Nr. of alpha_s-vetos: ", counter%n_veto_alpha_s
    if (counter%n_alpha_s > 0) &
      write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
        one * counter%n_veto_alpha_s / counter%n_alpha_s * 100, "%"
    call write_separator (u)

    write (u, "(A29,I10)") "Nr. of xi_max-veto calls: ", counter%n_xi_max
    write (u, "(A29,I10)") "Nr. of xi_max-vetos: ", counter%n_veto_xi_max
    if (counter%n_alpha_s > 0) &
      write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
        one * counter%n_veto_xi_max / counter%n_xi_max * 100, "%"
    call write_separator (u)

    write (u, "(A29,I10)") "Nr. of norm-veto calls: ", counter%n_norm
    write (u, "(A29,I10)") "Nr. of norm-vetos: ", counter%n_veto_norm
    if (counter%n_norm > 0) &
      write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
        one * counter%n_veto_norm / counter%n_norm * 100, "%"
    call write_separator (u)

    write (u, "(A29,I10)") "Nr. of sqme-veto calls: ", counter%n_sqme
    write (u, "(A29,I10)") "Nr. of sqme-vetos: ", counter%n_veto_sqme
    if (counter%n_sqme > 0) &
      write (u, "(A29,F9.2,A1)") "Fraction of vetoed points: ", &
        one * counter%n_veto_sqme / counter%n_sqme * 100, "%"
    call write_separator (u)
    write (u, "(A29,I10)") "Nr. of upper-bound failures: ", &
      counter%n_fail_ubf
    if (counter%n_sqme > 0) &
      write (u, "(A29,F9.2,A1)") "Fraction of failed points: ", &
        one * counter%n_fail_ubf / counter%n_sqme * 100, "%"
  end subroutine veto_counter_write

```

31.4.2 Upper bounding functions and sudakovs

Abstract version

This contains the pieces that depend on the radiation region α_r

```
<POWHEG matching: public>+≡
  public :: sudakov_t

<POWHEG matching: types>+≡
  type, abstract, extends (solver_function_t) :: sudakov_t
    type(process_deps_t), pointer :: process_deps => null()
    type(event_deps_t), pointer :: event_deps => null()
    type(powheg_settings_t), pointer :: powheg_settings => null()
    type(phs_fks_generator_t), pointer :: phs_fks_generator => null()
    type(qcd_t) :: qcd
    class(rng_t), pointer :: rng => null()
    real(default) :: xi2_max = zero
    real(default) :: norm_max = zero
    real(default) :: current_pt2_max = zero
    real(default) :: sum_log_rands = zero
    real(default) :: random = zero
    type(veto_counter_t) :: veto_counter
    integer :: i_phs = 0
  contains
    <POWHEG matching: sudakov: TBP>
  end type sudakov_t

<POWHEG matching: sudakov: TBP>≡
  procedure :: write => sudakov_write

<POWHEG matching: procedures>+≡
  subroutine sudakov_write (sudakov, unit)
    class(sudakov_t), intent(in) :: sudakov
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    write (u, "(3X,A," // FMT_19 // ")") "xi2_max = ", sudakov%xi2_max
    write (u, "(3X,A," // FMT_19 // ")") "norm_max = ", sudakov%norm_max
    write (u, "(3X,A," // FMT_19 // ")") &
      "current_pt2_max = ", sudakov%current_pt2_max
    write (u, "(3X,A," // FMT_19 // ")") "sum_log_rands = ", sudakov%sum_log_rands
    write (u, "(3X,A," // FMT_19 // ")") "random = ", sudakov%random
  end subroutine sudakov_write

To allow for arrays of this class
<POWHEG matching: public>+≡
  public :: sudakov_wrapper_t

<POWHEG matching: types>+≡
  type :: sudakov_wrapper_t
    class(sudakov_t), allocatable :: s
  end type sudakov_wrapper_t

<POWHEG matching: sudakov: TBP>+≡
  procedure :: init => sudakov_init
```

```

<POWHEG matching: procedures>+≡
  subroutine sudakov_init (sudakov, process_deps, event_deps, &
    powheg_settings, qcd, phs_fks_generator, rng)
    class(sudakov_t), intent(out) :: sudakov
    type(process_deps_t), target, intent(in) :: process_deps
    type(event_deps_t), target, intent(in) :: event_deps
    type(powheg_settings_t), target, intent(in) :: powheg_settings
    type(qcd_t), intent(in) :: qcd
    type(phs_fks_generator_t), target, intent(in) :: phs_fks_generator
    class(rng_t), target, intent(in), optional :: rng
    sudakov%process_deps => process_deps
    sudakov%event_deps => event_deps
    sudakov%powheg_settings => powheg_settings
    sudakov%qcd = qcd
    sudakov%phs_fks_generator => phs_fks_generator
    if (present (rng)) sudakov%rng => rng
  end subroutine sudakov_init

```

This has to be done after the grids are initialized.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: set_normalization => sudakov_set_normalization

<POWHEG matching: procedures>+≡
  pure subroutine sudakov_set_normalization (sudakov, norm_max)
    class(sudakov_t), intent(inout) :: sudakov
    real(default), intent(in) :: norm_max
    sudakov%norm_max = norm_max
  end subroutine sudakov_set_normalization

```

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: update_xi2_max => sudakov_update_xi2_max

<POWHEG matching: procedures>+≡
  pure subroutine sudakov_update_xi2_max (sudakov, xi2_max)
    class(sudakov_t), intent(inout) :: sudakov
    real(default), intent(in) :: xi2_max
    sudakov%xi2_max = xi2_max
  end subroutine sudakov_update_xi2_max

```

upper_bound_func does *not* contain the normalization N which is given by the grids. In the notation of 1002.2581, it is thus $\frac{1}{N}U(\xi, y)$

```

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_upper_bound_func), deferred :: upper_bound_func

<POWHEG matching: interfaces>≡
  abstract interface
    pure function sudakov_upper_bound_func (sudakov, xi, y, alpha_s) result (u)
    import
    real(default) :: u
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y, alpha_s
  end function sudakov_upper_bound_func
end interface

```

Similar to the `upper_bound_func`, this is $-\frac{1}{N} \log \Delta(p_T^2)$ where

$$\Delta^{(U)}(p_T) = \exp \left[- \int U(\xi, y) \theta(k_T - p_T) d\xi dy d\phi \right] \quad (31.3)$$

```

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_log_integrated_ubf), deferred :: log_integrated_ubf

<POWHEG matching: interfaces>+≡
  abstract interface
    pure function sudakov_log_integrated_ubf (sudakov, pt2) result (y)
    import
    real(default) :: y
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: pt2
  end function sudakov_log_integrated_ubf
end interface

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_generate_xi_and_y_and_phi), deferred :: generate_xi_and_y_and_phi

<POWHEG matching: interfaces>+≡
  abstract interface
    subroutine sudakov_generate_xi_and_y_and_phi (sudakov, r)
    import
    class(sudakov_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
  end subroutine sudakov_generate_xi_and_y_and_phi
end interface

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_kt2), deferred :: kt2

<POWHEG matching: interfaces>+≡
  abstract interface
    function sudakov_kt2 (sudakov, xi, y) result (kt2)
    import
    real(default) :: kt2
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y
  end function sudakov_kt2
end interface

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_kt2_max), deferred :: kt2_max

<POWHEG matching: interfaces>+≡
  abstract interface
    pure function sudakov_kt2_max (sudakov) result (kt2_max)
    import
    real(default) :: kt2_max
    class(sudakov_t), intent(in) :: sudakov
  end function sudakov_kt2_max
end interface

```


Veto routine for an overestimation of the UBF performed to simplify the log integrated UBF

```

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_reweight_ubf), deferred :: reweight_ubf
<POWHEG matching: interfaces>+≡
  abstract interface
    function sudakov_reweight_ubf (sudakov, pt2) result (accepted)
      import
      logical :: accepted
      class(sudakov_t), intent(inout) :: sudakov
      real(default), intent(in) :: pt2
    end function sudakov_reweight_ubf
  end interface

```

Veto routine to correct for an overestimation of ξ_{\max} performed in the case of massive emitters.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure (sudakov_reweight_xi_max), deferred :: reweight_xi_max
<POWHEG matching: interfaces>+≡
  abstract interface
    function sudakov_reweight_xi_max (sudakov, xi) result (accepted)
      import
      logical :: accepted
      class(sudakov_t), intent(in) :: sudakov
      real(default), intent(in) :: xi
    end function sudakov_reweight_xi_max
  end interface

```

In the generation of p_T^2 via `log_integrated_ubf`, we use the simplified version α_s^{rad} while the grids take the improved version.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: alpha_s => sudakov_alpha_s
<POWHEG matching: procedures>+≡
  function sudakov_alpha_s (sudakov, kT2, use_correct) result (a)
    real(default) :: a
    class(sudakov_t), intent(in) :: sudakov
    real(default), intent(in) :: kT2
    logical, intent(in), optional :: use_correct
    logical :: yorn
    yorn = .false.; if (present (use_correct)) yorn = use_correct
    if (yorn) then
      a = get_alpha (sudakov%qcd, kT2)
    else
      a = sudakov%alpha_s_rad (kT2)
    end if
  end function sudakov_alpha_s

```

To generate the transverse momentum, we have to solve the equation

$$\frac{\Delta^{(U)}(p_T)}{\Delta^{(U)}(p_T^{\max})} = r_1$$

iteratively for p_T . In log space and with initially $\Delta^{(U)}(p_T^{\max}) = 1$, this is

$$\log \Delta^{(U)}(p_T) = \log r_1$$

If no solution is found, we set $p_T = p_T^{\min}$ to exit the event generation loop and generate an emissionless event. If a solution is found but the current emission is not accepted, we set $p_T = p_T^{\max}$ and thus in the next step it is $\Delta^{(U)}(p_T^{\max}) = r_1$, so that we have to solve the equation

$$\log \Delta^{(U)}(p_T) = \log r_1 + \log r_2$$

using another random number r_2 . We use `sum_log_rands` to remember the sum of the logarithms of all previous random numbers used for this event.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: generate_pt2 => sudakov_generate_pt2

<POWHEG matching: procedures>+≡
  function sudakov_generate_pt2 (sudakov) result (pt2)
    real(default) :: pt2
    class(sudakov_t), intent(inout) :: sudakov
    logical :: success
    success = .false.
    if (sudakov%current_pt2_max > sudakov%powheg_settings%pt2_min) then
      call sudakov%rng%generate (sudakov%random)
      sudakov%sum_log_rands = sudakov%sum_log_rands + log(sudakov%random)
      pt2 = solve_interval (sudakov, &
        sudakov%powheg_settings%pt2_min, &
        sudakov%current_pt2_max, success, &
        0.001_default)
    end if
    if (.not. success) then
      pt2 = sudakov%powheg_settings%pt2_min
    end if
  end function sudakov_generate_pt2

```

This could be activated if `(debug_active (MATCHING))`.

```

<POWHEG matching: sudakov: TBP>+≡
  procedure :: check_solution_interval => sudakov_check_solution_interval

<POWHEG matching: procedures>+≡
  subroutine sudakov_check_solution_interval (sudakov)
    class(sudakov_t), intent(inout) :: sudakov
    real(default) :: r
    real(default), parameter :: dr = 0.05
    real(default) :: pt2
    logical :: success
    r = 0._default
    do
      r = r + dr
      sudakov%random = r
      pt2 = solve_interval (sudakov, &
        sudakov%powheg_settings%pt2_min, &
        sudakov%current_pt2_max, success, &
        0.001_default)
    end do
  end subroutine

```

```

    if (success) then
        print *, 'r: ', r, ' zero found'
    else
        print *, 'r: ', r, 'no zero found'
    end if
    if (r >= 1._default) exit
end do
end subroutine sudakov_check_solution_interval

```

Generates the FKS variables (ξ, y, ϕ) and sets the emission hardness scale. In debug mode, we assert that the `pt2` saved in the `radiation_t` and the massive hardness scale are equal. This should hold as we compute `kt2` with the `y` we got from generating `pt2` so that this is a full circle. It then initiates the generation of the transverse momentum followed by a sequence of veto steps to get the correct distribution.

(POWHEG matching: sudakov: TBP)+≡

```

    procedure :: generate_emission => sudakov_generate_emission

```

(POWHEG matching: procedures)+≡

```

subroutine sudakov_generate_emission (sudakov, r)
    class(sudakov_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    logical :: accepted
    sudakov%current_pt2_max = r%pt2
    if (debug_on) call msg_debug2 (D_MATCHING, "sudakov_generate_emission")
    if (debug_on) call msg_debug2 (D_MATCHING, "sqrt (sudakov%current_pt2_max)", &
        sqrt (sudakov%current_pt2_max))
    if (debug_on) call msg_debug2 (D_MATCHING, "sudakov%sum_log_rands", sudakov%sum_log_rands)
    LOOP_UNTIL_ACCEPTED: do
        if (signal_is_pending ()) return
        r%valid = .false.
        r%pt2 = sudakov%generate_pt2 ()
        if (debug_on) call msg_debug2 (D_MATCHING, "sudakov_generate_emission: after generate_pt2")
        if (debug_on) call msg_debug2 (D_MATCHING, "sqrt (r%pt2)", sqrt (r%pt2))
        if (debug_on) call msg_debug2 (D_MATCHING, "sudakov%sum_log_rands", sudakov%sum_log_rands)
        if (r%pt2 <= sudakov%powheg_settings%pt2_min) then
            exit
        end if
        accepted = sudakov%reweight_ubf (r%pt2)
        call sudakov%veto_counter%record_ubf (.not. accepted)
        if (.not. accepted) then
            sudakov%current_pt2_max = r%pt2
            cycle
        end if
        accepted = sudakov%reweight_alpha_s (r%pt2)
        call sudakov%veto_counter%record_alpha_s (.not. accepted)
        if (.not. accepted) then
            sudakov%current_pt2_max = r%pt2
            cycle
        end if
        call sudakov%generate_xi_and_y_and_phi (r)
        accepted = sudakov%reweight_xi_max (r%xi)
        call sudakov%veto_counter%record_xi_max (.not. accepted)
        if (.not. accepted) then

```

```

        sudakov%current_pt2_max = r%pt2
        cycle
    end if
    if (debug_active (D_MATCHING)) then
        call assert_equal (OUTPUT_UNIT, r%pt2, &
            sudakov%kt2 (r%xi, r%y), &
            "sudakov_generate_xi_and_y_and_phi: pt2 inconsistency")
    end if
    r%valid = .true.
    exit
end do LOOP_UNTIL_ACCEPTED
end subroutine sudakov_generate_emission

```

Evaluates the Sudakov as needed for `solve_interval` to generate a p_T value.

```

<POWHEG matching: sudakov: TBP>+≡
    procedure :: evaluate => sudakov_evaluate

<POWHEG matching: procedures>+≡
    function sudakov_evaluate (solver_f, x) result (f)
        complex(default) :: f
        class(sudakov_t), intent(in) :: solver_f
        real(default), intent(in) :: x
        f = solver_f%sum_log_rands + solver_f%norm_max * solver_f%log_integrated_ubf (x)
    end function sudakov_evaluate

```

```

<POWHEG matching: sudakov: TBP>+≡
    procedure :: associated_emitter => sudakov_associated_emitter

<POWHEG matching: procedures>+≡
    elemental function sudakov_associated_emitter (sudakov) result (emitter)
        integer :: emitter
        class(sudakov_t), intent(in) :: sudakov
        emitter = sudakov%process_deps%phs_identifiers(sudakov%i_phs)%emitter
    end function sudakov_associated_emitter

```

```

<POWHEG matching: sudakov: TBP>+≡
    procedure :: set_i_phs => sudakov_set_i_phs

<POWHEG matching: procedures>+≡
    subroutine sudakov_set_i_phs (sudakov, alr)
        class(sudakov_t), intent(inout) :: sudakov
        integer, intent(in) :: alr
        sudakov%i_phs = sudakov%process_deps%alr_to_i_phs(alr)
    end subroutine sudakov_set_i_phs

```

Simple FSR

This corresponds to Appendix C of 1002.2581

```

<POWHEG matching: public>+≡
    public :: sudakov_simple_fsr_t

```

```

<POWHEG matching: types>+≡
  type, extends (sudakov_t) :: sudakov_simple_fsr_t
  contains
    <POWHEG matching: sudakov simple fsr: TBP>
  end type sudakov_simple_fsr_t

```

The simplest upper bounding function for final-state radiation is

$$\text{upper_bound_func} = \frac{U(\xi, y)}{N} = \frac{\alpha_s}{\xi(1-y)} \quad (31.4)$$

```

<POWHEG matching: sudakov simple fsr: TBP>≡
  procedure :: upper_bound_func => sudakov_simple_fsr_upper_bound_func

<POWHEG matching: procedures>+≡
  pure function sudakov_simple_fsr_upper_bound_func (sudakov, xi, y, alpha_s) result (u)
    real(default) :: u
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y, alpha_s
    u = alpha_s / (xi * (1 - y))
  end function sudakov_simple_fsr_upper_bound_func

```

The above upper bounding function corresponds to the transverse momentum scale

$$k_T^2 = \frac{s}{2} \xi^2 (1-y). \quad (31.5)$$

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: kt2 => sudakov_simple_fsr_kt2

<POWHEG matching: procedures>+≡
  function sudakov_simple_fsr_kt2 (sudakov, xi, y) result (kt2)
    real(default) :: kt2
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi, y
    kt2 = sudakov%phs_fks_generator%real_kinematics%kt2 &
      (sudakov%i_phs, sudakov%associated_emitter (), UBF_FSR_SIMPLE, xi, y)
  end function sudakov_simple_fsr_kt2

```

For massless emitters, the upper bound on the radiated energy is

$$t_{\max} = \xi_{\max}^2 \hat{s}$$

We use this as largest possible scale for the radiation.

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: kt2_max => sudakov_simple_fsr_kt2_max

<POWHEG matching: procedures>+≡
  pure function sudakov_simple_fsr_kt2_max (sudakov) result (kt2_max)
    real(default) :: kt2_max
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default) :: s_hat
    s_hat = sudakov%event_deps%s_hat
    kt2_max = sudakov%xi2_max * s_hat
  end function sudakov_simple_fsr_kt2_max

```

This is

$$-\frac{\log \Delta^{(U)}(p_T)}{N} = \frac{\pi}{b_0} \theta \left(\xi_{\max}^2 - \frac{p_T^2}{s} \right) \left[\log \frac{\xi_{\max}^2 s}{\Lambda^2} \log \frac{\log \xi_{\max}^2 s / \Lambda^2}{\log p_T^2 / \Lambda^2} - \log \frac{\xi_{\max}^2 s}{p_T^2} \right] \quad (31.6)$$

with $p_{T,\max}^2 = \xi_{\max}^2 s$.

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: log_integrated_ubf => sudakov_simple_fsr_log_integrated_ubf

<POWHEG matching: procedures>+≡
  pure function sudakov_simple_fsr_log_integrated_ubf (sudakov, pt2) result (log_sudakov)
    real(default) :: log_sudakov
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: pt2
    real(default) :: kt2_max, kt2_max1, pt21
    logical :: within_boundaries
    within_boundaries = pt2 <= sudakov%kt2_max () &
      .and. pt2 >= sudakov%powheg_settings%pt2_min
    if (within_boundaries) then
      kt2_max = sudakov%kt2_max ()
      kt2_max1 = kt2_max / sudakov%process_deps%lambda2_gen
      pt21 = pt2 / sudakov%process_deps%lambda2_gen
      log_sudakov = pi / b0rad * (log (kt2_max1) * &
        log (log (kt2_max1) / log (pt21)) - &
        log (kt2_max / pt2))
    else
      log_sudakov = 0
    end if
  end function sudakov_simple_fsr_log_integrated_ubf

```

No further veto needed for this upper bounding function.

```

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: reweight_ubf => sudakov_simple_fsr_reweight_ubf

<POWHEG matching: procedures>+≡
  function sudakov_simple_fsr_reweight_ubf (sudakov, pt2) result (accepted)
    logical :: accepted
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    real(default), intent(in) :: pt2
    accepted = .true.
  end function sudakov_simple_fsr_reweight_ubf

<POWHEG matching: sudakov simple fsr: TBP>+≡
  procedure :: reweight_xi_max => sudakov_simple_fsr_reweight_xi_max

<POWHEG matching: procedures>+≡
  function sudakov_simple_fsr_reweight_xi_max (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_simple_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
    accepted = .true.
  end function sudakov_simple_fsr_reweight_xi_max

```

This depends on the choice of p_T and is tested in the assertion.

```

(POWHEG matching: sudakov simple fsr: TBP)+≡
  procedure :: generate_xi_and_y_and_phi => sudakov_simple_fsr_generate_xi_and_y_and_phi

(POWHEG matching: procedures)+≡
  subroutine sudakov_simple_fsr_generate_xi_and_y_and_phi (sudakov, r)
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    real(default) :: s
    s = sudakov%event_deps%s_hat
    call sudakov%generate_xi (r)
    r%y = one - (two * r%pt2) / (s * r%xi**2)
    call sudakov%rng%generate (sudakov%random)
    r%phi = sudakov%random * twopi
  end subroutine sudakov_simple_fsr_generate_xi_and_y_and_phi

```

We generate $\xi \in [\frac{p_T}{\sqrt{s}}, \xi_{\max}]$ with a density $1/\xi$ i.e. uniformly in $\log(\xi)$.

```

(POWHEG matching: sudakov simple fsr: TBP)+≡
  procedure :: generate_xi => sudakov_simple_fsr_generate_xi

(POWHEG matching: procedures)+≡
  subroutine sudakov_simple_fsr_generate_xi (sudakov, r)
    class(sudakov_simple_fsr_t), intent(inout) :: sudakov
    type(radiation_t), intent(inout) :: r
    real(default) :: s, xi2_max
    s = sudakov%event_deps%s_hat
    xi2_max = sudakov%xi2_max
    call sudakov%rng%generate (sudakov%random)
    r%xi = exp (((one - sudakov%random) * log (r%pt2 / s) + &
      sudakov%random * log (xi2_max)) / two)
  end subroutine sudakov_simple_fsr_generate_xi

```

Dijet production at lepton colliders

In the POWHEG method paper, $e^+e^- \rightarrow q\bar{q}$ requires a UBF different from the simple one to account for an additional divergence for $(\xi, y) \rightarrow (1, -1)$.

```

(POWHEG matching: public)+≡
  public :: sudakov_eeqq_fsr_t

(POWHEG matching: types)+≡
  type, extends (sudakov_t) :: sudakov_eeqq_fsr_t
  contains
    (POWHEG matching: sudakov eeqq fsr: TBP)
  end type sudakov_eeqq_fsr_t

```

This k_T measure is the same as in the case for simple FSR up to $\mathcal{O}(\theta^4)$ when $y = \cos(\theta)$. It differs by just a factor of 2 w.r.t. `sudakov_simple_fsr_kt2`.

```

(POWHEG matching: sudakov eeqq fsr: TBP)≡
  procedure :: kt2 => sudakov_eeqq_fsr_kt2

```

```

<POWHEG matching: procedures>+=
function sudakov_eeqq_fsr_kt2 (sudakov, xi, y) result (kt2)
  real(default) :: kt2
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y
  kt2 = sudakov%phs_fks_generator%real_kinematics%kt2 &
    (sudakov%i_phs, sudakov%associated_emitter(), UBF_FSR_MASSLESS_RECOIL, xi, y)
end function sudakov_eeqq_fsr_kt2

```

For eeqq, the shower starts at $k_{\max} = \frac{q^0}{2}$. (c.f. eq. (7.86) in [0709.2092].)

```

<POWHEG matching: sudakov eeqq fsr: TBP>+=
procedure :: kt2_max => sudakov_eeqq_fsr_kt2_max

<POWHEG matching: procedures>+=
pure function sudakov_eeqq_fsr_kt2_max (sudakov) result (kt2_max)
  real(default) :: kt2_max
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  kt2_max = 0.25_default * sudakov%event_deps%s_hat
end function sudakov_eeqq_fsr_kt2_max

```

This covers also the singularity at $(\xi, y) \rightarrow (1, -1)$ that occurs for a massless recoiling system.

```

<POWHEG matching: sudakov eeqq fsr: TBP>+=
procedure :: upper_bound_func => sudakov_eeqq_fsr_upper_bound_func

<POWHEG matching: procedures>+=
pure function sudakov_eeqq_fsr_upper_bound_func (sudakov, xi, y, alpha_s) result (u)
  real(default) :: u
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y, alpha_s
  u = alpha_s / (xi * (1 - y**2))
end function sudakov_eeqq_fsr_upper_bound_func

```

The logarithmic integrated UBF in the eeqq case as explained in [0709.2092], eq. (7.98), is given by

$$\begin{aligned}
-\frac{1}{N} \log [\Delta^U(p_T)] &= 2\pi \int_0^{k_{\max}} \alpha_s(k_T) \log \left[\frac{4k_{\max}^2}{k_T^2} \right] \theta(k_T - p_T) \frac{dk_T}{k_T} \\
&= \frac{\pi}{b_0} \left(\log \left[\frac{4k_{\max}^2}{k_T^2} \right] \log \left[\frac{\log(k_{\max}^2/\Lambda^2)}{\log(p_T^2/\Lambda^2)} \right] - \log \left[\frac{k_{\max}^2}{p_T^2} \right] \right)
\end{aligned}
\tag{31.7}$$

with $k_{\max} = \frac{q^0}{2}$. We see that for these logarithms to be well defined, we need to set a lower bound for the transverse momentum $p_{T,\min} > \Lambda = \text{lambda2_gen}$.

```

<POWHEG matching: sudakov eeqq fsr: TBP>+=
procedure :: log_integrated_ubf => sudakov_eeqq_fsr_log_integrated_ubf

<POWHEG matching: procedures>+=
pure function sudakov_eeqq_fsr_log_integrated_ubf (sudakov, pt2) result (log_sudakov)
  real(default) :: log_sudakov
  class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: pt2

```



```

real(default) :: k_max2, Lambda2
logical :: within_boundaries
k_max2 = sudakov%kt2_max ()
within_boundaries = pt2 >= sudakov%powheg_settings%pt2_min &
    .and. pt2 <= k_max2
if (within_boundaries) then
    Lambda2 = sudakov%process_deps%lambda2_gen
    log_sudakov = pi / b0rad * ( log (4 * k_max2 / Lambda2) * &
        log (log (k_max2/Lambda2) / log (pt2/Lambda2)) - log(k_max2/pt2) )
else
    log_sudakov = 0
end if
end function sudakov_eeqq_fsr_log_integrated_ubf

```

In order to arrive at the log integrated Sudakov implemented in `sudakov_eeqq_fsr_log_integrated_ubf`, we overestimated

$$\log \left[\frac{1 + \sqrt{1 - (k_T/k_{\max})^2}}{1 - \sqrt{1 - (k_T/k_{\max})^2}} \right] \leq \log \left[\frac{4k_{\max}^2}{k_T^2} \right]. \quad (31.8)$$

We correct for this in this veto step.

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
procedure :: reweight_ubf => sudakov_eeqq_fsr_reweight_ubf

<POWHEG matching: procedures>+≡
function sudakov_eeqq_fsr_reweight_ubf (sudakov, pt2) result (accepted)
    logical :: accepted
    class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
    real(default), intent(in) :: pt2
    real(default) :: log_bound, k_max2
    k_max2 = sudakov%kt2_max ()
    log_bound = log((1 + sqrt(1 - (pt2/k_max2))) &
        / (1 - sqrt(1 - (pt2/k_max2))))
    call sudakov%rng%generate (sudakov%random)
    accepted = sudakov%random * log( 4 * k_max2 / pt2 ) <= log_bound
end function sudakov_eeqq_fsr_reweight_ubf

```

In the eeqq case, we did not overestimate ξ with ξ_{\max} .

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
procedure :: reweight_xi_max => sudakov_eeqq_fsr_reweight_xi_max

<POWHEG matching: procedures>+≡
function sudakov_eeqq_fsr_reweight_xi_max (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_eeqq_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
    accepted = .true.
end function sudakov_eeqq_fsr_reweight_xi_max

```

In the eeqq case, we generate y from a random number and afterwards compute $\xi(p_T, y)$ so the sequence is reversed in comparison to the simple case.

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
procedure :: generate_xi_and_y_and_phi => sudakov_eeqq_fsr_generate_xi_and_y_and_phi

```

```

<POWHEG matching: procedures>+≡
subroutine sudakov_eeqq_fsr_generate_xi_and_y_and_phi (sudakov, r)
  class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  call sudakov%generate_y (r)
  call sudakov%generate_xi (r)
  call sudakov%generate_phi (r)
end subroutine sudakov_eeqq_fsr_generate_xi_and_y_and_phi

```

To generate y for the eeqq UBF, we take a random number

$$-\log \left[\frac{1 + \sqrt{1 - (p_T/k_{\max})^2}}{1 - \sqrt{1 - (p_T/k_{\max})^2}} \right] < r_y < \log \left[\frac{1 + \sqrt{1 - (p_T/k_{\max})^2}}{1 - \sqrt{1 - (p_T/k_{\max})^2}} \right] \quad (31.9)$$

and then compute

$$y(r_y) = \frac{e^{r_y} - 1}{e^{r_y} + 1} \quad (31.10)$$

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
  procedure :: generate_y => sudakov_eeqq_fsr_generate_y

<POWHEG matching: procedures>+≡
subroutine sudakov_eeqq_fsr_generate_y (sudakov, r)
  class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  real(default) :: k_max2, log_bound, r_y
  k_max2 = sudakov%kt2_max ()
  call sudakov%rng%generate (sudakov%random)
  log_bound = log((1 + sqrt(1 - (r%pt2/k_max2))) &
    / (1 - sqrt(1 - (r%pt2/k_max2))))
  r_y = -log_bound + sudakov%random * (two * log_bound)
  r%y = (exp(r_y) - 1) / (exp(r_y) + 1)
end subroutine sudakov_eeqq_fsr_generate_y

```

We generate ξ for the eeqq UBF according to

$$\xi(p_T, y) = \frac{2p_T}{\sqrt{s}\sqrt{1-y^2}} \quad (31.11)$$

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
  procedure :: generate_xi => sudakov_eeqq_fsr_generate_xi

<POWHEG matching: procedures>+≡
subroutine sudakov_eeqq_fsr_generate_xi (sudakov, r)
  class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  real(default) :: q0
  q0 = sqrt(sudakov%event_deps%s_hat)
  r%xi = (2 * sqrt(r%pt2)) / (q0 * sqrt(1 - r%y**2))
end subroutine sudakov_eeqq_fsr_generate_xi

```

Generate ϕ for the eeqq UBF

```

<POWHEG matching: sudakov eeqq fsr: TBP>+≡
  procedure :: generate_phi => sudakov_eeqq_fsr_generate_phi

```

```

<POWHEG matching: procedures>+≡
subroutine sudakov_eeqq_fsr_generate_phi (sudakov, r)
  class(sudakov_eeqq_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  call sudakov%rng%generate (sudakov%random)
  r%phi = sudakov%random * twopi
end subroutine sudakov_eeqq_fsr_generate_phi

```

Massive FSR

```

<POWHEG matching: public>+≡
public :: sudakov_massive_fsr_t

<POWHEG matching: types>+≡
type, extends (sudakov_t) :: sudakov_massive_fsr_t
  real(default) :: z, z1, z2 = 0._default
  real(default) :: xi_1, xi_min, xi_m = 0._default
  real(default) :: xi_max_extended = 1._default
contains
  <POWHEG matching: sudakov massive fsr: TBP>
end type sudakov_massive_fsr_t

```

According to eq. A.42 1202.0465, during the radiation generation, an alternative expression for ξ_{\max} ,

$$\xi_{\max} = 1 - \frac{(m + m_{\text{rec}})^2}{q^2},$$

is used, which corresponds to an extended Dalitz region. Phase space points outside of the original Dalitz region will be vetoed afterwards in `sudakov_massive_fsr_reweight_xi_max`.

```

<POWHEG matching: sudakov massive fsr: TBP>≡
procedure :: compute_xi_max_extended &
=> sudakov_massive_fsr_compute_xi_max_extended

<POWHEG matching: procedures>+≡
subroutine sudakov_massive_fsr_compute_xi_max_extended (sudakov, i_phs)
  class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  integer, intent(in) :: i_phs
  real(default) :: m, mrec
  real(default) :: q0
  type(vector4_t) :: p
  q0 = sqrt(sudakov%event_deps%s_hat)
  p = sudakov%event_deps%p_born_lab%get_momentum (1, sudakov%associated_emitter())
  m = p**1
  mrec = sqrt ((q0 - p%p(0))**2 - p%p(1)**2 - p%p(2)**2 - p%p(3)**2)
  sudakov%xi_max_extended = one - (m + mrec)**2 / q0**2
end subroutine sudakov_massive_fsr_compute_xi_max_extended

```

As described in 1202.0465, App. A.5., for massive emitters, the radiation variable ξ is constructed as follows. First,

$$\xi_{\min}(K_T^2) = \frac{\sqrt{K_T^2 (K_T^2 z_2^2 + 8\bar{p}^0 q (1 - z_2))} - K_T^2 z_2}{2q^2(1 - z_2)} \quad (31.12)$$

is computed where K_T is a hardness scale for the radiation that determines the upper limit of the integral for the Sudakov form factor and coincides with the usual one, i.e. the transverse momentum of the radiated particle, in the massless limit. Then ξ_1 is computed according to the same equation with $z_2 \leftrightarrow z_1$. Finally, ξ is generated according to

$$\xi = \frac{1}{q^2} \left(\exp \left[\log (\xi_{\min} q^2 - K_T^2) + r \log \frac{\xi_m q^2 - K_T^2}{\xi_{\min} q^2 - K_T^2} \right] + K_T^2 \right), \quad (31.13)$$

where $\xi_m = \min (\xi_{\max}, \xi_1)$.

(POWHEG matching: sudakov massive fsr: TBP)+≡

```
procedure :: generate_xi => sudakov_massive_fsr_generate_xi
```

(POWHEG matching: procedures)+≡

```
subroutine sudakov_massive_fsr_generate_xi (sudakov, r)
  class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  real(default) :: pt2, q0, q02
  real(default) :: E_em, xi_max_ext
  real(default) :: xi_1, xi_min, xi_m
  pt2 = r%pt2
  E_em = sudakov%event_deps%p_born_lab%get_energy &
    (1, sudakov%associated_emitter())
  q02 = sudakov%event_deps%s_hat; q0 = sqrt(q02)
  xi_max_ext = sudakov%xi_max_extended
  associate (z1 => sudakov%z1, z2 => sudakov%z2)
    xi_1 = (sqrt(pt2 * (pt2 * z1**2 + 8 * E_em * q0 * (one - z1))) - pt2 * z1) / &
      (two * q02 * (one - z1))
    xi_min = (sqrt(pt2 * (pt2 * z2**2 + 8 * E_em * q0 * (one - z2))) - pt2 * z2) / &
      (two * q02 * (one - z2))
  end associate
  xi_m = min (xi_max_ext, xi_1)
  call sudakov%rng%generate (sudakov%random)
  r%xi = (exp (log(xi_min * q02 - pt2) + sudakov%random * &
    log((xi_m * q02 - pt2) / (xi_min * q02 - pt2))) + pt2) / q02
end subroutine sudakov_massive_fsr_generate_xi
```

Generates the FKS variables in the case of a massive emitter and additionally computes z and $z_{1/2}$ as well as ξ_{\max} to be stored in the Sudakov for later use when reweighting ξ_{\max} and retrieving the norm from the POWHEG grid. The corresponding derivations can be found in 1202.0465, App. A.

(POWHEG matching: sudakov massive fsr: TBP)+≡

```
procedure :: generate_xi_and_y_and_phi => sudakov_massive_fsr_generate_xi_and_y_and_phi
```

(POWHEG matching: procedures)+≡

```
subroutine sudakov_massive_fsr_generate_xi_and_y_and_phi (sudakov, r)
  class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  type(radiation_t), intent(inout) :: r
  real(default) :: q0
  real(default) :: m2, mrec2, k0_rec_max
  real(default) :: E_em
  type(vector4_t) :: p_emitter

  q0 = sqrt (sudakov%event_deps%s_hat)
```

```

p_emitter = sudakov%event_deps%p_born_lab%get_momentum &
(1, sudakov%associated_emitter())
associate (p => p_emitter%p)
mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
E_em = p(0)
end associate
m2 = p_emitter**2
call compute_dalitz_bounds (q0, m2, mrec2, sudakov%z1, sudakov%z2, k0_rec_max)
call sudakov%generate_xi (r)

sudakov%z = (two * r%pt2 * E_em - r%xi**2 * q0**3) / &
(r%pt2 * r%xi * q0 - r%xi**2 * q0**3)
sudakov%xi2_max = - (q0**2 * sudakov%z**2 - two * q0 * k0_rec_max * sudakov%z + mrec2) / &
(q0**2 * sudakov%z * (one - sudakov%z))
sudakov%xi2_max = sudakov%xi2_max**2
r%y = two * (sudakov%z2 - sudakov%z) / (sudakov%z2 - sudakov%z1) - one
call sudakov%rng%generate (sudakov%random)
r%phi = sudakov%random * twopi
end subroutine sudakov_massive_fsr_generate_xi_and_y_and_phi

```

Computes the hardness scale as discussed in 1202.0465, App. A.2.

$$K_T^2 = \frac{\xi^2 q^3 (1-z)}{2\bar{p}_{\text{em}}^0 - z\xi q} \quad (31.14)$$

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
procedure :: kt2 => sudakov_massive_fsr_kt2

<POWHEG matching: procedures>+≡
function sudakov_massive_fsr_kt2 (sudakov, xi, y) result (kt2)
real(default) :: kt2
class(sudakov_massive_fsr_t), intent(in) :: sudakov
real(default), intent(in) :: xi, y
kt2 = sudakov%phs_fks_generator%real_kinematics%kt2 &
(sudakov%i_phs, sudakov%associated_emitter(), UBF_FSR_MASSIVE, xi, y)
end function sudakov_massive_fsr_kt2

```

For massive emitters, the upper bound on the radiated p_T is

$$t_{\text{max}} = \frac{\xi_{\text{max}}^2 q^3 (1-z_2)}{2 \cdot \bar{p}^0 - z_2 \xi_{\text{max}} q}$$

For this, we have to compute z_2 from the Dalitz bounds as `sudakov%z2` has not yet been set for the current event.

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
procedure :: kt2_max => sudakov_massive_fsr_kt2_max

<POWHEG matching: procedures>+≡
pure function sudakov_massive_fsr_kt2_max (sudakov) result (kt2_max)
real(default) :: kt2_max
class(sudakov_massive_fsr_t), intent(in) :: sudakov
real(default) :: q0, E_em, xi_max, z1, z2, m2, mrec2, k0_rec_max
type(vector4_t) :: p_emitter
q0 = sqrt(sudakov%event_deps%s_hat)

```

```

p_emitter = sudakov%event_deps%p_born_lab%get_momentum &
(1, sudakov%associated_emitter())
associate (p => p_emitter%p)
mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
E_em = p(0)
end associate
m2 = p_emitter**2
call compute_dalitz_bounds (q0, m2, mrec2, z1, z2, k0_rec_max)
xi_max = sudakov%xi_max_extended
kt2_max = (xi_max**2 * q0**3 * (one - z2)) / (two * E_em - z2 * xi_max * q0)
end function sudakov_massive_fsr_kt2_max

```

The upper bounding function for massive emitters according to Eq. A.56 in [1202.0465] (disregarding a possible factor of α_s) is

$$U(\xi, y) \sim \frac{\sqrt{s}}{\bar{p}_{\text{em}}} \frac{1}{\xi(1-z)} \quad (31.15)$$

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
procedure :: upper_bound_func => sudakov_massive_fsr_upper_bound_func

<POWHEG matching: procedures>+≡
pure function sudakov_massive_fsr_upper_bound_func (sudakov, xi, y, alpha_s) result (u)
  real(default) :: u
  class(sudakov_massive_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: xi, y, alpha_s
  real(default) :: q, p_em
  q = sqrt (sudakov%event_deps%s_hat)
  p_em = space_part_norm &
    (sudakov%event_deps%p_born_lab%get_momentum (1, &
      sudakov%associated_emitter()))
  u = alpha_s * q / p_em * one / (xi * (one - sudakov%z))
end function sudakov_massive_fsr_upper_bound_func

```

The integrated upper-bounding function for massive final-state emitters is given by

$$\begin{aligned}
I(t) = & \frac{q}{\bar{p}_{\text{em}}} \left[\log \xi \log \left[(1-z_2) \frac{q}{k_T^2} \right] + \frac{1}{2} \log^2 \xi + G(-k_T^2, q^2, \xi) - G(2\bar{p}_{\text{em}}, -q, \xi) \right]_{\xi_{\min}}^{\min(\xi_1(k_T^2), \xi_{\max})} \\
& + \frac{q}{\bar{p}_{\text{em}}} \theta(\xi_{\max} - \xi_1(k_T^2)) \log \frac{\xi_{\max}}{\xi_1(k_T^2)} \log \frac{1-z_2}{1-z_1},
\end{aligned}$$

where the function $G(a, b, \xi)$ is given by

$$G(a, b, \xi) = \log(a + b\xi) \log \left(1 - \frac{a + b\xi}{a} \right) + Li_2 \left(\frac{a + b\xi}{a} \right), \quad (31.16)$$

for $a < 0$ and by

$$G(a, b, \xi) = \log \left| \frac{b\xi}{a} \right| \log a - Li_2 \left(-\frac{b\xi}{a} \right) + \frac{\pi^2}{6}, \quad (31.17)$$

for $a > 0$.

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
procedure :: log_integrated_ubf => sudakov_massive_fsr_log_integrated_ubf

```

(POWHEG matching: procedures)+≡

```

pure function sudakov_massive_fsr_log_integrated_ubf (sudakov, pt2) result (log_sudakov)
  real(default) :: log_sudakov
  class(sudakov_massive_fsr_t), intent(in) :: sudakov
  real(default), intent(in) :: pt2
  real(default) :: xi, xi_max, xi_1, xi_min
  real(default) :: q0, p_em, E_em, m2, mrec2, k0_rec_max
  type(vector4_t) :: p_emitter
  real(default) :: log_sudakov_up, log_sudakov_down, z1, z2
  logical :: within_boundaries
  within_boundaries = pt2 >= sudakov%powheg_settings%pt2_min &
    .and. pt2 <= sudakov%kt2_max ()
  if (within_boundaries) then
    q0 = sqrt (sudakov%event_deps%s_hat)
    p_emitter = sudakov%event_deps%p_born_lab%get_momentum &
      (1, sudakov%associated_emitter())
    associate (p => p_emitter%p)
      mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
      E_em = p(0)
    end associate
    m2 = p_emitter**2
    call compute_dalitz_bounds (q0, m2, mrec2, z1, z2, k0_rec_max)
    p_em = space_part_norm (p_emitter)
    xi_max = sudakov%xi_max_extended
    xi_1 = (sqrt (pt2 * (pt2 * z1**2 + 8 * E_em * q0 * (one - z1))) - pt2 * z1) / &
      (two * q0**2 * (one - z1))
    xi_min = (sqrt (pt2 * (pt2 * z2**2 + 8 * E_em * q0 * (one - z2))) - pt2 * z2) / &
      (two * q0**2 * (one - z2))
    xi = min (xi_1, xi_max)
    log_sudakov_up = log(xi) * log((one - z2) * q0 / pt2) + log(xi)**2 / two + &
      G_FSR(-pt2, q0**2, xi) - G_FSR(two * E_em, -q0, xi)
    xi = xi_min
    log_sudakov_down = log(xi) * log((one - z2) * q0 / pt2) + log(xi)**2/two + &
      G_FSR(-pt2, q0**2, xi) - G_FSR(two * E_em, -q0, xi)
    log_sudakov = log_sudakov_up - log_sudakov_down
    if (xi_max > xi_1) &
      log_sudakov = log_sudakov + log(xi_max / xi_1) * log((one - z2) / (one - z1))
    log_sudakov = twopi * q0 / p_em * log_sudakov
  else
    log_sudakov = 0
  end if
end function sudakov_massive_fsr_log_integrated_ubf

```

No further ubf veto needed for now.

(POWHEG matching: sudakov massive fsr: TBP)+≡

```

procedure :: reweight_ubf => sudakov_massive_fsr_reweight_ubf

```

(POWHEG matching: procedures)+≡

```

function sudakov_massive_fsr_reweight_ubf (sudakov, pt2) result (accepted)
  logical :: accepted
  class(sudakov_massive_fsr_t), intent(inout) :: sudakov
  real(default), intent(in) :: pt2
  accepted = .true.
end function sudakov_massive_fsr_reweight_ubf

```

In the massive case, we generated $0 < \xi < \xi_{\text{max_extended}}$ and thus we need to veto values of ξ larger than ξ_{max} in this extra veto step.

```

<POWHEG matching: sudakov massive fsr: TBP>+≡
  procedure :: reweight_xi_max => sudakov_massive_fsr_reweight_xi_max

<POWHEG matching: procedures>+≡
  function sudakov_massive_fsr_reweight_xi_max (sudakov, xi) result (accepted)
    logical :: accepted
    class(sudakov_massive_fsr_t), intent(in) :: sudakov
    real(default), intent(in) :: xi
    accepted = xi < sqrt (sudakov%xi2_max)
  end function sudakov_massive_fsr_reweight_xi_max

```

Auxiliary functions

Implements the function $G(a, b, \xi)$ given in eq. (31.17) and eq. (31.16). Cannot be evaluated for $a = 0$.

```

<POWHEG matching: procedures>+≡
  elemental function G_FSR (a,b,xi)
    real(default) :: G_FSR
    real(default), intent(in) :: a, b, xi
    if (a > 0) then
      G_FSR = G_FSR_Plus (a,b,xi)
    else if (a < 0) then
      G_FSR = G_FSR_Minus (a,b,xi)
    end if
  end function G_FSR

  elemental function G_FSR_Minus (a,b,xi)
    real(default) :: G_FSR_Minus
    real(default), intent(in) :: a, b, xi
    G_FSR_Minus = log(a+b*xi)*log(one - (a+b*xi)/a) + Li2((a+b*xi)/a)
  end function G_FSR_Minus

  elemental function G_FSR_Plus (a,b,xi)
    real(default) :: G_FSR_Plus
    real(default), intent(in) :: a, b, xi
    G_FSR_Plus = log(abs(b*xi/a))*log(a) - Li2(-b*xi/a) + pi**2/6
  end function G_FSR_Plus

```

31.4.3 Main POWHEG class

```

<POWHEG matching: public>+≡
  public :: powheg_matching_t

<POWHEG matching: types>+≡
  type, extends(matching_t) :: powheg_matching_t
  type(grid_t) :: grid
  type(phs_fks_generator_t) :: phs_fks_generator
  type(powheg_settings_t) :: settings

```



```

        type(event_deps_t) :: event_deps
        type(process_deps_t) :: process_deps
        type(sudakov_wrapper_t), dimension(:), allocatable :: sudakov
        integer :: n_emissions = 0
        logical :: active = .true.
contains
    <POWHEG matching: powheg matching: TBP>
end type powheg_matching_t

<POWHEG matching: powheg matching: TBP>≡
    procedure :: get_method => powheg_matching_get_method

<POWHEG matching: procedures>+≡
    function powheg_matching_get_method (matching) result (method)
        type(string_t) :: method
        class(powheg_matching_t), intent(in) :: matching
        method = matching_method (MATCH_POWHEG)
    end function powheg_matching_get_method

<POWHEG matching: powheg matching: TBP>+≡
    procedure :: before_shower => powheg_matching_before_shower

<POWHEG matching: procedures>+≡
    subroutine powheg_matching_before_shower &
        (matching, particle_set, vetoed)
        class(powheg_matching_t), intent(inout) :: matching
        type(particle_set_t), intent(inout) :: particle_set
        logical, intent(out) :: vetoed
        if (debug_on) call msg_debug2 (D_MATCHING, "powheg_matching_before_shower")
        if (signal_is_pending ()) return
        if (.not. matching%active) return
        call matching%update (particle_set)
        if (matching%settings%test_sudakov) then
            call matching%test_sudakov ()
            stop
        end if
        if (.not. matching%settings%disable_sudakov) &
            call matching%generate_emission (particle_set = particle_set)
        vetoed = .false.
    end subroutine powheg_matching_before_shower

<POWHEG matching: powheg matching: TBP>+≡
    procedure :: first_event => powheg_matching_first_event

<POWHEG matching: procedures>+≡
    subroutine powheg_matching_first_event (matching)
        class(powheg_matching_t), intent(inout), target :: matching
        associate (instance => matching%process_instance)
            matching%process_deps%lab_is_cm = instance%lab_is_cm (1)
        end associate
        call matching%setup_grids ()
    end subroutine powheg_matching_first_event

```

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: after_shower => powheg_matching_after_shower

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_after_shower (matching, particle_set, vetoed)
    class(powheg_matching_t), intent(inout) :: matching
    type(particle_set_t), intent(inout) :: particle_set
    logical, intent(out) :: vetoed
    vetoed = .false.
  end subroutine powheg_matching_after_shower

```

Output

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: write => powheg_write

<POWHEG matching: procedures>+≡
  subroutine powheg_write (matching, unit)
    class(powheg_matching_t), intent(in) :: matching
    integer, intent(in), optional :: unit
    integer :: u, alr
    u = given_output_unit (unit); if (u < 0) return
    call write_separator (u, 2)
    write (u, "(1X,A)") "POWHEG Emission Generator"
    write (u, "(1X,A)") "Process name: " // char (matching%process_name)
    if (allocated (matching%rng)) then
      call matching%rng%write (u)
    else
      write (u, "(1X,A)") "RNG not allocated"
    end if
    call matching%qcd%write (u)
    call matching%settings%write (u)
    call matching%event_deps%write (u)
    call matching%process_deps%write (u)
    do alr = 1, size (matching%sudakov)
      call write_separator (u)
      write (u, "(1X,A,I12,A)") "sudakov (alr = ", alr, ")"
      call matching%sudakov(alr)%s%write (u)
    end do
    call write_separator (u, 2)
  end subroutine powheg_write

```

Finalization of the POWHEG matching. It creates a log file showing how many events failed at which stage of the POWHEG veto algorithm. It also issues a warning if too many POWHEG excess events occurred. If this is the case, the chosen upper-bounding function is unsuitable for the considered process.

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: final => powheg_matching_final

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_final (matching)
    class(powheg_matching_t), intent(in) :: matching
    integer :: u, alr, n_fail_ubf_total, n_sqme_total

```

```

real :: frac_ubf_fail
type(string_t) :: filename
n_fail_ubf_total = 0
n_sqme_total = 0
u = free_unit ()
filename = matching%process_name // "_veto.log"
open (file=char(filename), unit=u, action='write')
write (u, '(A)') "Summary of POWHEG veto procedure"
do alr = 1, matching%process_deps%n_alr
  write(u,'(A,I0)') 'alr: ', alr
  call matching%sudakov(alr)%s%veto_counter%write (u)
  call write_separator (u)
  n_fail_ubf_total = n_fail_ubf_total &
    + matching%sudakov(alr)%s%veto_counter%n_fail_ubf
  n_sqme_total = n_sqme_total &
    + matching%sudakov(alr)%s%veto_counter%n_sqme
end do
write (u,'(A,I0)') "Total number of events which radiate a gluon: ", &
  matching%n_emissions
close (u)
if (n_sqme_total > 0) then
  frac_ubf_fail = one * n_fail_ubf_total / n_sqme_total * 100
  if (frac_ubf_fail > 1) then
    write (msg_buffer, "(A16,I4,A2,F6.2,A24)") "There have been ", n_fail_ubf_total,&
      " (", frac_ubf_fail, "%) POWHEG grid excesses."
    call msg_warning
  end if
end if
end subroutine powheg_matching_final

```

Initialization and Finalization

Setup the POWHEG grids. As they are filled during integration using the POWHEG hook, we can load them from file here.

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: setup_grids => powheg_matching_setup_grids

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_setup_grids (matching)
    class(powheg_matching_t), intent(inout), target :: matching
    call matching%prepare_for_events ()
    if (matching%check_grids ()) then
      call matching%load_grids ()
    else
      call msg_fatal ("POWHEG: POWHEG grids are invalid.")
    end if
    call matching%grid%compute_and_write_mean_and_max ()
    call matching%import_norms_from_grid ()
  end subroutine powheg_matching_setup_grids

```

Sets up the Sudakovs and chooses the correct UBF type. To determine the UBF type, we check for massive or initial state emitters for each ALR. For

consistency, we thus also check the eeqq case for each ALR. Only FSR Sudakovs are supported so far.

```

(POWHEG matching: powheg matching: TBP)+≡
  procedure :: setup_sudakovs => powheg_matching_setup_sudakovs

(POWHEG matching: procedures)+≡
  subroutine powheg_matching_setup_sudakovs (powheg)
    class(powheg_matching_t), intent(inout), target :: powheg
    integer :: alr, ubf_type, n_in
    logical :: is_fsr, is_massive, is_eeqq
    allocate (powheg%sudakov (powheg%process_deps%n_alr))
    do alr = 1, powheg%process_deps%n_alr
      select type (pcm => powheg%process_instance%pcm)
        type is (pcm_nlo_t)
          associate(reg_data => pcm%region_data, &
            phs => powheg%phs_fks_generator)
            n_in = reg_data%get_n_in()
            is_fsr = reg_data%get_emitter (alr) > n_in
            is_massive = phs%is_massive (reg_data%get_emitter (alr))
            is_eeqq = n_in == 2 .and. &
              reg_data%n_legs_born == 4 .and. &
              .not. phs%is_massive(3) .and. &
              .not. phs%is_massive(4)
            ! (PS 2021-05-28) This includes FSR regions of pp -> jj.
          end associate
        end select
      if (is_fsr) then
        if (is_eeqq) then
          ubf_type = UBF_FSR_MASSLESS_RECOIL
        else if (is_massive) then
          ubf_type = UBF_FSR_MASSIVE
        else
          ubf_type = powheg%settings%upper_bound_func_type
        end if
        select case (ubf_type)
          case (UBF_FSR_SIMPLE)
            allocate (sudakov_simple_fsr_t :: powheg%sudakov(alr)%s)
          case (UBF_FSR_MASSLESS_RECOIL)
            allocate (sudakov_eeqq_fsr_t :: powheg%sudakov(alr)%s)
          case (UBF_FSR_MASSIVE)
            allocate (sudakov_massive_fsr_t :: powheg%sudakov(alr)%s)
          case default
            call msg_fatal ("powheg_setup_sudakovs: Please choose upper bounding function!")
          end select
      else
        call msg_fatal ("powheg_setup_sudakovs: ISR not implemented yet!")
      end if
      if (allocated (powheg%rng)) then
        !!! generator mode
        call powheg%sudakov(alr)%s%init (powheg%process_deps, &
          powheg%event_deps, powheg%settings, &
          powheg%qcd, powheg%phs_fks_generator, powheg%rng)
      else
        !!! lookup mode

```

```

        call powheg%sudakov(alr)%s%init (powheg%process_deps, &
            powheg%event_deps, powheg%settings, &
            powheg%qcd, powheg%phs_fks_generator)
    end if

    call powheg%sudakov(alr)%s%set_i_phs (alr)
end do
end subroutine powheg_matching_setup_sudakovs

<POWHEG matching: powheg matching: TBP>+≡
    procedure :: init => powheg_matching_init

<POWHEG matching: procedures>+≡
    subroutine powheg_matching_init (matching, var_list, process_name)
        class(powheg_matching_t), intent(out) :: matching
        <default matching init>
    end subroutine powheg_matching_init

<POWHEG matching: powheg matching: TBP>+≡
    generic :: update => update_momenta, &
        update_particle_set
    procedure :: update_momenta => powheg_matching_update_momenta
    procedure :: update_particle_set => powheg_matching_update_particle_set

<POWHEG matching: procedures>+≡
    subroutine powheg_matching_update_momenta (powheg, p_born)
        class(powheg_matching_t), intent(inout) :: powheg
        type(vector4_t), dimension(:), intent(in) :: p_born
        type(lorentz_transformation_t) :: lt_lab_to_cms
        real(default) :: sqme_born

        sqme_born = powheg%process_instance%get_sqme (powheg%process_deps%i_born)
        if (.not. powheg%process_deps%lab_is_cm) then
            lt_lab_to_cms = powheg%process_instance%get_boost_to_cms (1)
            call powheg%update_event_deps (sqme_born, p_born, lt_lab_to_cms)
        else
            call powheg%update_event_deps (sqme_born, p_born)
        end if
    end subroutine powheg_matching_update_momenta

    subroutine powheg_matching_update_particle_set (powheg, particle_set)
        class(powheg_matching_t), intent(inout) :: powheg
        type(particle_set_t), intent(in) :: particle_set
        integer, dimension(:), allocatable :: indices
        logical, dimension(:), allocatable :: in_out_mask
        integer :: i
        allocate (in_out_mask (particle_set%get_n_tot()))
        do i = 1, particle_set%get_n_tot()
            in_out_mask(i) = particle_set%prt(i)%get_status () == PRT_INCOMING &
                .or. particle_set%prt(i)%get_status () == PRT_OUTGOING
        end do
        allocate (indices (size (particle_set%get_indices (in_out_mask))))
        indices = particle_set%get_indices (in_out_mask)
        call powheg%update_momenta (particle_set%get_momenta (indices))
    end subroutine powheg_matching_update_particle_set

```

```

end subroutine powheg_matching_update_particle_set

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: update_event_deps => powheg_matching_update_event_deps

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_update_event_deps (powheg, sqme_born, p_born, lt_lab_to_cms)
    class(powheg_matching_t), intent(inout) :: powheg
    real(default), intent(in) :: sqme_born
    type(vector4_t), dimension(:), intent(in) :: p_born
    type(lorentz_transformation_t), intent(in), optional :: lt_lab_to_cms
    call powheg%event_deps%update (sqme_born, p_born, lt_lab_to_cms)
  end subroutine powheg_matching_update_event_deps

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: boost_preal_to_lab_frame => powheg_matching_boost_preal_to_lab_frame

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_boost_preal_to_lab_frame (powheg, i_phs)
    class(powheg_matching_t), intent(inout) :: powheg
    type(lorentz_transformation_t) :: lt_cms_to_lab
    integer, intent(in) :: i_phs
    associate (event_deps => powheg%event_deps)
      if (powheg%process_deps%lab_is_cm) then
        event_deps%p_real_lab%phs_point(i_phs) = event_deps%p_real_cms%phs_point(i_phs)
      else
        lt_cms_to_lab = powheg%process_instance%get_boost_to_lab (1)
        event_deps%p_real_lab%phs_point(i_phs) = &
          lt_cms_to_lab * event_deps%p_real_cms%phs_point(i_phs)
      end if
    end associate
  end subroutine powheg_matching_boost_preal_to_lab_frame

```

This is the last step of the Sudakov veto algorithm removing the dependence on the normalization factor N and the upper bounding function U from the final result.

In cases where the Born kinematic failed the cuts, \mathcal{B} was artificially set to zero, so we cannot use it in a denominator. We assume that the generator cuts applied for parton showering are weak cuts to avoid divergent phase space regions, thus \mathcal{B} would have been large and the reweighting would have failed.

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: reweight_matrix_elements => powheg_matching_reweight_matrix_elements

<POWHEG matching: procedures>+≡
  function powheg_matching_reweight_matrix_elements (powheg, r) result (accepted)
    logical :: accepted
    class(powheg_matching_t), intent(inout) :: powheg
    type(radiation_t), intent(in) :: r
    integer :: emitter, i_phs
    real(default) :: sqme_real_x_jacobian, sqme_born
    real(default) :: norm, ubf, ubound, random, weight
    real(default) :: alpha_s
    type(vector4_t), dimension(:), allocatable :: p_real

```

```

if (debug_on) call msg_debug (D_MATCHING, "reweight_matrix_elements")
call powheg%rng%generate (random)
i_phs = powheg%process_deps%alr_to_i_phs (r%alr)
p_real = powheg%event_deps%p_real_cms%phs_point(i_phs)
! TODO wk 19-02-28 p_real is INOUT in this call, or rather OUT?
select type (pcm => powheg%process_instance%pcm)
type is (pcm_nlo_t)
  emitter = pcm%region_data%get_emitter (r%alr)
end select
call powheg%phs_fks_generator%generate_fsr_from_xi_and_y (r%xi, r%y, &
  r%phi, emitter, i_phs, powheg%event_deps%p_born_cms%get_momenta(1), &
  p_real)
powheg%event_deps%p_real_cms%phs_point(i_phs) = p_real
call powheg%boost_preal_to_lab_frame (i_phs)
call powheg%copy_momenta ()
norm = powheg%norm_from_xi_and_y (r)
associate (s => powheg%sudakov(r%alr)%s)
  alpha_s = s%alpha_s (s%kt2 (r%xi, r%y), use_correct=.true.)
  ubf = s%upper_bound_func (r%xi, r%y, alpha_s)
  sqme_real_x_jacobian = powheg%compute_sqme_real (r%alr, alpha_s)
  sqme_born = powheg%event_deps%sqme_born
  if (sqme_born == 0) then
    accepted = .false.
    return
  end if
  ubound = sqme_born * ubf * norm
  weight = sqme_real_x_jacobian / ubound
  if (weight > 1) call s%veto_counter%record_ubf_fail()
  if (debug_active (D_MATCHING)) then
    if (weight < 0) call msg_warning ("R/B < 0!")
  end if
  accepted = random < weight
end associate
if (debug_active (D_MATCHING)) then
  print *, ' r%alr = ', r%alr
  print *, ' r%xi = ', r%xi
  print *, ' r%y = ', r%y
  print *, ' emitter = ', emitter
  print *, ' random = ', random
  print *, ' sqme_real_x_jacobian = ', sqme_real_x_jacobian
  print *, ' sqme_born = ', sqme_born
  print *, ' ubf = ', ubf
  print *, ' norm = ', norm
  print *, ' ubound = ', ubound
  print *, ' matrix element accepted = ', accepted
end if
end function powheg_matching_reweight_matrix_elements

```

Generation algorithm and grid initialization

compute_sqme_real is the projected real matrix element $R_{\alpha_r} = S_{\alpha_r} R$ whereby the current α_r is implied by the emitter. Furthermore, it is multiplied by the

Jacobian.

(POWHEG matching: powheg matching: TBP)+≡

```
procedure :: compute_sqme_real => powheg_matching_compute_sqme_real
```

(POWHEG matching: procedures)+≡

```
function powheg_matching_compute_sqme_real (powheg, alr, alpha_s) result (sqme)
  real(default) :: sqme
  class(powheg_matching_t), intent(inout) :: powheg
  integer, intent(in) :: alr
  real(default), intent(in) :: alpha_s
  integer :: i_phs, i_term
  select type (pcm_work => powheg%process_instance%pcm_work)
  class is (pcm_nlo_workspace_t)
    i_phs = powheg%process_deps%alr_to_i_phs (alr)
    i_term = powheg%process_deps%i_real(i_phs)
    associate (instance => powheg%process_instance)
      call instance%compute_sqme_rad (i_term, i_phs, .false., alpha_s)
      sqme = instance%get_sqme (i_term)
    end associate
  end select
end function powheg_matching_compute_sqme_real
```

(POWHEG matching: powheg matching: TBP)+≡

```
procedure :: set_scale => powheg_matching_set_scale
```

(POWHEG matching: procedures)+≡

```
subroutine powheg_matching_set_scale (powheg, pT2)
  class(powheg_matching_t), intent(inout) :: powheg
  real(default), intent(in) :: pT2
  call powheg%process_instance%set_fac_scale (sqrt(pT2))
end subroutine powheg_matching_set_scale
```

(POWHEG matching: powheg matching: TBP)+≡

```
procedure :: update_sudakovs => powheg_matching_update_sudakovs
```

(POWHEG matching: procedures)+≡

```
subroutine powheg_matching_update_sudakovs (powheg, alr, i_phs, y)
  class(powheg_matching_t), intent(inout) :: powheg
  integer, intent(in) :: alr, i_phs
  real(default), intent(in) :: y
  real(default) :: q0, m2, mrec2, k0_rec_max
  type(vector4_t) :: p_emitter
  select type (s => powheg%sudakov(alr)%s)
  type is (sudakov_massive_fsr_t)
    q0 = sqrt (s%event_deps%s_hat)
    p_emitter = s%event_deps%p_born_lab%get_momentum (1, &
      s%associated_emitter ())
    associate (p => p_emitter%p)
      mrec2 = (q0 - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
    end associate
    m2 = p_emitter**2
    call compute_dalitz_bounds (q0, m2, mrec2, s%z1, s%z2, k0_rec_max)
    s%z = s%z2 - (s%z2 - s%z1) * (one + y) / two
  end select
```



```
end subroutine powheg_matching_update_sudakovs
```

```
<POWHEG matching: powheg matching: TBP>+≡
  procedure :: import_norms_from_grid => powheg_matching_import_norms_from_grid

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_import_norms_from_grid (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
    integer :: alr
    real(default) :: norm_max
    do alr = 1, powheg%process_deps%n_alr
      norm_max = powheg%grid%get_maximum_in_3d (alr)
      call powheg%sudakov(alr)%s%set_normalization (norm_max)
    end do
  end subroutine powheg_matching_import_norms_from_grid
```

We save the POWHEG grid to a file to be used for the event generation. If it has no non-zero entries, we assume that the integration was skipped because there were existing VAMP(2) and POWHEG grid files.

```
<POWHEG matching: powheg matching: TBP>+≡
  procedure :: save_grids => powheg_matching_save_grids

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_save_grids (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
    type(string_t) :: filename, n_points
    filename = powheg%process_name // ".pg"
    if (powheg%grid%has_non_zero_entries()) then
      call powheg%grid%save_to_file (char (filename))
    else
      call msg_warning("POWHEG grid not saved to file. An existing " // &
        & char(filename) // " will be used for the events.")
    end if
  end subroutine powheg_matching_save_grids
```

```
<POWHEG matching: powheg matching: TBP>+≡
  procedure :: load_grids => powheg_matching_load_grids

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_load_grids (powheg)
    class(powheg_matching_t), intent(inout) :: powheg
    type(string_t) :: filename, n_points
    filename = powheg%process_name // ".pg"
    call powheg%grid%load_from_file (char (filename))
    if (powheg%grid%has_non_zero_entries()) then
      write (msg_buffer, "(A,A,A)") "POWHEG: using grids from file '", &
        char (filename), "'"
    else
      call msg_fatal("POWHEG grid in " // char(filename) // &
        & " is zero and cannot be used for event generation.")
    end if
    call msg_message ()
  end subroutine powheg_matching_load_grids
```

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: check_grids => powheg_matching_check_grids

<POWHEG matching: procedures>+≡
  function powheg_matching_check_grids (powheg) result (ok)
    logical :: ok
    class(powheg_matching_t), intent(in) :: powheg
    type(string_t) :: filename, n_points
    filename = powheg%process_name // ".pg"
    ok = os_file_exist (filename) .and. &
        verify_points_for_grid (char (filename), &
            [powheg%settings%size_grid_xi, &
            powheg%settings%size_grid_y, &
            powheg%process_deps%n_alr])
  end function powheg_matching_check_grids

```

This routine implements the Sudakov veto algorithm as explained in [1002.2581], Sec. 7.1 and Bijans thesis, Sec. 3.3 and B.2. Here, we veto in order to correct for

1. an overestimation of parts of the upper bounding function for complicated UBFs in `reweight_ubf`
2. the usage of α_s^{rad} instead of α_s^{true} in `reweight_alpha_s`
3. the usage of `xi_max_extended` instead of `xi_max` in `reweight_xi_max` which is only non-trivial for massive FSR.
4. using the maximum of the entire POWHEG normalization grid N_{max} when generating p_T instead of the correct bin value $N(\xi_i, y_i)$ in `reweight_norm`.
5. the normalization grid and the upper bounding function in the first place in `reweight_matrix_elements` to retrieve the correct fraction $\frac{\mathcal{R}(\xi, y) \mathcal{J}(\xi, y)}{\mathcal{B}}$.

By keeping the radiation with the largest `pt2`, we are effectively implementing the highest bid procedure. This means that we generate values (f_B) .

We need to compute `xi2_max` before `kt2_max` here. In the simple case, it is given by $\xi_{\text{max}} = \frac{s - M_{\text{rec}}^2}{s}$ but we can also take the ξ_{max} from the phase space computed before; they coincide. In the eeqq case, $M_{\text{rec}} = 0$, so $x_{i_{\text{max}}} = 1$ and in the massive case, we compute an extended $\xi_{\text{max}} = 1 - \frac{(m + M_{\text{rec}})^2}{q^2}$.

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: generate_emission => powheg_matching_generate_emission

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_generate_emission (powheg, particle_set, pt2_generated)
    class(powheg_matching_t), intent(inout) :: powheg
    type(particle_set_t), intent(inout), optional :: particle_set
    real(default), intent(out), optional :: pt2_generated
    type(radiation_t) :: r, r_max
    real(default) :: xi2_max
    integer :: alr, emitter
    logical :: accepted
    type(vector4_t), dimension(:), allocatable :: p_real_max
    if (signal_is_pending ()) return

```

```

r_max%pt2 = zero
r_max%alr = 0
if (debug_on) call msg_debug (D_MATCHING, "powheg_matching_generate_emission")
select type (pcm => powheg%process_instance%pcm)
type is (pcm_nlo_t)
  allocate (p_real_max (pcm%region_data%n_legs_real))
end select
select type (pcm_work => powheg%process_instance%pcm_work)
class is (pcm_nlo_workspace_t)
  do alr = 1, powheg%process_deps%n_alr
    if (signal_is_pending ()) return
    associate (sudakov => powheg%sudakov(alr)%s)
    select type (sudakov)
    type is (sudakov_simple_fsr_t)
      xi2_max = pcm_work%get_xi_max (alr)**2
      call sudakov%update_xi2_max (xi2_max)
      if (debug2_active (D_MATCHING)) then
        call check_xi2_max (sudakov)
      end if
    type is (sudakov_eeqq_fsr_t)
      call sudakov%update_xi2_max (one)
    type is (sudakov_massive_fsr_t)
      call sudakov%compute_xi_max_extended (sudakov%i_phs)
    end select
    r%alr = alr
    r%pt2 = sudakov%kt2_max ()
    sudakov%sum_log_rands = 0
    if (debug_on) call msg_debug (D_MATCHING, "Starting evolution at r%pt2", r%pt2)
    PT_EVOLUTION: do
      if (signal_is_pending ()) return
      call sudakov%generate_emission (r)
      if (signal_is_pending ()) return
      if (r%valid) then
        accepted = powheg%reweight_norm (r)
        call sudakov%veto_counter%record_norm (.not. accepted)
        if (.not. accepted) cycle PT_EVOLUTION
        accepted = powheg%reweight_matrix_elements (r)
        call sudakov%veto_counter%record_sqme (.not. accepted)
        if (.not. accepted) cycle PT_EVOLUTION
      end if
      exit
    end do PT_EVOLUTION
    if (r%pt2 > r_max%pt2 .and. r%valid) then
      r_max = r
      p_real_max = powheg%event_deps%p_real_lab%get_momenta (sudakov%i_phs)
    end if
  end associate
end do
if (r_max%pt2 > powheg%settings%pt2_min) then
  powheg%n_emissions = powheg%n_emissions + 1
  call powheg%set_scale (r_max%pt2)
  if (present (particle_set)) then
    select type (pcm => powheg%process_instance%pcm)
    type is (pcm_nlo_t)

```

```

        emitter = pcm%region_data%get_emitter (r_max%alr)
        call powheg%build_particle_set (particle_set, &
            powheg%event_deps%p_born_lab%get_momenta (1), &
            p_real_max, emitter)
    end select
end if
if (present (pt2_generated)) pt2_generated = r_max%pt2
else
    call powheg%set_scale (powheg%settings%pt2_min)
    if (present (pt2_generated)) pt2_generated = powheg%settings%pt2_min
end if
end select
contains
subroutine check_xi2_max (sudakov)
    class(sudakov_t), intent(in) :: sudakov
    real(default) :: s_hat, mrec2, xi2_max
    type(vector4_t) :: p_emitter
    s_hat = sudakov%event_deps%s_hat
    p_emitter = sudakov%event_deps%p_born_lab%get_momentum &
        (1, sudakov%associated_emitter())
    associate (p => p_emitter%p)
        mrec2 = (sqrt(s_hat) - p(0))**2 - p(1)**2 - p(2)**2 - p(3)**2
    end associate
    xi2_max = (s_hat - mrec2) / s_hat
    xi2_max = xi2_max**2
    call assert_equal (OUTPUT_UNIT, sudakov%xi2_max, xi2_max, &
        "powheg_matching_generate_emission: xi_max inconsistent")
end subroutine check_xi2_max
end subroutine powheg_matching_generate_emission

```

(POWHEG matching: powheg matching: TBP)+≡

```

    procedure :: build_particle_set => powheg_matching_build_particle_set

```

(POWHEG matching: procedures)+≡

```

subroutine powheg_matching_build_particle_set &
    (powheg, particle_set, p_born, p_real, emitter)
    class(powheg_matching_t), intent(inout) :: powheg
    type(particle_set_t), intent(inout) :: particle_set
    type(vector4_t), dimension(:), intent(in) :: p_born, p_real
    integer, intent(in) :: emitter
    integer, dimension(:), allocatable :: flv_radiated
    real(default) :: r_col
    select type (pcm => powheg%process_instance%pcm)
    type is (pcm_nlo_t)
        allocate (flv_radiated (size (pcm%region_data%get_flv_states_real (1))))
        flv_radiated = pcm%region_data%get_flv_states_real (1)
    end select
    call powheg%rng%generate (r_col)
    call particle_set%build_radiation (p_real, emitter, flv_radiated, &
        powheg%process_instance%process%get_model_ptr (), r_col)
end subroutine powheg_matching_build_particle_set

```

When generating the transverse momentum in `sudakov_generate_pt2`, we used N^{\max} as normalization. In this veto step, we correct for this by keeping events

with probability

$$\frac{N(\xi_i, y_i)}{N^{\max}}.$$

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: reweight_norm => powheg_matching_reweight_norm

<POWHEG matching: procedures>+≡
  function powheg_matching_reweight_norm (powheg, r) result (accepted)
    logical :: accepted
    class(powheg_matching_t), intent(inout) :: powheg
    type(radiation_t), intent(in) :: r
    real(default) :: random, norm_max, norm_true
    if (debug_on) call msg_debug2 (D_MATCHING, "reweight_norm")
    call powheg%rng%generate (random)
    norm_true = powheg%norm_from_xi_and_y (r)
    norm_max = powheg%sudakov(r%alr)%s%norm_max
    accepted = random < norm_true / norm_max
    if (debug2_active (D_MATCHING)) then
      print *, ' r%alr = ', r%alr
      print *, ' random = ', random
      print *, ' norm_true = ', norm_true
      print *, ' norm_max = ', norm_max
      print *, ' norm accepted = ', accepted
    end if
    if (debug_active (D_MATCHING)) then
      if (.not. (zero < r%xi .and. &
        r%xi < sqrt(powheg%sudakov(r%alr)%s%xi2_max))) then
        call msg_bug ("powheg_matching_reweight_norm: xi is out of bounds")
      end if
      if (norm_true > norm_max) then
        call msg_bug ("powheg_matching_reweight_norm: norm shouldnt be larger than norm_max")
      end if
    end if
  end function powheg_matching_reweight_norm

```

Retrieves the value of the norm for given ξ and y from the pre-computed POWHEG grid. To find the correct bin in the grid, we need to invert the generation of ξ and y from their corresponding random numbers. As the grid is filled during integration, the formulas here are the inverse of those in `compute_y_from_emitter` instead of those specific for POWHEG matching. There, we coompute y with $y = (\text{one} - \text{two} * r.y)$ and $y = 1.5_default * (y - y**3 / 3)$. The inverse of this operation is given by

$$r_y = \begin{cases} \frac{1}{4} \left[(i\sqrt{3} - 1)A^{\frac{1}{3}} - (i\sqrt{3} + 1)A^{-\frac{1}{3}} + 2 \right] & \text{for } y < 0 \\ \frac{1}{4} \left[-(i\sqrt{3} + 1)A^{\frac{1}{3}} + (i\sqrt{3} - 1)A^{-\frac{1}{3}} + 2 \right] & \text{for } y > 0 \end{cases}$$

with $A = \sqrt{y^2 - 1} + y$ (31.18)

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: norm_from_xi_and_y => powheg_matching_norm_from_xi_and_y

<POWHEG matching: procedures>+≡
  function powheg_matching_norm_from_xi_and_y (powheg, r) result (norm_true)

```

```

real(default) :: norm_true
class(powheg_matching_t), intent(inout) :: powheg
type(radiation_t), intent(in) :: r
real(default) :: f_alr
real(default), dimension(2) :: rands
real(default) :: beta
f_alr = (one * r%alr) / powheg%process_deps%n_alr - tiny_07
rands(I_XI) = r%xi / sqrt (powheg%sudakov(r%alr)%s%xi2_max)
select type (s => powheg%sudakov(r%alr)%s)
type is (sudakov_simple_fsr_t)
  rands(I_Y) = map_y_to_rands_massless(r%y)
type is (sudakov_massive_fsr_t)
  beta = beta_emitter (sqrt (powheg%event_deps%s_hat), &
    powheg%event_deps%p_born_lab%get_momentum (1, s%associated_emitter()))
  rands(I_Y) = - log((one - r%y * beta) / (one + beta)) / &
    log((one + beta) / (one - beta))
type is (sudakov_eeqq_fsr_t)
  rands(I_Y) = map_y_to_rands_massless(r%y)
end select
norm_true = powheg%grid%get_value ([rands, f_alr])
contains
function map_y_to_rands_massless (y) result (r_y)
  real(default), intent(in) :: y
  real(default) :: r_y
  complex(default) :: y_cmplx, A, r_y_cmplx
  y_cmplx = cmplx(y, 0, default)
  A = sqrt(y_cmplx**2 - 1) + y_cmplx
  if (y < 0) then
    r_y_cmplx = 0.25_default * (cmplx(-one,sqrt(three)) * A**(one/three) &
      - cmplx(one,sqrt(three)) * A**(-one/three) + two)
  else if (y == 0) then
    r_y_cmplx = cmplx(0.5_default,0)
  else if (y > 0) then
    r_y_cmplx = 0.25_default * (-cmplx(one,sqrt(three)) * A**(one/three) &
      + cmplx(-one,sqrt(three)) * A**(-one/three) + two)
  end if
  r_y = real(r_y_cmplx)
end function map_y_to_rands_massless
end function powheg_matching_norm_from_xi_and_y

```

31.4.4 α_s and its reweighting

The main point to ensure here is that the simple fixed-flavor-1-loop expression α_s^{rad} is larger than the more accurate α_s such that we can use a reweighting veto and use α_s^{rad} for the generation of the emission. This can be done by setting

$$\alpha_s^{\text{rad}}(\mu_0) = \alpha_s(\mu_0) \quad (31.19)$$

whereby μ_0^2 is the `scale_to_relate2` that is taken to be $p_{T,\min}^2$.

(POWHEG matching: powheg matching: TBP) +=

```

procedure :: prepare_for_events => powheg_matching_prepare_for_events

```

```

<POWHEG matching: procedures>+≡
subroutine powheg_matching_prepare_for_events (matching)
  class(powheg_matching_t), intent(inout), target :: matching
  if (debug_on) call msg_debug (D_MATCHING, "powheg_matching_prepare_for_events")
  call matching%setup_nlo_environment ()
  call matching%grid%init ([matching%settings%size_grid_xi, &
    matching%settings%size_grid_y, matching%process_deps%n_alr])
  call matching%compute_lambda2_gen ()
  call matching%setup_sudakovs ()
end subroutine powheg_matching_prepare_for_events

```

Computes the scale Λ used for the (log integrated) UBFs. By construction, it is always $p_{T,\min} > \Lambda$.

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: compute_lambda2_gen => powheg_matching_compute_lambda2_gen

```

```

<POWHEG matching: procedures>+≡
subroutine powheg_matching_compute_lambda2_gen (matching)
  class(powheg_matching_t), intent(inout) :: matching
  real(default) :: scale_to_relate2, alpha_s
  scale_to_relate2 = matching%settings%pt2_min
  alpha_s = get_alpha (matching%qcd, scale_to_relate2)
  matching%process_deps%lambda2_gen = exp (- one / (b0rad * alpha_s)) * &
    scale_to_relate2
end subroutine powheg_matching_compute_lambda2_gen

```

```

<POWHEG matching: powheg matching: TBP>+≡
  procedure :: setup_nlo_environment => powheg_matching_setup_nlo_environment

```

```

<POWHEG matching: procedures>+≡
subroutine powheg_matching_setup_nlo_environment (matching)
  class(powheg_matching_t), intent(inout) :: matching
  integer :: n_tot_born, n_tot_real
  integer :: i, i_real, i_term
  integer :: n_phs, nlo_type
  if (debug_on) call msg_debug (D_MATCHING, "powheg_matching_setup_nlo_environment")
  select type (pcm_work => matching%process_instance%pcm_work)
  class is (pcm_nlo_workspace_t)
    matching%process_deps%sqrts = matching%process_instance%get_sqrts ()
    select type (pcm => matching%process_instance%pcm)
    type is (pcm_nlo_t)
      matching%process_deps%n_alr = pcm%region_data%n_regions
      n_tot_born = pcm%region_data%n_legs_born
      n_tot_real = pcm%region_data%n_legs_real
      call pcm%setup_phs_generator (pcm_work, &
        matching%phs_fks_generator, matching%process_deps%sqrts, &
        singular_jacobian = matching%settings%singular_jacobian)
    end select
  end select
  associate (process => matching%process_instance%process)
    i_real = process%get_first_real_component ()
  end associate
  associate (process_deps => matching%process_deps)
    select type (phs => matching%process_instance%kin(i_real)%phs)
    type is (phs_fks_t)

```

```

        n_phs = size (phs%phs_identifiers)
        allocate (process_deps%phs_identifiers (n_phs))
        process_deps%phs_identifiers = phs%phs_identifiers
    end select
    allocate (matching%process_deps%alr_to_i_phs &
        (size (pcm_work%real_kinematics%alr_to_i_phs)))
    process_deps%alr_to_i_phs = pcm_work%real_kinematics%alr_to_i_phs
    allocate (process_deps%i_real (n_phs))
    i = 1
    do i_term = 1, size (matching%process_instance%term)
        nlo_type = matching%process_instance%term(i_term)%nlo_type
        if (nlo_type == BORN) then
            process_deps%i_born = i_term
        else if (nlo_type == NLO_REAL) then
            if (matching%process_instance%kin(i_term)%emitter >= 0) then
                process_deps%i_real(i) = i_term
                i = i + 1
            end if
        end if
    end do
end associate
call matching%event_deps%p_born_lab%init (n_tot_born, 1)
call matching%event_deps%p_born_cms%init (n_tot_born, 1)
call matching%event_deps%p_real_lab%init (n_tot_real, n_phs)
call matching%event_deps%p_real_cms%init (n_tot_real, n_phs)
end select
end subroutine powheg_matching_setup_nlo_environment

```

Copy momenta from `event_deps` to `real_kinematics`. So far this is only valid if the center-of-mass system is equal to the lab frame, i.e. for FSR processes without beamstrahlung or structure functions.

(POWHEG matching: powheg matching: TBP)+≡

```

    procedure :: copy_momenta => powheg_matching_copy_momenta

```

(POWHEG matching: procedures)+≡

```

    subroutine powheg_matching_copy_momenta (matching)
        class(powheg_matching_t), intent(inout) :: matching
        integer :: i_phs
        select type (pcm_work => matching%process_instance%pcm_work)
        class is (pcm_nlo_workspace_t)
            !!! Too much redundancy!
            do i_phs = 1, matching%event_deps%p_real_cms%get_n_phs ()
                call pcm_work%real_kinematics%p_real_cms%set_momenta &
                    (i_phs, matching%event_deps%p_real_cms%get_momenta (i_phs))
                call pcm_work%real_kinematics%p_real_lab%set_momenta &
                    (i_phs, matching%event_deps%p_real_lab%get_momenta (i_phs))
            end do
        end select
    end subroutine powheg_matching_copy_momenta

```

`qcd%alpha%get` should implement a variable-flavor result and optionally return `n_flavors` that are active at the scale...

(POWHEG matching: procedures)+≡


```

function get_alpha (qcd, scale2) result (alpha_s)
  real(default) :: alpha_s
  class(qcd_t), intent(in) :: qcd
  real(default), intent(in) :: scale2
  integer :: nf, order
  ! TODO: (bcn 2015-01-30) implement variable flavor alpha_s
  alpha_s = qcd%alpha%get (sqrt(scale2))
  select type (alpha => qcd%alpha)
  type is (alpha_qcd_from_scale_t)
    nf = alpha%nf
    order = alpha%order
  type is (alpha_qcd_from_lambda_t)
    nf = alpha%nf
    order = alpha%order
  class default
    call msg_warning ("get_alpha: QCD type is not running!" // &
      "Assuming 5-flavors and L0 (1-loop) running!")
    nf = 5
    order = 0
  end select
  if (order > 0) alpha_s = improve_nll_accuracy (alpha_s, nf)
end function get_alpha

```

See Eq. (4.31) in 0709.2092. Should be used everywhere in the Sudakov exponent.

```

<POWHEG matching: procedures>+≡
pure function improve_nll_accuracy (alpha_s, n_flavors) result (alpha_s_imp)
  real(default) :: alpha_s_imp
  real(default), intent(in) :: alpha_s
  integer, intent(in) :: n_flavors
  alpha_s_imp = alpha_s * (one + alpha_s / (two*pi) * &
    ((67.0_default/18 - pi**2/6) * CA - five/9 * n_flavors))
end function improve_nll_accuracy

```

This is fixed to $n_f = 5$ for radiation generation. It will be reweighted to the more precise α_s .

```

<POWHEG matching: parameters>≡
real(default), parameter :: b0rad = (33 - 2 * 5) / (12 * pi)

<POWHEG matching: sudakov: TBP>+≡
procedure :: alpha_s_rad => sudakov_alpha_s_rad

<POWHEG matching: procedures>+≡
elemental function sudakov_alpha_s_rad (sudakov, scale2) result (y)
  real(default) :: y
  class(sudakov_t), intent(in) :: sudakov
  real(default), intent(in) :: scale2
  y = one / (b0rad * log (scale2 / sudakov%process_deps%lambda2_gen))
end function sudakov_alpha_s_rad

```

```

<POWHEG matching: sudakov: TBP>+≡
procedure :: reweight_alpha_s => sudakov_reweight_alpha_s

```

```

<POWHEG matching: procedures>+≡
function sudakov_reweight_alpha_s (sudakov, pt2) result (accepted)
  logical :: accepted
  class(sudakov_t), intent(inout) :: sudakov
  real(default), intent(in) :: pt2
  real(default) :: alpha_s_true, alpha_s_rad
  logical :: alpha_s_equal
  if (debug_on) call msg_debug2 (D_MATCHING, "reweight_alpha_s")
  alpha_s_true = get_alpha (sudakov%qcd, pt2)
  alpha_s_rad = sudakov%alpha_s_rad (pt2)
  call sudakov%rng%generate (sudakov%random)
  alpha_s_equal = nearly_equal (alpha_s_true, alpha_s_rad)
  accepted = alpha_s_equal .or. sudakov%random < alpha_s_true / alpha_s_rad
  if (debug2_active (D_MATCHING)) then
    print *, ' sudakov%random = ', sudakov%random
    print *, ' alpha_s_true = ', alpha_s_true
    print *, ' alpha_s_rad = ', alpha_s_rad
    print *, ' alpha_s accepted = ', accepted
    if (alpha_s_rad < alpha_s_true .and. .not. alpha_s_equal) then
      print *, 'pt2 = ', pt2
      print *, 'sudakov%process_deps%lambda2_gen = ', &
        sudakov%process_deps%lambda2_gen
      call msg_fatal ("sudakov_reweight_alpha_s: This should never happen. &
        &Have you chosen a running alpha_s?")
    end if
  end if
end function sudakov_reweight_alpha_s

```

31.4.5 POWHEG hook

We provide a POWHEG hook to be called by `process_instance_evaluate` to prefill the adaptation grid.

We store the actual `powheg` object, which does the computations.

```

<POWHEG matching: public>+≡
public :: powheg_matching_hook_t

<POWHEG matching: types>+≡
type, extends(process_instance_hook_t) :: powheg_matching_hook_t
  type(string_t) :: process_name
  type(powheg_matching_t) :: powheg
contains
  <POWHEG matching: powheg matching hook: TBP>
end type powheg_matching_hook_t

```

Init the hook. The init procedure will be called in `setup_process`, after everything is set up.

Additionally, we have to include `var_list` in order to retrieve the grid size in `xi` and `y`.

```

<POWHEG matching: powheg matching hook: TBP>≡
procedure :: init => powheg_matching_hook_init

```

```

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_hook_init (hook, var_list, instance)
    class(powheg_matching_hook_t), intent(inout), target :: hook
    type(var_list_t), intent(in) :: var_list
    class(process_instance_t), intent(in), target :: instance
    if (debug_on) call msg_debug (D_MATCHING, "powheg_matching_hook_init")
    hook%process_name = instance%get_process_name ()
    call hook%powheg%init (var_list, hook%process_name)
    hook%powheg%qcd = instance%get_qcd ()
    call hook%powheg%connect (instance)
    hook%powheg%process_deps%lab_is_cm = &
      hook%powheg%process_instance%lab_is_cm (1)
    call hook%powheg%prepare_for_events ()
  end subroutine powheg_matching_hook_init

```

We save the filled grid to file, such that it can be retrieved later on. The hook object will be deallocated when the instance gets deallocated.

```

<POWHEG matching: powheg matching hook: TBP>+≡
  procedure :: final => powheg_matching_hook_final

<POWHEG matching: procedures>+≡
  subroutine powheg_matching_hook_final (hook)
    class(powheg_matching_hook_t), intent(inout) :: hook
    type(string_t) :: filename
    if (debug_on) call msg_debug (D_MATCHING, "powheg_matching_hook_final")
    <POWHEG matching: powheg matching hook final: reduce>
    call hook%powheg%save_grids ()
  end subroutine powheg_matching_hook_final

```

<POWHEG matching: powheg matching hook final: reduce>≡

Reduce all grids to a single grid by using MPI_MAX on each element.

```

<MPI: POWHEG matching: powheg matching hook final: reduce>≡
  call hook%powheg%grid%mpi_reduce (MPI_MAX)

```

This routine fills each bin of the POWHEG normalization grid $\{\tilde{\xi}, \tilde{y}\}$ such that

$$N(\{\tilde{\xi}, \tilde{y}\}) = \max_{\forall \xi, y \in \{\tilde{\xi}, \tilde{y}\}} \frac{\mathcal{R}(\xi, y) \mathcal{J}(\xi, y)}{\mathcal{B} U(\xi, y, \alpha_s^{\text{true}})} \quad (31.20)$$

where $\mathcal{R}(\xi, y)$ is the real cross section `sqme_real`, \mathcal{B} is the Born cross section `sqme_born`, \mathcal{J} is the Jacobian and U the upper bounding function `ubf`.

For each underlying Born f_b , there is a number of radiation regions. A radiation region `rr` may correspond to multiple α_r s. The phase space only depends upon the radiation region kinematics `rr` and not on the specific α_r . α_r can be picked in the set $\{\alpha_r | f_b, rr\}$ proportional to their R_{α_r} . For now, we simplify things though and just work with the α_r .

References:

-

1002.2581

, Sec. 7.1

- Bijans Thesis, Sec. 3.3 and B.2

In cases where just the Born kinematic failed the cuts, \mathcal{B} was artificially set to zero. Unfortunately, we lost information about the value of `sqme_born` in these cases but we assume that the generator cuts applied for parton showering are weak cuts to avoid divergent phase space regions, thus \mathcal{B} is large and does not influence N so we can skip these phase space points.

A more appropriate way to solve this problem of Born zeroes is given by the real partition. With real partition, there are two possible cases if $\mathcal{B} = 0$: if the real phase space point belongs to the real singular, the real kinematic is Born-like and very likely also fails the cuts. If the real kinematic is not Born-like, it belongs to the real finite. In both cases, it is $\mathcal{R} = \mathcal{B} = 0$ and we can safely skip the phase space point.

In cases where just the real kinematic failed the cuts, \mathcal{R} was artificially set to zero and we have no way to recover it. We skip these phase space points too. If we apply the same cuts during integration and event generation, these points are not relevant.

```

(POWHEG matching: powheg matching hook: TBP)+≡
  procedure :: evaluate => powheg_matching_hook_evaluate
(POWHEG matching: procedures)+≡
  subroutine powheg_matching_hook_evaluate (hook, instance)
    class(powheg_matching_hook_t), intent(inout) :: hook
    class(process_instance_t), intent(in), target :: instance
    type(vector4_t), dimension(:), allocatable :: p_hard
    real(default), dimension(:), allocatable :: x
    real(default) :: xi, y
    real(default) :: sqme_real, sqme_born, alpha_s
    real(default) :: f_alr, norm, ubf
    integer :: alr, i_phs, i_real, n_x
    if (instance%get_active_component_type () == COMP_REAL_FIN) return
    associate (powheg => hook%powheg)
      allocate (p_hard (size (instance%get_p_hard (1))))
      p_hard = instance%get_p_hard (1)
      call powheg%update (p_hard)
      i_real = instance%process%get_first_real_component ()
      do alr = 1, powheg%process_deps%n_alr
        i_phs = powheg%process_deps%alr_to_i_phs (alr)
        select type (phs => instance%kin( &
          powheg%process_deps%i_real(i_phs))%phs)
          type is (phs_fks_t)
            call phs%generator%get_radiation_variables (i_phs, xi, y)
          end select
          call powheg%update_sudakovs (alr, i_phs, y)
          sqme_born = instance%get_sqme (powheg%process_deps%i_born)
          sqme_real = instance%get_sqme (powheg%process_deps%i_real(i_phs))
          if (sqme_born == 0 .or. sqme_real == 0) then
            cycle
          end if
          if (powheg%sudakov(alr)%s%kt2 (xi, y) >= powheg%settings%pt2_min) then
            associate (s => powheg%sudakov(alr)%s)
              alpha_s = s%alpha_s (s%kt2(xi, y), use_correct=.true.)
              ubf = s%upper_bound_func (xi, y, alpha_s)
            end associate
          end if
        end do
      end associate
    end subroutine

```

```

        norm = sqme_real / (sqme_born * ubf)
        f_alr = (one * alr) / powheg%process_deps%n_alr - tiny_07
        if (.not. allocated (x)) &
            allocate (x(size (instance%get_x_process ())))
        x = instance%get_x_process ()
        n_x = size (x)
        call powheg%grid%update_maxima &
            ([x(n_x - 2 : n_x - 1), f_alr], norm)
    end if
end do
end associate
end subroutine powheg_matching_hook_evaluate

```

31.4.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<powheg_matching_ut.f90>≡
<File header>

module powheg_matching_ut
    use unit_tests
    use powheg_matching_util

    <Standard module head>

    <POWHEG matching: public test>

contains

    <POWHEG matching: test driver>

end module powheg_matching_ut

<powheg_matching_util.f90>≡
<File header>

module powheg_matching_util

    <Use kinds>
    <Use strings>
    use constants, only: zero, one
    use lorentz
    use physics_defs, only: LAMBDA_QCD_REF
    use sm_qcd
    use subevents, only: PRT_INCOMING, PRT_OUTGOING
    use model_data
    use particles
    use rng_base
    use variables
    use shower_base
    use shower_core

    use powheg_matching

```

```

    use rng_base_ut, only: rng_test_factory_t

    <Standard module head>

    <POWHEG matching: test declarations>

contains

    <POWHEG matching: tests>

end module powheg_matching_utl
API: driver for the unit tests below.
<POWHEG matching: public test>≡
    public :: powheg_test
<POWHEG matching: test driver>≡
    subroutine powheg_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <POWHEG matching: execute tests>
    end subroutine powheg_test

```

Initialization

There are no Powheg unit tests so far.

Compare generated emission with Sudakov form factor

This is a nontrivial test of the generation algorithm and should be independent of the used upper bounding function (as long as all singularities are included).

It runs for an extensive amount of time generating a file `sudakov.dat` containing a histogram for the Sudakov factor in bins of the radiation's transverse momentum p_T^2 .

So far, it is only designed to work for lepton collisions without beam spectra and cuts. In its current state however, it fills the histogram with either 1 or NaN as the `p_hard` received in `term_instance_evaluate_interaction` is identically zero.

```

<POWHEG matching: powheg matching: TBP>+≡
    procedure :: test_sudakov => powheg_test_sudakov

<POWHEG matching: procedures>+≡
    subroutine powheg_test_sudakov (powheg)
        class(powheg_matching_t), intent(inout) :: powheg
        integer :: n_calls1, n_calls2
        integer, parameter :: n_bins = 20
        real(default) :: sqme_real_x_jacobian, sqme_born
        type(vector4_t), dimension(:), allocatable :: p_born
        real(default), dimension(3) :: random
        real(default) :: xi, y
        integer :: i_call, i_bin, alr, emitter, i_phs
        real(default) :: alpha_s, kt2, weight
    end subroutine powheg_test_sudakov

```

```

real(default) :: pt2_min, s, random_jacobian
real(default), dimension(n_bins) :: histo1, histo2, histo1sq, histo2sq
real(default), dimension(n_bins) :: tmp
integer :: i_strip, n_in_strip, n_strips
real(default), dimension(n_bins) :: average, average_sq, error
real(default), dimension(n_bins) :: &
    sudakov_0, sudakov_p, sudakov_m, rel_error
integer :: u

p_born = powheg%event_deps%p_born_lab%get_momenta (1)
sqme_born = powheg%event_deps%sqme_born
s = powheg%event_deps%s_hat
pt2_min = powheg%settings%pt2_min
n_calls1 = 100000; n_calls2 = 1000000
histo1 = zero; histo2 = zero; histo1sq = zero; histo2sq = zero
n_strips = 10

call compute_integrals ()
call generate_emissions ()
call write_to_screen_and_file ()

contains

<POWHEG matching: powheg test sudakov: procedures>

end subroutine powheg_test_sudakov

```

This determines the binning of the Sudakov histogram. Linear and logarithmic binning are available.

<POWHEG matching: powheg test sudakov: procedures>≡

```

pure function binning (i) result (pt2)
    real(default) :: pt2
    integer, intent(in) :: i
    !pt2 = pt2_min + (s-pt2_min) * (i-1) / (n_bins-1)
    pt2 = pt2_min * exp (log (s / pt2_min) * (i-1) / (n_bins-1))
end function

```

<POWHEG matching: powheg test sudakov: procedures>+≡

```

subroutine compute_integrals ()
    write (msg_buffer, "(A)") "POWHEG: test_sudakov: Computing integrals"
    call msg_message ()
    select type (pcm_work => powheg%process_instance%pcm_work)
    class is (pcm_nlo_workspace_t)
        associate (fks => powheg%phs_fks_generator)
            do i_call = 1, n_calls1
                do alr = 1, powheg%process_deps%n_alr
                    call powheg%rng%generate (random)
                    select type (pcm => powheg%process_instance%pcm)
                    type is (pcm_nlo_t)
                        emitter = pcm%region_data%get_emitter (alr)
                        i_phs = powheg%process_deps%alr_to_i_phs(alr)
                    end select
                end do
            end do
        end associate
    end select
    !!! The sudakov test works only with lepton collisions without beam spectra

```

```

!!! so we can identify the cms and lab momenta.
powheg%event_deps%p_real_lab = powheg%event_deps%p_real_cms
call powheg%copy_momenta ()
call fks%get_radiation_variables (i_phs, xi, y)
kT2 = powheg%sudakov(alr)%s%kt2(xi, y)
if (kT2 >= pt2_min .and. xi < one - tiny_07) then
  alpha_s = get_alpha (powheg%qcd, kT2)
  sqme_real_x_jacobian = powheg%compute_sqme_real (alr, alpha_s)
  random_jacobian = pcm_work%real_kinematics%jac_rand (emitter)
  weight = sqme_real_x_jacobian * random_jacobian / sqme_born
  do i_bin = 1, n_bins
    if (kT2 > binning(i_bin)) then
      histo1(i_bin) = histo1(i_bin) + weight
      histo1sq(i_bin) = histo1sq(i_bin) + weight**2
    end if
  end do
end if
! Do not cycle since there is a Heaviside in the exponent
end do
call msg_show_progress (i_call, n_calls1)
end do
end associate
end select
average = histo1 / n_calls1
average_sq = histo1sq / n_calls1
error = sqrt ((average_sq - average**2) / n_calls1)
sudakov_0 = exp(-average)
sudakov_p = exp(-(average + error))
sudakov_m = exp(-(average - error))
rel_error = (sudakov_m - sudakov_p) / (2 * sudakov_0) * 100
end subroutine compute_integrals

```

(POWHEG matching: powheg test sudakov: procedures)+≡

```

subroutine generate_emissions ()
  write (msg_buffer, "(A)") "POWHEG: test_sudakov: Generating emissions"
  call msg_message ()
  do i_strip = 1, n_strips
    tmp = 0
    n_in_strip = n_calls2 / n_strips
    do i_call = 1, n_in_strip
      if (signal_is_pending ()) return
      call powheg%generate_emission (pt2_generated = kT2)
      do i_bin = 1, n_bins
        if (kT2 > binning(i_bin)) then
          tmp(i_bin) = tmp(i_bin) + 1
        end if
      end do
    end do
    tmp = one - (one * tmp) / n_in_strip
    histo2 = histo2 + tmp
    histo2sq = histo2sq + tmp**2
    call msg_show_progress (i_strip, n_strips)
  end do
  average = histo2 / n_strips

```



```

        average_sq = histo2sq / n_strips
        error = sqrt ((average_sq - average**2) / n_strips)
    end subroutine generate_emissions

```

(POWHEG matching: powheg test sudakov: procedures)+≡

```

subroutine write_to_screen_and_file ()
    u = free_unit ()
    open (file='sudakov.dat', unit=u, action='write')
    print *, 'exp(-Integrated R/B)-distribution: '
    print *, 'pT2  sudakov_+  sudakov_0  sudakov_-  rel_err[%]: '
    do i_bin = 1, n_bins
        print *, binning(i_bin), &
            sudakov_p(i_bin), sudakov_0(i_bin), sudakov_m(i_bin), &
            rel_error(i_bin)
        write (u, "(6(" // FMT_16 // ",2X))" binning(i_bin), &
            sudakov_p(i_bin), sudakov_0(i_bin), sudakov_m(i_bin), &
            average(i_bin), error(i_bin)
    end do
    close (u)
    print *, '*****'
    print *, 'Noemission probability: '
    do i_bin = 1, n_bins
        print *, binning (i_bin), average (i_bin), error(i_bin)
    end do
end subroutine write_to_screen_and_file

```

Chapter 32

Event Implementation

With a process object and the associated methods at hand, we can generate events for elementary processes and, by subsequent transformation, for complete physical processes.

We have the following modules:

event_transforms Abstract base type for transforming a physical process with process instance and included evaluators, etc., into a new object. The following modules extend this base type.

resonance_insertion Insert a resonance history into an event record, based on kinematical and matrix-element information.

recoil_kinematics Common kinematics routines for the ISR and EPA handlers.

isr_photon_handler Transform collinear kinematics, as it results from applying ISR radiation, to non-collinear kinematics with a reasonable transverse-momentum distribution of the radiated photons, and also of the recoiling partonic event.

epa_beam_handler For photon-initiated processes where the effective photon approximation is used in integration, to add in beam-particle recoil. Analogous to the ISR handler.

decays Combine the elementary process with elementary decay processes and thus transform the elementary event into a decayed event, still at the parton level.

showers Create QED/QCD showers out of the partons that are emitted by elementary processes. This should be interleaved with showering of radiated particles (structure functions) and multiple interactions.

hadrons (not implemented yet) Apply hadronization to the partonic events, interleaved with hadron decays. (The current setup relies on hadronizing partonic events externally.)

tau_decays (not implemented yet) Let τ leptons decay taking full spin correlations into account.

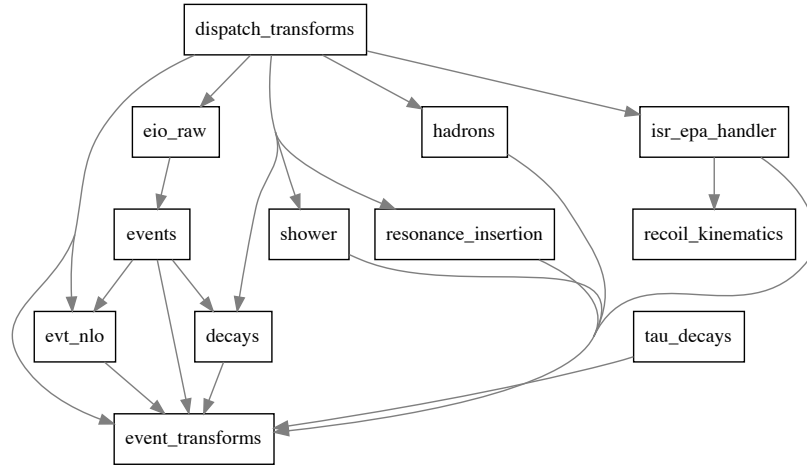


Figure 32.1: Module dependencies in `src/transforms`.

evt_nlo Handler for fixed-order NLO events.

events Combine all pieces to generate full events.

eio_raw Raw I/O for complete events.

32.1 Abstract Event Transforms

```

<event_transforms.f90>≡
  <File header>

  module event_transforms

    <Use kinds>
    <Use strings>
    use io_units
    use format_utils, only: write_separator
    use diagnostics
    use model_data
    use interactions
    use particles
    use subevents
    use rng_base
    use quantum_numbers, only: quantum_numbers_t
    use process, only: process_t
    use instances, only: process_instance_t
    use process_stacks

    <Standard module head>

```

```

    <Event transforms: public>

    <Event transforms: types>

    <Event transforms: interfaces>

contains

    <Event transforms: procedures>

end module event_transforms

```

32.1.1 Abstract base type

Essentially, all methods are abstract, but some get minimal base versions. We know that there will be a random-number generator at top level, and that we will relate to an elementary process.

The model is stored separately. It may contain modified settings that differ from the model instance stored in the process object.

Each event transform contains a particle set that it can fill for further use. There is a flag that indicates this.

We will collect event transforms in a list, therefore we include `previous` and `next` pointers.

```

<Event transforms: public>≡
    public :: evt_t

<Event transforms: types>≡
    type, abstract :: evt_t
        type(process_t), pointer :: process => null ()
        type(process_instance_t), pointer :: process_instance => null ()
        class(model_data_t), pointer :: model => null ()
        class(rng_t), allocatable :: rng
        integer :: rejection_count = 0
        logical :: particle_set_exists = .false.
        type(particle_set_t) :: particle_set
        class(evt_t), pointer :: previous => null ()
        class(evt_t), pointer :: next => null ()
        logical :: only_weighted_events = .false.
    contains
        <Event transforms: evt: TBP>
    end type evt_t

```

Finalizer. In any case, we finalize the r.n.g. The process instance is a pointer and should not be finalized here.

```

<Event transforms: evt: TBP>≡
    procedure :: final => evt_final
    procedure :: base_final => evt_final

<Event transforms: procedures>≡
    subroutine evt_final (evt)
        class(evt_t), intent(inout) :: evt

```

```

    if (allocated (evt%rng)) call evt%rng%final ()
    if (evt%particle_set_exists) &
        call evt%particle_set%final ()
end subroutine evt_final

```

Print out the type of the evt.

```

<Event transforms: evt: TBP>+≡
    procedure (evt_write_name), deferred :: write_name

```

```

<Event transforms: interfaces>≡
    abstract interface
        subroutine evt_write_name (evt, unit)
            import
            class(evt_t), intent(in) :: evt
            integer, intent(in), optional :: unit
        end subroutine evt_write_name
    end interface

```

```

<Event transforms: evt: TBP>+≡
    procedure (evt_write), deferred :: write

```

```

<Event transforms: interfaces>+≡
    abstract interface
        subroutine evt_write (evt, unit, verbose, more_verbose, testflag)
            import
            class(evt_t), intent(in) :: evt
            integer, intent(in), optional :: unit
            logical, intent(in), optional :: verbose, more_verbose, testflag
        end subroutine evt_write
    end interface

```

Output. We can print r.n.g. info.

```

<Event transforms: evt: TBP>+≡
    procedure :: base_write => evt_base_write

```

```

<Event transforms: procedures>+≡
    subroutine evt_base_write (evt, unit, testflag, show_set)
        class(evt_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag, show_set
        integer :: u
        logical :: show
        u = given_output_unit (unit)
        show = .true.; if (present (show_set)) show = show_set
        if (associated (evt%process)) then
            write (u, "(3x,A,A,A)") "Associated process: '", &
                char (evt%process%get_id ()), "'"
        end if
        if (allocated (evt%rng)) then
            call evt%rng%write (u, 1)
            write (u, "(3x,A,I0)") "Number of tries = ", evt%rejection_count
        end if
        if (show) then
            if (evt%particle_set_exists) then

```

```

        call write_separator (u)
        call evt%particle_set%write (u, testflag = testflag)
    end if
end if
end subroutine evt_base_write

```

Connect the transform with a process instance (and thus with the associated process). Use this to allocate the master random-number generator.

This is not an initializer; we may initialize the transform by implementation-specific methods.

```

<Event transforms: evt: TBP>+≡
    procedure :: connect => evt_connect
    procedure :: base_connect => evt_connect

<Event transforms: procedures>+≡
    subroutine evt_connect (evt, process_instance, model, process_stack)
        class(evt_t), intent(inout), target :: evt
        type(process_instance_t), intent(in), target :: process_instance
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
        evt%process => process_instance%process
        evt%process_instance => process_instance
        evt%model => model
        call evt%process%make_rng (evt%rng)
    end subroutine evt_connect

```

Reset internal state.

```

<Event transforms: evt: TBP>+≡
    procedure :: reset => evt_reset
    procedure :: base_reset => evt_reset

<Event transforms: procedures>+≡
    subroutine evt_reset (evt)
        class(evt_t), intent(inout) :: evt
        evt%rejection_count = 0
        call evt%particle_set%final ()
        evt%particle_set_exists = .false.
    end subroutine evt_reset

```

Prepare for a new event: reset internal state, if necessary. We provide MCI and term index of the parent process.

```

<Event transforms: evt: TBP>+≡
    procedure (evt_prepare_new_event), deferred :: prepare_new_event

<Event transforms: interfaces>+≡
    interface
        subroutine evt_prepare_new_event (evt, i_mci, i_term)
            import
            class(evt_t), intent(inout) :: evt
            integer, intent(in) :: i_mci, i_term
        end subroutine evt_prepare_new_event
    end interface

```

Generate a weighted event, using a valid initiator event in the process instance, and the random-number generator. The returned event probability should be a number between zero and one that we can use for rejection.

```

(Event transforms: evt: TBP)+≡
  procedure (evt_generate_weighted), deferred :: generate_weighted

(Event transforms: interfaces)+≡
  abstract interface
    subroutine evt_generate_weighted (evt, probability)
      import
      class(evt_t), intent(inout) :: evt
      real(default), intent(inout) :: probability
    end subroutine evt_generate_weighted
  end interface

```

The unweighted event generation routine is actually implemented. It uses the random-number generator for simple rejection. Of course, the implementation may override this and implement a different way of generating an unweighted event.

```

(Event transforms: evt: TBP)+≡
  procedure :: generate_unweighted => evt_generate_unweighted
  procedure :: base_generate_unweighted => evt_generate_unweighted

(Event transforms: procedures)+≡
  subroutine evt_generate_unweighted (evt)
    class(evt_t), intent(inout) :: evt
    real(default) :: p, x
    evt%rejection_count = 0
    REJECTION: do
      evt%rejection_count = evt%rejection_count + 1
      call evt%generate_weighted (p)
      if (signal_is_pending ()) return
      call evt%rng%generate (x)
      if (x < p) exit REJECTION
    end do REJECTION
  end subroutine evt_generate_unweighted

```

Make a particle set. This should take the most recent evaluator (or whatever stores the event), factorize the density matrix if necessary, and store as a particle set.

If applicable, the factorization should make use of the `factorization_mode` and `keep_correlations` settings.

The values `r`, if set, should control the factorization in more detail, e.g., bypassing the random-number generator.

```

(Event transforms: evt: TBP)+≡
  procedure (evt_make_particle_set), deferred :: make_particle_set

(Event transforms: interfaces)+≡
  interface
    subroutine evt_make_particle_set &
      (evt, factorization_mode, keep_correlations, r)
    import
    class(evt_t), intent(inout) :: evt
  end interface

```

```

        integer, intent(in) :: factorization_mode
        logical, intent(in) :: keep_correlations
        real(default), dimension(:), intent(in), optional :: r
    end subroutine evt_make_particle_set
end interface

```

Copy an existing particle set into the event record. This bypasses all methods to evaluate the internal state, but may be sufficient for further processing.

<Event transforms: evt: TBP>+≡

```

    procedure :: set_particle_set => evt_set_particle_set

```

<Event transforms: procedures>+≡

```

    subroutine evt_set_particle_set (evt, particle_set, i_mci, i_term)
        class(evt_t), intent(inout) :: evt
        type(particle_set_t), intent(in) :: particle_set
        integer, intent(in) :: i_term, i_mci
        call evt%prepare_new_event (i_mci, i_term)
        evt%particle_set = particle_set
        evt%particle_set_exists = .true.
    end subroutine evt_set_particle_set

```

This procedure can help in the previous task, if the particles are available in the form of an interaction object. We need two interactions, one with color summed over, the `int_matrix`, and one with the probability distributed among flows, the `int_flows`.

We use the two values from the random number generator saved in `r` for factorizing the state. For testing purposes, we can provide those numbers explicitly.

The optional `qn_select` allows to limit the number of quantum numbers to choose from when factorizing. If only a single set of quantum numbers is given, it effectively dictates the quantum numbers chosen for the event.

<Event transforms: evt: TBP>+≡

```

    procedure :: factorize_interactions => evt_factorize_interactions

```

<Event transforms: procedures>+≡

```

    subroutine evt_factorize_interactions &
        (evt, int_matrix, int_flows, factorization_mode, &
         keep_correlations, r, qn_select)
        class(evt_t), intent(inout) :: evt
        type(interaction_t), intent(in), target :: int_matrix, int_flows
        integer, intent(in) :: factorization_mode
        logical, intent(in) :: keep_correlations
        real(default), dimension(:), intent(in), optional :: r
        type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
        real(default), dimension(2) :: x
        if (present (r)) then
            if (size (r) == 2) then
                x = r
            else
                call msg_bug ("event factorization: size of r array must be 2")
            end if
        else
            call evt%rng%generate (x)

```



```

end if
call evt%particle_set%init (evt%particle_set_exists, &
    int_matrix, int_flows, factorization_mode, x, &
    keep_correlations, keep_virtual=.true., qn_select = qn_select)
evt%particle_set_exists = .true.
end subroutine evt_factorize_interactions

```

<Event transforms: public>+≡

```

public :: make_factorized_particle_set

```

<Event transforms: procedures>+≡

```

subroutine make_factorized_particle_set (evt, factorization_mode, &
    keep_correlations, r, ii_term, qn_select)
class(evt_t), intent(inout) :: evt
integer, intent(in) :: factorization_mode
logical, intent(in) :: keep_correlations
real(default), dimension(:), intent(in), optional :: r
integer, intent(in), optional :: ii_term
type(quantum_numbers_t), dimension(:), intent(in), optional :: qn_select
integer :: i_term
type(interaction_t), pointer :: int_matrix, int_flows
if (evt%process_instance%is_complete_event ()) then
    if (present (ii_term)) then
        i_term = ii_term
    else
        i_term = evt%process_instance%select_i_term ()
    end if
    int_matrix => evt%process_instance%get_matrix_int_ptr (i_term)
    int_flows => evt%process_instance%get_flows_int_ptr (i_term)
    call evt%factorize_interactions (int_matrix, int_flows, &
        factorization_mode, keep_correlations, r, qn_select)
    call evt%tag_incoming ()
else
    call msg_bug ("Event factorization: event is incomplete")
end if
end subroutine make_factorized_particle_set

```

Mark the incoming particles as incoming in the particle set. This is necessary because in the interaction objects they are usually marked as virtual.

In the inquiry functions we set the term index to one; the indices of beams and incoming particles should be identical for all process terms.

We use the initial elementary process for obtaining the indices. Thus, we implicitly assume that the beam and incoming indices stay the same across event transforms. If this is not true for a transform (say, MPI), it should override this method.

<Event transforms: evt: TBP>+≡

```

procedure :: tag_incoming => evt_tag_incoming

```

<Event transforms: procedures>+≡

```

subroutine evt_tag_incoming (evt)
class(evt_t), intent(inout) :: evt
integer :: i_term, n_in
integer, dimension(:), allocatable :: beam_index, in_index

```

```

n_in = evt%process%get_n_in ()
i_term = 1
allocate (beam_index (n_in))
call evt%process_instance%get_beam_index (i_term, beam_index)
call evt%particle_set%reset_status (beam_index, PRT_BEAM)
allocate (in_index (n_in))
call evt%process_instance%get_in_index (i_term, in_index)
call evt%particle_set%reset_status (in_index, PRT_INCOMING)
end subroutine evt_tag_incoming

```

32.1.2 Implementation: Trivial transform

This transform contains just a pointer to process and process instance. The `generate` methods do nothing.

```

<Event transforms: public>+≡
  public :: evt_trivial_t

<Event transforms: types>+≡
  type, extends (evt_t) :: evt_trivial_t
  contains
    <Event transforms: evt trivial: TBP>
  end type evt_trivial_t

<Event transforms: evt trivial: TBP>≡
  procedure :: write_name => evt_trivial_write_name

<Event transforms: procedures>+≡
  subroutine evt_trivial_write_name (evt, unit)
    class(evt_trivial_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: trivial (hard process)"
  end subroutine evt_trivial_write_name

```

The finalizer is trivial. Some output:

```

<Event transforms: evt trivial: TBP>+≡
  procedure :: write => evt_trivial_write

<Event transforms: procedures>+≡
  subroutine evt_trivial_write (evt, unit, verbose, more_verbose, testflag)
    class(evt_trivial_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    call evt%write_name (u)
    call write_separator (u)
    call evt%base_write (u, testflag = testflag)
    !!! More readable but wider output; in line with evt_resonance_write
    !   if (verbose .and. evt%particle_set_exists) then

```

```

!      call evt%particle_set%write &
!      (u, summary = .true., compressed = .true., testflag = testflag)
!      call write_separator (u)
!      end if
end subroutine evt_trivial_write

```

Nothing to do here:

```

<Event transforms: evt trivial: TBP>+≡
  procedure :: prepare_new_event => evt_trivial_prepare_new_event

<Event transforms: procedures>+≡
  subroutine evt_trivial_prepare_new_event (evt, i_mci, i_term)
    class(evt_trivial_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    call evt%reset ()
  end subroutine evt_trivial_prepare_new_event

```

The weighted generator is, surprisingly, trivial.

```

<Event transforms: evt trivial: TBP>+≡
  procedure :: generate_weighted => evt_trivial_generate_weighted

<Event transforms: procedures>+≡
  subroutine evt_trivial_generate_weighted (evt, probability)
    class(evt_trivial_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
    probability = 1
  end subroutine evt_trivial_generate_weighted

```

This routine makes a particle set, using the associated process instance as-is. Note that it is a potential risk to tolerate a non-existent particle set at this point. We should remove it once the flavors are determined correctly in all cases. It is currently necessary if we are keeping failed events `?keep_failed_events = .true.`. For these events, we do not compute the matrix elements, so the factorization fails trying to determine the quantum numbers. Additionally, it is necessary for the trivial event transformation preceeding the event transformations required for POWHEG matching.

```

<Event transforms: evt trivial: TBP>+≡
  procedure :: make_particle_set => evt_trivial_make_particle_set

<Event transforms: procedures>+≡
  subroutine evt_trivial_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_trivial_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
    call make_factorized_particle_set (evt, factorization_mode, &
      keep_correlations, r)
    evt%particle_set_exists = .true.
  end subroutine evt_trivial_make_particle_set

```

32.1.3 Unit tests

Test module, followed by the corresponding implementation module.

```
(event_transforms_ut.f90)≡
  ⟨File header⟩

  module event_transforms_ut
    use unit_tests
    use event_transforms_uti

    ⟨Standard module head⟩

    ⟨Event transforms: public test⟩

    contains

    ⟨Event transforms: test driver⟩

  end module event_transforms_ut

(event_transforms_uti.f90)≡
  ⟨File header⟩

  module event_transforms_uti

    ⟨Use kinds⟩
    ⟨Use strings⟩
    use format_utils, only: write_separator
    use os_interface
    use sm_qcd
    use models
    use state_matrices, only: FM_IGNORE_HELICITY
    use interactions, only: reset_interaction_counter
    use process_libraries
    use rng_base
    use mci_base
    use mci_midpoint
    use phs_base
    use phs_single
    use prc_core
    use prc_test, only: prc_test_create_library

    use process, only: process_t
    use instances, only: process_instance_t

    use event_transforms

    use rng_base_ut, only: rng_test_factory_t

    ⟨Standard module head⟩

    ⟨Event transforms: test declarations⟩

    contains
```

⟨Event transforms: tests⟩

⟨Event transforms: test auxiliary⟩

end module event_transforms_util

API: driver for the unit tests below.

⟨Event transforms: public test⟩≡

public :: event_transforms_test

⟨Event transforms: test driver⟩≡

subroutine event_transforms_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

⟨Event transforms: execute tests⟩

end subroutine event_transforms_test

Test trivial event transform

The trivial transform, as an instance of the abstract transform, does nothing but to trigger event generation for an elementary process.

⟨Event transforms: execute tests⟩≡

call test (event_transforms_1, "event_transforms_1", &
"trivial event transform", &
u, results)

⟨Event transforms: test declarations⟩≡

public :: event_transforms_1

⟨Event transforms: tests⟩≡

subroutine event_transforms_1 (u)

integer, intent(in) :: u

type(os_data_t) :: os_data

type(model_t), target :: model

type(process_library_t), target :: lib

type(string_t) :: libname, procname1

class(phs_config_t), allocatable :: phs_config_template

real(default) :: sqrts

type(process_t), allocatable, target :: process

type(process_instance_t), allocatable, target :: process_instance

class(evt_t), allocatable :: evt

integer :: factorization_mode

logical :: keep_correlations

write (u, "(A)") " * Test output: event_transforms_1"

write (u, "(A)") " * Purpose: handle trivial transform"

write (u, "(A)")

write (u, "(A)") " * Initialize environment and parent process"

write (u, "(A)")

call os_data%init ()

```

libname = "event_transforms_1_lib"
procname1 = "event_transforms_1_p"

call prc_test_create_library (libname, lib, &
    scattering = .true., procname1 = procname1)
call reset_interaction_counter ()

call model%init_test ()

allocate (process)
call process%init (procname1, lib, os_data, model)
call process%setup_test_cores ()

allocate (phs_single_config_t :: phs_config_template)
call process%init_components (phs_config_template)

sqrts = 1000
call process%setup_beams_sqrts (sqrts, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_test_midpoint)
call process%setup_terms ()

allocate (process_instance)
call process_instance%init (process)
call process_instance%integrate (1, n_it=1, n_calls=100)
call process_instance%final_integration (1)
call process_instance%final ()
deallocate (process_instance)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
call process_instance%init_simulation (1)

write (u, "(A)")  "* Initialize trivial event transform"
write (u, "(A)")

allocate (evt_trivial_t :: evt)
call evt%connect (process_instance, process%get_model_ptr ())

write (u, "(A)")  "* Generate event and subsequent transform"
write (u, "(A)")

call process_instance%generate_unweighted_event (1)
call process_instance%evaluate_event_data ()

call evt%prepare_new_event (1, 1)
call evt%generate_unweighted ()

call write_separator (u, 2)
call evt%write (u)
call write_separator (u, 2)

write (u, "(A)")

```

```

write (u, "(A)")  "* Obtain particle set"
write (u, "(A)")

factorization_mode = FM_IGNORE_HELICITY
keep_correlations = .false.

call evt%make_particle_set (factorization_mode, keep_correlations)

call write_separator (u, 2)
call evt%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt%final ()
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Test output end: event_transforms_1"

end subroutine event_transforms_1

```

MCI record prepared for midpoint integrator.

```

<Event transforms: test auxiliary>≡
subroutine dispatch_mci_test_midpoint (mci, var_list, process_id, is_nlo)
  use variables, only: var_list_t
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
  allocate (mci_midpoint_t :: mci)
end subroutine dispatch_mci_test_midpoint

```

32.2 Hadronization interface

```

<hadrons.f90>≡
<File header>

module hadrons

  <Use kinds with double>
  <Use strings>
  <Use debug>
  use constants
  use diagnostics
  use event_transforms
  use format_utils, only: write_separator
  use helicities
  use hep_common

```

```

use io_units
use lorentz
use model_data
use models
use numeric_utils, only: vanishes
use particles
use physics_defs
use process, only: process_t
use instances, only: process_instance_t
use process_stacks
use pythia8
use rng_base, only: rng_t
use shower_base
use shower_pythia6
use sm_qcd
use subevents
use variables
use whizard_lha

```

⟨Standard module head⟩

⟨Hadrons: public⟩

⟨Hadrons: parameters⟩

⟨Hadrons: types⟩

⟨Hadrons: interfaces⟩

contains

⟨Hadrons: procedures⟩

end module hadrons

32.2.1 Hadronization implementations

⟨Hadrons: public⟩≡

```
public :: HADRONS_UNDEFINED, HADRONS_WHIZARD, HADRONS_PYTHIA6, HADRONS_PYTHIA8
```

⟨Hadrons: parameters⟩≡

```
integer, parameter :: HADRONS_UNDEFINED = 0
integer, parameter :: HADRONS_WHIZARD = 1
integer, parameter :: HADRONS_PYTHIA6 = 2
integer, parameter :: HADRONS_PYTHIA8 = 3
```

A dictionary

⟨Hadrons: public⟩+≡

```
public :: hadrons_method
```

⟨Hadrons: interfaces⟩≡

```
interface hadrons_method
  module procedure hadrons_method_of_string
  module procedure hadrons_method_to_string
end interface
```



```

⟨Hadrons: procedures⟩≡
  elemental function hadrons_method_of_string (string) result (i)
    integer :: i
    type(string_t), intent(in) :: string
    select case (char(string))
    case ("WHIZARD")
      i = HADRONS_WHIZARD
    case ("PYTHIA6")
      i = HADRONS_PYTHIA6
    case ("PYTHIA8")
      i = HADRONS_PYTHIA8
    case default
      i = HADRONS_UNDEFINED
    end select
  end function hadrons_method_of_string

  elemental function hadrons_method_to_string (i) result (string)
    type(string_t) :: string
    integer, intent(in) :: i
    select case (i)
    case (HADRONS_WHIZARD)
      string = "WHIZARD"
    case (HADRONS_PYTHIA6)
      string = "PYTHIA6"
    case (HADRONS_PYTHIA8)
      string = "PYTHIA8"
    case default
      string = "UNDEFINED"
    end select
  end function hadrons_method_to_string

```

32.2.2 Hadronization settings

These are the general settings and parameters for the different shower methods.

```

⟨Hadrons: public⟩+≡
  public :: hadron_settings_t

⟨Hadrons: types⟩≡
  type :: hadron_settings_t
    logical :: active = .false.
    integer :: method = HADRONS_UNDEFINED
    real(default) :: enhanced_fraction = 0
    real(default) :: enhanced_width = 0
  contains
    ⟨Hadrons: hadron settings: TBP⟩
  end type hadron_settings_t

```

Read in the hadronization settings.

```

⟨Hadrons: hadron settings: TBP⟩≡
  procedure :: init => hadron_settings_init

```

```

<Hadrons: procedures>+≡
subroutine hadron_settings_init (hadron_settings, var_list)
  class(hadron_settings_t), intent(out) :: hadron_settings
  type(var_list_t), intent(in) :: var_list
  hadron_settings%active = &
    var_list%get_lval (var_str ("?hadronization_active"))
  hadron_settings%method = hadrons_method_of_string ( &
    var_list%get_sval (var_str ("$hadronization_method")))
  hadron_settings%enhanced_fraction = &
    var_list%get_rval (var_str ("hadron_enhanced_fraction"))
  hadron_settings%enhanced_width = &
    var_list%get_rval (var_str ("hadron_enhanced_width"))
end subroutine hadron_settings_init

```

```

<Hadrons: hadron settings: TBP>+≡
procedure :: write => hadron_settings_write

```

```

<Hadrons: procedures>+≡
subroutine hadron_settings_write (settings, unit)
  class(hadron_settings_t), intent(in) :: settings
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  write (u, "(1x,A)") "Hadronization settings:"
  call write_separator (u)
  write (u, "(1x,A)") "Master switches:"
  write (u, "(3x,A,1x,L1)") &
    "active" = ", settings%active
  write (u, "(1x,A)") "General settings:"
  if (settings%active) then
    write (u, "(3x,A)") &
      "hadron_method" = " // &
      char (hadrons_method_to_string (settings%method))
  else
    write (u, "(3x,A)") " [Hadronization off]"
  end if
  write (u, "(1x,A)") "pT generation parameters"
  write (u, "(3x,A,1x,ES19.12)") &
    "enhanced_fraction" = ", settings%enhanced_fraction
  write (u, "(3x,A,1x,ES19.12)") &
    "enhanced_width" = ", settings%enhanced_width
end subroutine hadron_settings_write

```

32.2.3 Abstract Hadronization Type

The model is the fallback model including all hadrons

```

<Hadrons: types>+≡
type, abstract :: hadrons_t
  class(rng_t), allocatable :: rng
  type(shower_settings_t) :: shower_settings
  type(hadron_settings_t) :: hadron_settings
  type(model_t), pointer :: model => null()

```

```

contains
  <Hadrons: hadrons: TBP>
end type hadrons_t

<Hadrons: hadrons: TBP>≡
  procedure (hadrons_init), deferred :: init

<Hadrons: interfaces>+≡
  abstract interface
    subroutine hadrons_init &
      (hadrons, shower_settings, hadron_settings, model_hadrons)
    import
    class(hadrons_t), intent(out) :: hadrons
    type(shower_settings_t), intent(in) :: shower_settings
    type(hadron_settings_t), intent(in) :: hadron_settings
    type(model_t), target, intent(in) :: model_hadrons
  end subroutine hadrons_init
end interface

<Hadrons: hadrons: TBP>+≡
  procedure (hadrons_hadronize), deferred :: hadronize

<Hadrons: interfaces>+≡
  abstract interface
    subroutine hadrons_hadronize (hadrons, particle_set, valid)
    import
    class(hadrons_t), intent(inout) :: hadrons
    type(particle_set_t), intent(in) :: particle_set
    logical, intent(out) :: valid
  end subroutine hadrons_hadronize
end interface

<Hadrons: hadrons: TBP>+≡
  procedure (hadrons_make_particle_set), deferred :: make_particle_set

<Hadrons: interfaces>+≡
  abstract interface
    subroutine hadrons_make_particle_set (hadrons, particle_set, &
      model, valid)
    import
    class(hadrons_t), intent(in) :: hadrons
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    logical, intent(out) :: valid
  end subroutine hadrons_make_particle_set
end interface

<Hadrons: hadrons: TBP>+≡
  procedure :: import_rng => hadrons_import_rng

<Hadrons: procedures>+≡
  pure subroutine hadrons_import_rng (hadrons, rng)
  class(hadrons_t), intent(inout) :: hadrons
  class(rng_t), intent(inout), allocatable :: rng
  call move_alloc (from = rng, to = hadrons%rng)

```

```
end subroutine hadrons_import_rng
```

32.2.4 WHIZARD Hadronization Type

Hadronization can be (incompletely) performed through WHIZARD's internal routine.

```

<Hadrons: public>+≡
  public :: hadrons_hadrons_t

<Hadrons: types>+≡
  type, extends (hadrons_t) :: hadrons_hadrons_t
    contains
      <Hadrons: hadrons hadrons: TBP>
    end type hadrons_hadrons_t

<Hadrons: hadrons hadrons: TBP>≡
  procedure :: init => hadrons_hadrons_init

<Hadrons: procedures>+≡
  subroutine hadrons_hadrons_init &
    (hadrons, shower_settings, hadron_settings, model_hadrons)
    class(hadrons_hadrons_t), intent(out) :: hadrons
    type(shower_settings_t), intent(in) :: shower_settings
    type(hadron_settings_t), intent(in) :: hadron_settings
    type(model_t), intent(in), target :: model_hadrons
    hadrons%model => model_hadrons
    hadrons%shower_settings = shower_settings
    hadrons%hadron_settings = hadron_settings
    call msg_message &
      ("Hadronization: WHIZARD model for hadronization and decays")
  end subroutine hadrons_hadrons_init

<Hadrons: hadrons hadrons: TBP>+≡
  procedure :: hadronize => hadrons_hadrons_hadronize

<Hadrons: procedures>+≡
  subroutine hadrons_hadrons_hadronize (hadrons, particle_set, valid)
    class(hadrons_hadrons_t), intent(inout) :: hadrons
    type(particle_set_t), intent(in) :: particle_set
    logical, intent(out) :: valid
    integer, dimension(:), allocatable :: cols, acol, octs
    integer :: n
    if (signal_is_pending ()) return
    if (debug_on) call msg_debug (D_TRANSFORMS, "hadrons_hadrons_hadronize")
    call particle_set%write (6, compressed=.true.)
    n = particle_set%get_n_tot ()
    allocate (cols (n), acol (n), octs (n))
    call extract_color_systems (particle_set, cols, acol, octs)
    print *, "size(cols) = ", size (cols)
    if (size(cols) > 0) then
      print *, "cols = ", cols
    end if
  end subroutine

```

```

print *, "size(acols) = ", size(acols)
if (size(acols) > 0) then
    print *, "acols = ", acols
end if
print *, "size(octs) = ", size(octs)
if (size(octs) > 0) then
    print *, "octs = ", octs
end if
!!! if all arrays are empty, i.e. zero particles found, nothing to do
end subroutine hadrons_hadrons_hadronize

```

This type contains a flavor selector for the creation of hadrons, including parameters for the special handling of baryons.

```

<Hadrons: public>+≡
    public :: had_flav_t

<Hadrons: types>+≡
    type had_flav_t
end type had_flav_t

```

This is the type for the ends of Lund strings.

```

<Hadrons: public>+≡
    public :: lund_end

<Hadrons: types>+≡
    type lund_end
        logical :: from_pos
        integer :: i_end
        integer :: i_max
        integer :: id_had
        integer :: i_pos_old
        integer :: i_neg_old
        integer :: i_pos_new
        integer :: i_neg_new
        real(default) :: px_old
        real(default) :: py_old
        real(default) :: px_new
        real(default) :: py_new
        real(default) :: px_had
        real(default) :: py_had
        real(default) :: m_had
        real(default) :: mT2_had
        real(default) :: z_had
        real(default) :: gamma_old
        real(default) :: gamma_new
        real(default) :: x_pos_old
        real(default) :: x_pos_new
        real(default) :: x_pos_had
        real(default) :: x_neg_old
        real(default) :: x_neg_new
        real(default) :: x_neg_had
        type(had_flav_t) :: old_flav
        type(had_flav_t) :: new_flav
        type(vector4_t) :: p_had
    end type lund_end

```

```

        type(vector4_t) :: p_pre
    end type lund_end

```

Generator for transverse momentum for the fragmentation.

```

<Hadrons: public>+≡

```

```

    public :: lund_pt_t

```

```

<Hadrons: types>+≡

```

```

    type lund_pt_t
        real(default) :: sigma_min
        real(default) :: sigma_q
        real(default) :: enhanced_frac
        real(default) :: enhanced_width
        real(default) :: sigma_to_had
        class(rng_t), allocatable :: rng
    contains
        <Hadrons: lund pT: TBP>
    end type lund_pt_t

```

```

<Hadrons: lund pT: TBP>≡

```

```

    procedure :: init => lund_pt_init

```

```

<Hadrons: procedures>+≡

```

```

    subroutine lund_pt_init (lund_pt, settings)
        class (lund_pt_t), intent(out) :: lund_pt
        type(hadron_settings_t), intent(in) :: settings
    end subroutine lund_pt_init

```

```

<Hadrons: hadrons hadrons: TBP>+≡

```

```

    procedure :: make_particle_set => hadrons_hadrons_make_particle_set

```

```

<Hadrons: procedures>+≡

```

```

    subroutine hadrons_hadrons_make_particle_set &
        (hadrons, particle_set, model, valid)
        class(hadrons_hadrons_t), intent(in) :: hadrons
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model
        logical, intent(out) :: valid
        if (signal_is_pending ()) return
        valid = .false.
        if (valid) then
        else
            call msg_fatal ("WHIZARD hadronization not yet implemented")
        end if
    end subroutine hadrons_hadrons_make_particle_set

```

```

<Hadrons: procedures>+≡

```

```

    subroutine extract_color_systems (p_set, cols, acol, octs)
        type(particle_set_t), intent(in) :: p_set
        integer, dimension(:), allocatable, intent(out) :: cols, acol, octs
        logical, dimension(:), allocatable :: mask
        integer :: i, n, n_cols, n_acol, n_oct
        n = p_set%get_n_tot ()

```

```

allocate (mask (n))
do i = 1, n
    mask(i) = p_set%prt(i)%col%get_col () /= 0 .and. &
        p_set%prt(i)%col%get_acl () == 0 .and. &
        p_set%prt(i)%get_status () == PRT_OUTGOING
end do
n_cols = count (mask)
allocate (cols (n_cols))
cols = p_set%get_indices (mask)
do i = 1, n
    mask(i) = p_set%prt(i)%col%get_col () == 0 .and. &
        p_set%prt(i)%col%get_acl () /= 0 .and. &
        p_set%prt(i)%get_status () == PRT_OUTGOING
end do
n_acols = count (mask)
allocate (acols (n_acols))
acols = p_set%get_indices (mask)
do i = 1, n
    mask(i) = p_set%prt(i)%col%get_col () /= 0 .and. &
        p_set%prt(i)%col%get_acl () /= 0 .and. &
        p_set%prt(i)%get_status () == PRT_OUTGOING
end do
n_octs = count (mask)
allocate (octs (n_octs))
octs = p_set%get_indices (mask)
end subroutine extract_color_systems

```

32.2.5 PYTHIA6 Hadronization Type

Hadronization via PYTHIA6 is at another option for hadronization within WHIZARD.

```

<Hadrons: public>+≡
    public :: hadrons_pythia6_t

<Hadrons: types>+≡
    type, extends (hadrons_t) :: hadrons_pythia6_t
        contains
        <Hadrons: hadrons pythia6: TBP>
    end type hadrons_pythia6_t

<Hadrons: hadrons pythia6: TBP>≡
    procedure :: init => hadrons_pythia6_init

<Hadrons: procedures>+≡
    subroutine hadrons_pythia6_init &
        (hadrons, shower_settings, hadron_settings, model_hadrons)
        class(hadrons_pythia6_t), intent(out) :: hadrons
        type(shower_settings_t), intent(in) :: shower_settings
        type(hadron_settings_t), intent(in) :: hadron_settings
        type(model_t), intent(in), target :: model_hadrons
        logical :: pygive_not_set_by_shower
        hadrons%model => model_hadrons
        hadrons%shower_settings = shower_settings
        hadrons%hadron_settings = hadron_settings
    end subroutine

```

```

pygive_not_set_by_shower = .not. (shower_settings%method == PS_PYTHIA6 &
    .and. (shower_settings%isr_active .or. shower_settings%fsr_active))
if (pygive_not_set_by_shower) then
    call pythia6_set_verbose (shower_settings%verbose)
    call pythia6_set_config (shower_settings%pythia6_pygive)
end if
call msg_message &
    ("Hadronization: Using PYTHIA6 interface for hadronization and decays")
end subroutine hadrons_pythia6_init

```

Assume that the event record is still in the PYTHIA COMMON BLOCKS transferred there by the WHIZARD or PYTHIA6 shower routines.

<Hadrons: hadrons pythia6: TBP>+≡

```

procedure :: hadronize => hadrons_pythia6_hadronize

```

<Hadrons: procedures>+≡

```

subroutine hadrons_pythia6_hadronize (hadrons, particle_set, valid)
    class(hadrons_pythia6_t), intent(inout) :: hadrons
    type(particle_set_t), intent(in) :: particle_set
    logical, intent(out) :: valid
    integer :: N, NPAD, K
    real(double) :: P, V
    common /PYJETS/ N, NPAD, K(4000,5), P(4000,5), V(4000,5)
    save /PYJETS/
    if (signal_is_pending ()) return
    if (debug_on) call msg_debug (D_TRANSFORMS, "hadrons_pythia6_hadronize")
    call pygive ("MSTP(111)=1")    !!! Switch on hadronization and decays
    call pygive ("MSTJ(1)=1")    !!! String fragmentation
    call pygive ("MSTJ(21)=2")    !!! String fragmentation keeping resonance momentum
    call pygive ("MSTJ(28)=0")    !!! Switch off tau decays
    if (debug_active (D_TRANSFORMS)) then
        call msg_debug (D_TRANSFORMS, "N", N)
        call pylist(2)
        print *, ' line 7 : ', k(7,1:5), p(7,1:5)
    end if
    call pyedit (12)
    call pythia6_set_last_treated_line (N)
    call pyexec ()
    call pyedit (12)
    valid = .true.
end subroutine hadrons_pythia6_hadronize

```

<Hadrons: hadrons pythia6: TBP>+≡

```

procedure :: make_particle_set => hadrons_pythia6_make_particle_set

```

<Hadrons: procedures>+≡

```

subroutine hadrons_pythia6_make_particle_set &
    (hadrons, particle_set, model, valid)
    class(hadrons_pythia6_t), intent(in) :: hadrons
    type(particle_set_t), intent(inout) :: particle_set
    class(model_data_t), intent(in), target :: model
    logical, intent(out) :: valid
    if (signal_is_pending ()) return
    valid = pythia6_handle_errors ()

```



```

    if (valid) then
        call pythia6_combine_with_particle_set &
            (particle_set, model, hadrons%model, hadrons%shower_settings)
    end if
end subroutine hadrons_pythia6_make_particle_set

```

32.2.6 PYTHIA8 Hadronization

```

<Hadrons: public>+≡
    public :: hadrons_pythia8_t

```

```

<Hadrons: types>+≡
    type, extends (hadrons_t) :: hadrons_pythia8_t
        type(pythia8_t) :: pythia
        type(whizard_lha_t) :: lhaup
        logical :: user_process_set = .false.
        logical :: pythia_initialized = .false., &
            lhaup_initialized = .false.
    contains
        <Hadrons: hadrons pythia8: TBP>
    end type hadrons_pythia8_t

```

```

<Hadrons: hadrons pythia8: TBP>≡
    procedure :: init => hadrons_pythia8_init

```

```

<Hadrons: procedures>+≡
    subroutine hadrons_pythia8_init &
        (hadrons, shower_settings, hadron_settings, model_hadrons)
        class(hadrons_pythia8_t), intent(out) :: hadrons
        type(shower_settings_t), intent(in) :: shower_settings
        type(hadron_settings_t), intent(in) :: hadron_settings
        type(model_t), intent(in), target :: model_hadrons
        hadrons%model => model_hadrons
        hadrons%shower_settings = shower_settings
        hadrons%hadron_settings = hadron_settings
        call msg_message &
            ("Hadronization: Using PYTHIA8 interface for hadronization and decays.")
        ! TODO sbrass which verbose?
        call hadrons%pythia%init (verbose = shower_settings%verbose)
        call hadrons%lhaup%init ()
    end subroutine hadrons_pythia8_init

```

Transfer hadron settings to PYTHIA8.

```

<Hadrons: hadrons pythia8: TBP>+≡
    procedure, private :: transfer_settings => hadrons_pythia8_transfer_settings

```

```

<Hadrons: procedures>+≡
    subroutine hadrons_pythia8_transfer_settings (hadrons)
        class(hadrons_pythia8_t), intent(inout), target :: hadrons
        real(default) :: r
        if (debug_on) call msg_debug (D_TRANSFORMS, "hadrons_pythia8_transfer_settings")
        if (debug_on) call msg_debug2 (D_TRANSFORMS, "pythia_initialized", hadrons%pythia_initialized)
        if (hadrons%pythia_initialized) return
    end subroutine hadrons_pythia8_transfer_settings

```

```

call hadrons%pythia%import_rng (hadrons%rng)
call hadrons%pythia%parse_and_set_config (hadrons%shower_settings%pythia8_config)
if (len (hadrons%shower_settings%pythia8_config_file) > 0) &
    call hadrons%pythia%read_file (hadrons%shower_settings%pythia8_config_file)
call hadrons%pythia%read_string (var_str ("Beams:frameType = 5"))
call hadrons%pythia%read_string (var_str ("ProcessLevel:all = off"))
if (.not. hadrons%shower_settings%verbose) then
    call hadrons%pythia%read_string (var_str ("Print:quiet = on"))
end if
call hadrons%pythia%set_lhaup_ptr (hadrons%lhaup)
call hadrons%pythia%init_pythia ()
hadrons%pythia_initialized = .true.
end subroutine hadrons_pythia8_transfer_settings

```

Set user process for the LHA interface.

```

<Hadrons: hadrons pythia8: TBP>+≡
    procedure, private :: set_user_process => hadrons_pythia8_set_user_process

```

```

<Hadrons: procedures>+≡
    subroutine hadrons_pythia8_set_user_process (hadrons, pset)
        class(hadrons_pythia8_t), intent(inout) :: hadrons
        type(particle_set_t), intent(in) :: pset
        integer, dimension(2) :: beam_pdg
        real(default), dimension(2) :: beam_energy
        integer, parameter :: process_id = 0, n_processes = 0
        if (debug_on) call msg_debug (D_TRANSFORMS, "hadrons_pythia8_set_user_process")
        beam_pdg = [pset%prt(1)%get_pdg (), pset%prt(2)%get_pdg ()]
        beam_energy = [energy(pset%prt(1)%p), energy(pset%prt(2)%p)]
        call hadrons%lhaup%set_init (beam_pdg, beam_energy, &
            n_processes, unweighted = .false., negative_weights = .false.)
        call hadrons%lhaup%set_process_parameters (process_id = process_id, &
            cross_section = one, error = one)
    end subroutine hadrons_pythia8_set_user_process

```

Import particle set.

```

<Hadrons: hadrons pythia8: TBP>+≡
    procedure, private :: import_particle_set => hadrons_pythia8_import_particle_set

<Hadrons: procedures>+≡
    subroutine hadrons_pythia8_import_particle_set (hadrons, particle_set)
        class(hadrons_pythia8_t), target, intent(inout) :: hadrons
        type(particle_set_t), intent(in) :: particle_set
        type(particle_set_t) :: pset_reduced
        integer, parameter :: PROCESS_ID = 1
        if (debug_on) call msg_debug (D_TRANSFORMS, "hadrons_pythia8_import_particle_set")
        if (.not. hadrons%user_process_set) then
            call hadrons%set_user_process (particle_set)
            hadrons%user_process_set = .true.
        end if
        call hadrons%lhaup%set_event_process (process_id = PROCESS_ID, scale = -one, &
            alpha_qcd = -one, alpha_qed = -one, weight = -one)
        call hadrons%lhaup%set_event (process_id = PROCESS_ID, particle_set = particle_set, &
            polarization = .true.)
        if (debug_active (D_TRANSFORMS)) then

```

```

        call hadrons%lhaup%list_init ()
    end if
end subroutine hadrons_pythia8_import_particle_set

<Hadrons: hadrons pythia8: TBP>+≡
    procedure :: hadronize => hadrons_pythia8_hadronize

<Hadrons: procedures>+≡
    subroutine hadrons_pythia8_hadronize (hadrons, particle_set, valid)
        class(hadrons_pythia8_t), intent(inout) :: hadrons
        type(particle_set_t), intent(in) :: particle_set
        logical, intent(out) :: valid
        if (signal_is_pending ()) return
        call hadrons%import_particle_set (particle_set)
        if (.not. hadrons%pythia_initialized) &
            call hadrons%transfer_settings ()
        call hadrons%pythia%next (valid)
        if (debug_active (D_TRANSFORMS)) then
            call hadrons%pythia%list_event ()
            call particle_set%write (summary=.true., compressed=.true.)
        end if
    end subroutine hadrons_pythia8_hadronize

<Hadrons: hadrons pythia8: TBP>+≡
    procedure :: make_particle_set => hadrons_pythia8_make_particle_set

<Hadrons: procedures>+≡
    subroutine hadrons_pythia8_make_particle_set &
        (hadrons, particle_set, model, valid)
        class(hadrons_pythia8_t), intent(in) :: hadrons
        type(particle_set_t), intent(inout) :: particle_set
        class(model_data_t), intent(in), target :: model
        logical, intent(out) :: valid
        type(particle_t), dimension(:), allocatable :: beam
        if (debug_on) call msg_debug (D_TRANSFORMS, "hadrons_pythia8_make_particle_set")
        if (signal_is_pending ()) return
        associate (settings => hadrons%shower_settings)
            if (debug_active (D_TRANSFORMS)) then
                call msg_debug (D_TRANSFORMS, 'Combine PYTHIA8 with particle set')
                call msg_debug (D_TRANSFORMS, 'Particle set before replacing')
                call particle_set%write (summary=.true., compressed=.true.)
                call hadrons%pythia%list_event ()
                call msg_debug (D_TRANSFORMS, string = "settings%hadron_collision", &
                    value = settings%hadron_collision)
            end if
            call hadrons%pythia%get_hadron_particles (&
                model, hadrons%model, particle_set, &
                helicity = PRT_DEFINITE_HELICITY)
        end associate
        if (debug_active (D_TRANSFORMS)) then
            print *, 'Particle set after replacing'
            call particle_set%write (summary=.true., compressed=.true.)
        end if
        valid = .true.

```

```
end subroutine hadrons_pythia8_make_particle_set
```

32.2.7 Hadronization Event Transform

This is the type for the hadronization event transform. It does not depend on the specific hadronization implementation of `hadrons_t`.

```
<Hadrons: public>+≡
  public :: evt_hadrons_t

<Hadrons: types>+≡
  type, extends (evt_t) :: evt_hadrons_t
    class(hadrons_t), allocatable :: hadrons
    type(model_t), pointer :: model_hadrons => null()
    type(qcd_t) :: qcd
    logical :: is_first_event
  contains
    <Hadrons: evt hadrons: TBP>
  end type evt_hadrons_t
```

Initialize the parameters. The `model_hadrons` is supposed to be the SM variant that contains all hadrons that may be generated in the shower.

```
<Hadrons: evt hadrons: TBP>≡
  procedure :: init => evt_hadrons_init

<Hadrons: procedures>+≡
  subroutine evt_hadrons_init (evt, model_hadrons)
    class(evt_hadrons_t), intent(out) :: evt
    type(model_t), intent(in), target :: model_hadrons
    evt%model_hadrons => model_hadrons
    evt%is_first_event = .true.
  end subroutine evt_hadrons_init

<Hadrons: evt hadrons: TBP>+≡
  procedure :: write_name => evt_hadrons_write_name

<Hadrons: procedures>+≡
  subroutine evt_hadrons_write_name (evt, unit)
    class(evt_hadrons_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: hadronization"
  end subroutine evt_hadrons_write_name
```

Output.

```
<Hadrons: evt hadrons: TBP>+≡
  procedure :: write => evt_hadrons_write
```

<Hadrons: procedures>+≡

```

subroutine evt_hadrons_write (evt, unit, verbose, more_verbose, testflag)
  class(evt_hadrons_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose, more_verbose, testflag
  integer :: u
  u = given_output_unit (unit)
  call write_separator (u, 2)
  call evt%write_name (u)
  call write_separator (u)
  call evt%base_write (u, testflag = testflag, show_set = .false.)
  if (evt%particle_set_exists) &
    call evt%particle_set%write &
      (u, summary = .true., compressed = .true., testflag = testflag)
  call write_separator (u)
  call evt%hadrons%shower_settings%write (u)
  call write_separator (u)
  call evt%hadrons%hadron_settings%write (u)
end subroutine evt_hadrons_write

```

<Hadrons: evt hadrons: TBP>+≡

```

procedure :: first_event => evt_hadrons_first_event

```

<Hadrons: procedures>+≡

```

subroutine evt_hadrons_first_event (evt)
  class(evt_hadrons_t), intent(inout) :: evt
  if (debug_on) call msg_debug (D_TRANSFORMS, "evt_hadrons_first_event")
  associate (settings => evt%hadrons%shower_settings)
    settings%hadron_collision = .false.
    !!! !!! !!! Workaround for PGF90 16.1
    !!! if (all (evt%particle_set%prt(1:2)%flv%get_pdg_abs () <= 39)) then
    if (evt%particle_set%prt(1)%flv%get_pdg_abs () <= 39 .and. &
      evt%particle_set%prt(2)%flv%get_pdg_abs () <= 39) then
      settings%hadron_collision = .false.
    !!! else if (all (evt%particle_set%prt(1:2)%flv%get_pdg_abs () >= 100)) then
    else if (evt%particle_set%prt(1)%flv%get_pdg_abs () >= 100 .and. &
      evt%particle_set%prt(2)%flv%get_pdg_abs () >= 100) then
      settings%hadron_collision = .true.
    else
      call msg_fatal ("evt_hadrons didn't recognize beams setup")
    end if
    if (debug_on) call msg_debug (D_TRANSFORMS, "hadron_collision", settings%hadron_collision)
    if (.not. (settings%isr_active .or. settings%fsr_active)) then
      call msg_fatal ("Hadronization without shower is not supported")
    end if
  end associate
  evt%is_first_event = .false.
end subroutine evt_hadrons_first_event

```

Here we take the particle set from the previous event transform and apply the hadronization. The result is stored in the `evt%hadrons` object. We always return a probability of unity as we don't have the analytic weight of the hadronization. Invalid events have to be discarded by the caller which is why

we mark the particle set as invalid.

```

<Hadrons: evt hadrons: TBP>+≡
  procedure :: generate_weighted => evt_hadrons_generate_weighted

<Hadrons: procedures>+≡
  subroutine evt_hadrons_generate_weighted (evt, probability)
    class(evt_hadrons_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
    logical :: valid
    if (signal_is_pending ()) return
    evt%particle_set = evt%previous%particle_set
    if (evt%is_first_event) then
      call evt%first_event ()
    end if
    call evt%hadrons%hadronize (evt%particle_set, valid)
    probability = 1
    evt%particle_set_exists = valid
  end subroutine evt_hadrons_generate_weighted

```

The factorization parameters are irrelevant.

```

<Hadrons: evt hadrons: TBP>+≡
  procedure :: make_particle_set => evt_hadrons_make_particle_set

<Hadrons: procedures>+≡
  subroutine evt_hadrons_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_hadrons_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
    logical :: valid
    call evt%hadrons%make_particle_set (evt%particle_set, evt%model, valid)
    evt%particle_set_exists = evt%particle_set_exists .and. valid
  end subroutine evt_hadrons_make_particle_set

```

Connect the process with the hadrons object.

```

<Hadrons: evt hadrons: TBP>+≡
  procedure :: connect => evt_hadrons_connect

<Hadrons: procedures>+≡
  subroutine evt_hadrons_connect &
    (evt, process_instance, model, process_stack)
    class(evt_hadrons_t), intent(inout), target :: evt
    type(process_instance_t), intent(in), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    call evt%base_connect (process_instance, model, process_stack)
    call evt%make_rng (evt%process)
  end subroutine evt_hadrons_connect

```

Create RNG instances, spawned by the process object.

```

<Hadrons: evt hadrons: TBP>+≡
  procedure :: make_rng => evt_hadrons_make_rng

```

```

<Hadrons: procedures>+≡
  subroutine evt_hadrons_make_rng (evt, process)
    class(evt_hadrons_t), intent(inout) :: evt
    type(process_t), intent(inout) :: process
    class(rng_t), allocatable :: rng
    call process%make_rng (rng)
    call evt%hadrons%import_rng (rng)
  end subroutine evt_hadrons_make_rng

<Hadrons: evt hadrons: TBP>+≡
  procedure :: prepare_new_event => evt_hadrons_prepare_new_event

<Hadrons: procedures>+≡
  subroutine evt_hadrons_prepare_new_event (evt, i_mci, i_term)
    class(evt_hadrons_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    call evt%reset ()
  end subroutine evt_hadrons_prepare_new_event

```

32.3 Resonance Insertion

```

<resonance_insertion.f90>≡
  <File header>

  module resonance_insertion

    <Use kinds>
    <Use strings>
    use io_units
    use format_utils, only: write_separator
    use format_defs, only: FMT_12
    use rng_base, only: rng_t
    use selectors, only: selector_t
    use sm_qcd
    use model_data
    use interactions, only: interaction_t
    use particles, only: particle_t, particle_set_t
    use subevents, only: PRT_RESONANT
    use models
    use resonances, only: resonance_history_set_t
    use resonances, only: resonance_tree_t
    use instances, only: process_instance_ptr_t
    use event_transforms

    <Standard module head>

    <Resonance insertion: public>

    <Resonance insertion: types>

    contains

```

<Resonance insertion: procedures>

end module resonance_insertion

32.3.1 Resonance-Insertion Event Transform

This is the type for the event transform that applies resonance insertion. The resonance history set describe the resonance histories that we may consider. There is a process library with process objects that correspond to the resonance histories. Library creation, compilation etc. is done outside the scope of this module.

<Resonance insertion: public>≡

public :: evt_resonance_t

<Resonance insertion: types>≡

```
type, extends (evt_t) :: evt_resonance_t
  type(resonance_history_set_t), dimension(:), allocatable :: res_history_set
  integer, dimension(:), allocatable :: index_offset
  integer :: selected_component = 0
  type(string_t) :: libname
  type(string_t), dimension(:), allocatable :: proc_id
  real(default) :: on_shell_limit = 0
  real(default) :: on_shell_turnoff = 0
  real(default) :: background_factor = 1
  logical :: selector_active = .false.
  type(selector_t) :: selector
  integer :: selected_history = 0
  type(process_instance_ptr_t), dimension(:), allocatable :: instance
contains
  <Resonance insertion: evt resonance: TBP>
end type evt_resonance_t
```

<Resonance insertion: evt resonance: TBP>≡

procedure :: write_name => evt_resonance_write_name

<Resonance insertion: procedures>≡

```
subroutine evt_resonance_write_name (evt, unit)
  class(evt_resonance_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  integer :: u
  u = given_output_unit (unit)
  write (u, "(1x,A)") "Event transform: resonance insertion"
end subroutine evt_resonance_write_name
```

Output.

<Resonance insertion: evt resonance: TBP>+≡

procedure :: write => evt_resonance_write

<Resonance insertion: procedures>+≡

```
subroutine evt_resonance_write (evt, unit, verbose, more_verbose, testflag)
  class(evt_resonance_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose, more_verbose, testflag
```



```

integer :: u, i
u = given_output_unit (unit)
call write_separator (u, 2)
call evt%write_name (u)
call write_separator (u, 2)
write (u, "(1x,A,A,A)") "Process library = ', char (evt%libname), "'
if (allocated (evt%res_history_set)) then
  do i = 1, size (evt%res_history_set)
    if (i == evt%selected_component) then
      write (u, "(1x,A,I0,A)") "Component #", i, ": *"
    else
      write (u, "(1x,A,I0,A)") "Component #", i, ":"
    end if
    call evt%res_history_set(i)%write (u, indent=1)
  end do
end if
call write_separator (u)
if (allocated (evt%instance)) then
  write (u, "(1x,A)") "Subprocess instances: allocated"
else
  write (u, "(1x,A)") "Subprocess instances: not allocated"
end if
if (evt%particle_set_exists) then
  if (evt%selected_history > 0) then
    write (u, "(1x,A,I0)") "Selected: resonance history #", &
      evt%selected_history
  else
    write (u, "(1x,A)") "Selected: no resonance history"
  end if
else
  write (u, "(1x,A)") "Selected: [none]"
end if
write (u, "(1x,A,1x," // FMT_12 // ")") &
  "On-shell limit    =", evt%on_shell_limit
write (u, "(1x,A,1x," // FMT_12 // ")") &
  "On-shell turnoff =", evt%on_shell_turnoff
write (u, "(1x,A,1x," // FMT_12 // ")") &
  "Background factor =", evt%background_factor
call write_separator (u)
if (evt%selector_active) then
  write (u, "(2x)", advance="no")
  call evt%selector%write (u, testflag=testflag)
  call write_separator (u)
end if
call evt%base_write (u, testflag = testflag, show_set = .false.)
call write_separator (u)
if (evt%particle_set_exists) then
  call evt%particle_set%write &
    (u, summary = .true., compressed = .true., testflag = testflag)
  call write_separator (u)
end if
end subroutine evt_resonance_write

```

32.3.2 Set contained data

Insert the resonance data, in form of a pre-generated resonance history set. Accumulate the number of histories for each set, to initialize an array of index offsets for lookup.

```
(Resonance insertion: evt resonance: TBP)+≡
  procedure :: set_resonance_data => evt_resonance_set_resonance_data

(Resonance insertion: procedures)+≡
  subroutine evt_resonance_set_resonance_data (evt, res_history_set)
    class(evt_resonance_t), intent(inout) :: evt
    type(resonance_history_set_t), dimension(:), intent(in) :: res_history_set
    integer :: i
    evt%res_history_set = res_history_set
    allocate (evt%index_offset (size (evt%res_history_set)), source = 0)
    do i = 2, size (evt%res_history_set)
      evt%index_offset(i) = &
        evt%index_offset(i-1) + evt%res_history_set(i-1)%get_n_history ()
    end do
  end subroutine evt_resonance_set_resonance_data
```

Set the library that contains the resonant subprocesses.

```
(Resonance insertion: evt resonance: TBP)+≡
  procedure :: set_library => evt_resonance_set_library

(Resonance insertion: procedures)+≡
  subroutine evt_resonance_set_library (evt, libname)
    class(evt_resonance_t), intent(inout) :: evt
    type(string_t), intent(in) :: libname
    evt%libname = libname
  end subroutine evt_resonance_set_library
```

Assign pointers to subprocess instances. Once a subprocess has been selected, the instance is used for generating the particle set with valid quantum-number assignments, ready for resonance insertion.

```
(Resonance insertion: evt resonance: TBP)+≡
  procedure :: set_subprocess_instances &
    => evt_resonance_set_subprocess_instances

(Resonance insertion: procedures)+≡
  subroutine evt_resonance_set_subprocess_instances (evt, instance)
    class(evt_resonance_t), intent(inout) :: evt
    type(process_instance_ptr_t), dimension(:), intent(in) :: instance
    evt%instance = instance
  end subroutine evt_resonance_set_subprocess_instances
```

Set the on-shell limit, the relative distance from a resonance that is still considered to be on-shell. The probability for being considered on-shell can be reduced by the turnoff parameter below. For details, see the **resonances** module.

```
(Resonance insertion: evt resonance: TBP)+≡
  procedure :: set_on_shell_limit => evt_resonance_set_on_shell_limit
```

```

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_set_on_shell_limit (evt, on_shell_limit)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: on_shell_limit
    evt%on_shell_limit = on_shell_limit
  end subroutine evt_resonance_set_on_shell_limit

```

Set the Gaussian on-shell turnoff parameter, the width of the weighting factor for the resonance squared matrix element. If the resonance is off shell, this factor reduces the weight of the matrix element in the selector, such that the probability for considered resonant is reduced. The factor is applied only if the offshellness is less than the `on_shell_limit` above. For details, see the `resonances` module.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: set_on_shell_turnoff => evt_resonance_set_on_shell_turnoff

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_set_on_shell_turnoff (evt, on_shell_turnoff)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: on_shell_turnoff
    evt%on_shell_turnoff = on_shell_turnoff
  end subroutine evt_resonance_set_on_shell_turnoff

```

Reweight (suppress) the background contribution if there is a resonance history that applies. The event will be registered as background if there is no applicable resonance history, or if the background configuration has been selected based on (reweighted) squared matrix elements.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: set_background_factor => evt_resonance_set_background_factor

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_set_background_factor (evt, background_factor)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(in) :: background_factor
    evt%background_factor = background_factor
  end subroutine evt_resonance_set_background_factor

```

32.3.3 Selector

Manually import a random-number generator object. This should be done only for testing purposes. The standard procedure is to `connect` a process to an event transform; this will create an appropriate `rng` from the RNG factory in the process object.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: import_rng => evt_resonance_import_rng

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_import_rng (evt, rng)
    class(evt_resonance_t), intent(inout) :: evt
    class(rng_t), allocatable, intent(inout) :: rng
    call move_alloc (from = rng, to = evt%rng)
  end subroutine evt_resonance_import_rng

```

```
end subroutine evt_resonance_import_rng
```

We use a standard selector object to choose from the available resonance histories. If the selector is inactive, we do not insert resonances.

```
<Resonance insertion: evt resonance: TBP>+≡
  procedure :: write_selector => evt_resonance_write_selector

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_write_selector (evt, unit, testflag)
    class(evt_resonance_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: u
    u = given_output_unit (unit)
    if (evt%selector_active) then
      call evt%selector%write (u, testflag)
    else
      write (u, "(1x,A)") "Selector: [inactive]"
    end if
  end subroutine evt_resonance_write_selector
```

The selector is initialized with relative weights of histories which need not be normalized. Channels with weight zero are ignored.

The `offset` will normally be -1 , so we count from zero, and zero is a valid result from the selector. Selecting the zero entry implies no resonance insertion. However, this behavior is not hard-coded here (without `offset`, no resonance is not possible as a result).

```
<Resonance insertion: evt resonance: TBP>+≡
  procedure :: init_selector => evt_resonance_init_selector

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_init_selector (evt, weight, offset)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), dimension(:), intent(in) :: weight
    integer, intent(in), optional :: offset
    if (any (weight > 0)) then
      call evt%selector%init (weight, offset = offset)
      evt%selector_active = .true.
    else
      evt%selector_active = .false.
    end if
  end subroutine evt_resonance_init_selector
```

Return all selector weights, for inspection. Note that the index counts from zero.

```
<Resonance insertion: evt resonance: TBP>+≡
  procedure :: get_selector_weights => evt_resonance_get_selector_weights

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_get_selector_weights (evt, weight)
    class(evt_resonance_t), intent(in) :: evt
    real(default), dimension(0:), intent(out) :: weight
    integer :: i
```

```

do i = 0, ubound (weight,1)
  weight(i) = evt%selector%get_weight (i)
end do
end subroutine evt_resonance_get_selector_weights

```

32.3.4 Runtime calculations

Use the associated master process instance and the subprocess instances to distribute the current momentum set, then compute the squared matrix elements weights for all subprocesses.

NOTE: Procedures in this subsection are not covered by unit tests in this module, but by unit tests of the `restricted_subprocesses` module.

Fill the particle set, so the momentum configuration can be used by the subprocess instances. The standard workflow is to copy from the previous particle set.

```

<Resonance insertion: evt_resonance: TBP>+≡
  procedure :: fill_momenta => evt_resonance_fill_momenta

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_fill_momenta (evt)
    class(evt_resonance_t), intent(inout) :: evt
    integer :: i, n
    if (associated (evt%previous)) then
      evt%particle_set = evt%previous%particle_set
    else if (associated (evt%process_instance)) then
      ! this branch only for unit test
      call evt%process_instance%get_trace &
        (evt%particle_set, i_term=1, n_incoming=evt%process%get_n_in ())
    end if
  end subroutine evt_resonance_fill_momenta

```

Return the indices of those subprocesses which can be considered on-shell. The result depends on the stored particle set (outgoing momenta) and on the on-shell limit value.

The index `evt%selected_component` identifies the particular history set that corresponds to the given process component. Recall that process components may have different external particles, so they have distinct history sets.

```

<Resonance insertion: evt_resonance: TBP>+≡
  procedure :: determine_on_shell_histories &
    => evt_resonance_determine_on_shell_histories

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_determine_on_shell_histories &
    (evt, index_array)
    class(evt_resonance_t), intent(in) :: evt
    integer, dimension(:), allocatable, intent(out) :: index_array
    integer :: i
    i = evt%selected_component
    call evt%res_history_set(i)%determine_on_shell_histories &
      (evt%particle_set%get_outgoing_momenta (), &
        evt%on_shell_limit, &

```

```

        index_array)
    end subroutine evt_resonance_determine_on_shell_histories

```

Evaluate selected subprocesses. (In actual operation, the ones that have been tagged as on-shell.)

We assume that the MCI, term, and channel indices for the subprocesses can all be set to 1.

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: evaluate_subprocess => evt_resonance_evaluate_subprocess

<Resonance insertion: procedures>+≡
    subroutine evt_resonance_evaluate_subprocess (evt, index_array)
        class(evt_resonance_t), intent(inout) :: evt
        integer, dimension(:), intent(in) :: index_array
        integer :: k, i
        if (allocated (evt%instance)) then
            do k = 1, size (index_array)
                i = index_array(k)
                associate (instance => evt%instance(i)%p)
                    call instance%choose_mci (1)
                    call instance%set_trace (evt%particle_set, 1, check_match=.false.)
                    call instance%recover (channel = 1, i_term = 1, &
                        update_sqme = .true., recover_phs = .false.)
                end associate
            end do
        end if
    end subroutine evt_resonance_evaluate_subprocess

```

Return the current squared matrix-element value of the master process, and of the selected resonant subprocesses, respectively.

```

<Resonance insertion: evt resonance: TBP>+≡
    procedure :: get_master_sqme => evt_resonance_get_master_sqme
    procedure :: get_subprocess_sqme => evt_resonance_get_subprocess_sqme

<Resonance insertion: procedures>+≡
    function evt_resonance_get_master_sqme (evt) result (sqme)
        class(evt_resonance_t), intent(in) :: evt
        real(default) :: sqme
        sqme = evt%process_instance%get_sqme ()
    end function evt_resonance_get_master_sqme

    subroutine evt_resonance_get_subprocess_sqme (evt, sqme, index_array)
        class(evt_resonance_t), intent(in) :: evt
        real(default), dimension(:), intent(out) :: sqme
        integer, dimension(:), intent(in), optional :: index_array
        integer :: k, i
        if (present (index_array)) then
            sqme = 0
            do k = 1, size (index_array)
                call get_sqme (index_array(k))
            end do
        else
            do i = 1, size (evt%instance)

```

```

        call get_sqme (i)
    end do
end if
contains
    subroutine get_sqme (i)
        integer, intent(in) :: i
        associate (instance => evt%instance(i)%p)
            sqme(i) = instance%get_sqme ()
        end associate
    end subroutine get_sqme
end subroutine evt_resonance_get_subprocess_sqme

```

Apply a turnoff factor for off-shell kinematics to the `sqme` values. The `sqme` array indices are offset from the resonance history set entries.

```

<Resonance insertion: evt_resonance: TBP>+=
    procedure :: apply_turnoff_factor => evt_resonance_apply_turnoff_factor

<Resonance insertion: procedures>+=
    subroutine evt_resonance_apply_turnoff_factor (evt, sqme, index_array)
        class(evt_resonance_t), intent(in) :: evt
        real(default), dimension(:), intent(inout) :: sqme
        integer, dimension(:), intent(in) :: index_array
        integer :: k, i_res, i_prc
        do k = 1, size (index_array)
            i_res = evt%selected_component
            i_prc = index_array(k) + evt%index_offset(i_res)
            sqme(i_prc) = sqme(i_prc) &
                * evt%res_history_set(i_res)%evaluate_gaussian &
                & (evt%particle_set%get_outgoing_momenta (), &
                & evt%on_shell_turnoff, index_array(k))
        end do
    end subroutine evt_resonance_apply_turnoff_factor

```

We use the calculations of resonant matrix elements to determine probabilities for all applicable resonance configurations. This method combines the steps implemented above.

First, we determine the selected process component.

TODO: the version below selects the first component which is found active. This make sense only for standard LO process components, where exactly one component corresponds to a MCI set.

For the selected process component, we query the kinematics and determine the applicable resonance histories. We collect squared matrix elements for those resonance histories and compare them to the master-process squared matrix element.

The result is the probability for each resonance history together with the probability for non-resonant background (zeroth entry). The latter is defined as the difference between the complete process result and the sum of the resonances, ignoring the possibility for interference. If the complete process result is actually undershooting the sum of resonances, we nevertheless count the background with positive probability.

When looking up the subprocess `sqme`, we must add the `index_offset` to the resulting array, since the indices returned by the individual history set all count

from one, while the subprocess instances that belong to process components are collected in one flat array.

After determining matrix elements and background, we may reduce the weight of the matrix elements in the selector by applying a turnoff factor.

The factor **background_factor** indicates whether to include the background contribution at all, as long as there is a nonvanishing resonance contribution. Note that instead of setting background to zero, we just multiply it by a very small number. This ensures that indices are assigned correctly, and that background will eventually be selected if smooth turnoff is chosen.

```

<Resonance insertion: evt resonance: TBP>+=
  procedure :: compute_probabilities => evt_resonance_compute_probabilities

<Resonance insertion: procedures>+=
  subroutine evt_resonance_compute_probabilities (evt)
    class(evt_resonance_t), intent(inout) :: evt
    integer, dimension(:), allocatable :: index_array
    real(default) :: sqme_master, sqme_sum, sqme_bg
    real(default), dimension(:), allocatable :: sqme_res
    integer :: n, ic
    if (.not. associated (evt%process_instance)) return
    n = size (evt%instance)
    call evt%select_component (0)
    FIND_ACTIVE_COMPONENT: do ic = 1, evt%process%get_n_components ()
      if (evt%process%component_is_selected (ic)) then
        call evt%select_component (ic)
        exit FIND_ACTIVE_COMPONENT
      end if
    end do FIND_ACTIVE_COMPONENT
    if (evt%selected_component > 0) then
      call evt%determine_on_shell_histories (index_array)
    else
      allocate (index_array (0))
    end if
    call evt%evaluate_subprocess &
      (index_array + evt%index_offset(evt%selected_component))
    allocate (sqme_res (n), source = 0._default)
    call evt%get_subprocess_sqme &
      (sqme_res, index_array + evt%index_offset(evt%selected_component))
    sqme_master = evt%get_master_sqme ()
    sqme_sum = sum (sqme_res)
    sqme_bg = abs (sqme_master - sqme_sum)
    if (evt%on_shell_turnoff > 0) then
      call evt%apply_turnoff_factor (sqme_res, index_array)
    end if
    if (any (sqme_res > 0)) then
      sqme_bg = sqme_bg * evt%background_factor
    end if
    call evt%init_selector ([sqme_bg, sqme_res], offset = -1)
  end subroutine evt_resonance_compute_probabilities

```

Set the selected component (unit tests).

```

<Resonance insertion: evt resonance: TBP>+=
  procedure :: select_component => evt_resonance_select_component

```



```

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_select_component (evt, i_component)
    class(evt_resonance_t), intent(inout) :: evt
    integer, intent(in) :: i_component
    evt%selected_component = i_component
  end subroutine evt_resonance_select_component

```

32.3.5 Sanity check

Check the color assignment, which may be wrong for the inserted resonances. Delegated to the particle-set component. Return offending particle indices and, optionally, particles as arrays.

This is done in a unit test. The current algorithm, i.e., selecting the color assignment from the resonant-subprocess instance, should not generate invalid color assignments.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: find_prt_invalid_color => evt_resonance_find_prt_invalid_color

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_find_prt_invalid_color (evt, index, prt)
    class(evt_resonance_t), intent(in) :: evt
    integer, dimension(:), allocatable, intent(out) :: index
    type(particle_t), dimension(:), allocatable, intent(out), optional :: prt
    if (evt%particle_set_exists) then
      call evt%particle_set%find_prt_invalid_color (index, prt)
    else
      allocate (prt (0))
    end if
  end subroutine evt_resonance_find_prt_invalid_color

```

32.3.6 API implementation

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: prepare_new_event => evt_resonance_prepare_new_event

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_prepare_new_event (evt, i_mci, i_term)
    class(evt_resonance_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    call evt%reset ()
  end subroutine evt_resonance_prepare_new_event

```

Select one of the histories, based on the momentum array from the current particle set. Compute the probabilities for all resonant subprocesses and initialize the selector accordingly. Then select one resonance history, or none.

```

<Resonance insertion: evt resonance: TBP>+≡
  procedure :: generate_weighted => evt_resonance_generate_weighted

```

```

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_generate_weighted (evt, probability)
    class(evt_resonance_t), intent(inout) :: evt
    real(default), intent(inout) :: probability
    call evt%fill_momenta ()
    call evt%compute_probabilities ()
    call evt%selector%generate (evt%rng, evt%selected_history)
    probability = 1
  end subroutine evt_resonance_generate_weighted

```

Here take the current particle set and insert resonance intermediate states if applicable. The resonance history has already been chosen by the generator above. If no resonance history applies, just retain the particle set.

If a resonance history applies, we factorize the exclusive interaction of the selected (resonance-process) process instance. With a temporary particle set `prt_set` as workspace, we insert the resonances, reinstate parent-child relations and set colors and momenta for the resonances. The temporary is then copied back.

Taking the event data from the resonant subprocess instead of the master process, guarantees that all flavor, helicity, and color assignments are valid for the selected resonance history. Note that the transform may thus choose a quantum-number combination that is different from the one chosen by the master process.

The `i_term` value for the selected subprocess instance is always 1. We support only LO process. For those, the master process may have several terms (= components) that correspond to different external states. The subprocesses are distinct, each one corresponds to a definite master component, and by itself it consists of a single component/term.

However, if the selector chooses resonance history #0, i.e., no resonance, we just copy the particle set from the previous (i.e., trivial) event transform and ignore all subprocess data.

```

<Resonance insertion: evt_resonance: TBP>+≡
  procedure :: make_particle_set => evt_resonance_make_particle_set

<Resonance insertion: procedures>+≡
  subroutine evt_resonance_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_resonance_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
    type(particle_set_t), target :: prt_set
    type(particle_t), dimension(:), allocatable :: prt
    integer :: n_beam, n_in, n_vir, n_res, n_out, i, i_res, i_term, i_tree
    type(interaction_t), pointer :: int_matrix, int_flows
    integer, dimension(:), allocatable :: map
    type(resonance_tree_t) :: res_tree
    if (associated (evt%previous)) then
      if (evt%previous%particle_set_exists) then
        if (evt%selected_history > 0) then
          if (allocated (evt%instance)) then
            associate (instance => evt%instance(evt%selected_history)%p)

```

```

        call instance%evaluate_event_data (weight = 1._default)
        i_term = 1
        int_matrix => instance%get_matrix_int_ptr (i_term)
        int_flows => instance%get_flows_int_ptr (i_term)
        call evt%factorize_interactions (int_matrix, int_flows, &
            factorization_mode, keep_correlations, r)
        call evt%tag_incoming ()
    end associate
else ! this branch only for unit test
    evt%particle_set = evt%previous%particle_set
end if
i_tree = evt%selected_history &
    - evt%index_offset(evt%selected_component)
call evt%res_history_set(evt%selected_component)%get_tree &
    (i_tree, res_tree)
n_beam = evt%particle_set%get_n_beam ()
n_in = evt%particle_set%get_n_in ()
n_vir = evt%particle_set%get_n_vir ()
n_out = evt%particle_set%get_n_out ()
n_res = res_tree%get_n_resonances ()
allocate (map (n_beam + n_in + n_vir + n_out))
map(1:n_beam+n_in+n_vir) &
    = [(i, i = 1, n_beam+n_in+n_vir)]
map(n_beam+n_in+n_vir+1:n_beam+n_in+n_vir+n_out) &
    = [(i + n_res, &
        & i = n_beam+n_in+n_vir+1, &
        & n_beam+n_in+n_vir+n_out)]
call prt_set%transfer (evt%particle_set, n_res, map)
do i = 1, n_res
    i_res = n_beam + n_in + n_vir + i
    call prt_set%insert (i_res, &
        PRT_RESONANT, &
        res_tree%get_flv (i), &
        res_tree%get_children (i, &
            & n_beam+n_in+n_vir, n_beam+n_in+n_vir+n_res))
end do
do i = n_res, 1, -1
    i_res = n_beam + n_in + n_vir + i
    call prt_set%recover_color (i_res)
end do
call prt_set%set_momentum &
    (map(:), evt%particle_set%get_momenta (), on_shell = .true.)
do i = n_res, 1, -1
    i_res = n_beam + n_in + n_vir + i
    call prt_set%recover_momentum (i_res)
end do
call evt%particle_set%final ()
evt%particle_set = prt_set
call prt_set%final ()
evt%particle_set_exists = .true.
else ! retain particle set, as copied from previous evt
    evt%particle_set_exists = .true.
end if
else

```

```

        evt%particle_set_exists = .false.
    end if
else
    evt%particle_set_exists = .false.
end if
end subroutine evt_resonance_make_particle_set

```

32.3.7 Unit tests

Test module, followed by the corresponding implementation module.

```

<resonance_insertion_ut.f90>≡
  <File header>

```

```

module resonance_insertion_ut
  use unit_tests
  use resonance_insertion_uti

```

```

  <Standard module head>

```

```

  <Resonance insertion: public test>

```

```

contains

```

```

  <Resonance insertion: test driver>

```

```

end module resonance_insertion_ut

```

```

<resonance_insertion_uti.f90>≡
  <File header>

```

```

module resonance_insertion_uti

```

```

  <Use kinds>

```

```

  <Use strings>

```

```

  use format_utils, only: write_separator
  use os_interface
  use lorentz
  use rng_base, only: rng_t
  use flavors, only: flavor_t
  use colors, only: color_t
  use models, only: syntax_model_file_init, syntax_model_file_final
  use models, only: model_list_t, model_t
  use particles, only: particle_t, particle_set_t

```

```

  use resonances, only: resonance_info_t
  use resonances, only: resonance_history_t
  use resonances, only: resonance_history_set_t

```

```

  use event_transforms
  use resonance_insertion

```

```

  use rng_base_ut, only: rng_test_t

```

```

    <Standard module head>

    <Resonance insertion: test declarations>

contains

    <Resonance insertion: tests>

end module resonance_insertion_util

```

API: driver for the unit tests below.

```

<Resonance insertion: public test>≡
    public :: resonance_insertion_test

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

```

Test resonance insertion as event transform

Insert a resonance (W boson) into an event with momentum assignment.

```

<Resonance insertion: execute tests>≡
    call test (resonance_insertion_1, "resonance_insertion_1", &
        "simple resonance insertion", &
        u, results)

<Resonance insertion: test declarations>≡
    public :: resonance_insertion_1

<Resonance insertion: tests>≡
    subroutine resonance_insertion_1 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(particle_set_t) :: pset
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        type(flavor_t) :: fw
        type(color_t) :: col
        real(default) :: mw, ew, pw
        type(vector4_t), dimension(5) :: p
        class(rng_t), allocatable :: rng
        real(default) :: probability
        integer, dimension(:), allocatable :: i_invalid
        type(particle_t), dimension(:), allocatable :: prt_invalid
        integer :: i
    end subroutine resonance_insertion_1

```

```

write (u, "(A)")  "* Test output: resonance_insertion_1"
write (u, "(A)")  "* Purpose: apply simple resonance insertion"
write (u, "(A)")

write (u, "(A)")  "* Initialize environment"
write (u, "(A)")

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
       os_data, model)
! reset slightly in order to avoid a rounding ambiguity
call model%set_real (var_str ("mW"), 80.418_default)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 3, &
      pdg = [1, -1, 1, -2, 24], model = model)

call fw%init (24, model)

mw = fw%get_mass ()
ew = 200._default
pw = sqrt (ew**2 - mw**2)

p(1) = vector4_moving (ew, ew, 3)
p(2) = vector4_moving (ew, -ew, 3)
p(3) = vector4_moving (ew/2, vector3_moving ([pw/2, mw/2, 0._default]))
p(4) = vector4_moving (ew/2, vector3_moving ([pw/2, -mw/2, 0._default]))
p(5) = vector4_moving (ew, vector3_moving ([-pw, 0._default, 0._default]))

call pset%set_momentum (p, on_shell = .true.)

call col%init_col_acl (1,0)
call pset%set_color (1, col)

call col%init_col_acl (0,1)
call pset%set_color (2, col)

call col%init_col_acl (2,0)
call pset%set_color (3, col)

call col%init_col_acl (0,2)
call pset%set_color (4, col)

call col%init_col_acl (0,0)
call pset%set_color (5, col)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()

```

```

call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, -24, model, 2)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%init_selector ([1._default])
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (0, .false.)

call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
call evt_resonance%find_prt_invalid_color (i_invalid, prt_invalid)
write (u, "(A)")  "Particles with invalid color:"
select case (size (prt_invalid))
case (0)
    write (u, "(2x,A)")  "[none]"
case default
    do i = 1, size (prt_invalid)
        write (u, "(1x,A,1x,I0)", advance="no")  "Particle", i_invalid(i)
        call prt_invalid(i)%write (u)
    end do
end select

```

```

        end do
    end select

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"

    call evt_resonance%final ()
    call evt_trivial%final ()
    call syntax_model_file_final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: resonance_insertion_1"

end subroutine resonance_insertion_1

```

Resonance insertion with color mismatch

Same as previous test (but no momenta); resonance insertion should fail because of color mismatch: W boson is color-neutral.

```

<Resonance insertion: execute tests>+≡
    call test (resonance_insertion_2, "resonance_insertion_2", &
        "resonance color mismatch", &
        u, results)

<Resonance insertion: test declarations>+≡
    public :: resonance_insertion_2

<Resonance insertion: tests>+≡
    subroutine resonance_insertion_2 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(particle_set_t) :: pset
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        type(color_t) :: col
        class(rng_t), allocatable :: rng
        real(default) :: probability
        type(particle_t), dimension(:), allocatable :: prt_invalid
        integer, dimension(:), allocatable :: i_invalid
        integer :: i

        write (u, "(A)")  "* Test output: resonance_insertion_2"
        write (u, "(A)")  "* Purpose: resonance insertion with color mismatch"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")
    end subroutine resonance_insertion_2

```



```

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
    os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 3, &
    pdg = [1, -1, 1, -2, 24], model = model)

call col%init_col_acl (1,0)
call pset%set_color (1, col)

call col%init_col_acl (0,2)
call pset%set_color (2, col)

call col%init_col_acl (1,0)
call pset%set_color (3, col)

call col%init_col_acl (0,2)
call pset%set_color (4, col)

call col%init_col_acl (0,0)
call pset%set_color (5, col)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, -24, model, 2)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

```

```

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%init_selector ([1._default])
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (0, .false.)

call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
call evt_resonance%find_prt_invalid_color (i_invalid, prt_invalid)
write (u, "(A)")  "Particles with invalid color:"
select case (size (prt_invalid))
case (0)
  write (u, "(2x,A)")  "[none]"
case default
  do i = 1, size (prt_invalid)
    write (u, "(1x,A,1x,I0)", advance="no")  "Particle", i_invalid(i)
    call prt_invalid(i)%write (u)
  end do
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_insertion_2"

end subroutine resonance_insertion_2

```

Complex resonance history

This is the resonance history $u\bar{u} \rightarrow (t \rightarrow W^+b) + (\bar{t} \rightarrow (h \rightarrow b\bar{b}) + (\bar{t}^* \rightarrow W^- \bar{b}))$.

(Resonance insertion: execute tests)+≡

```

call test (resonance_insertion_3, "resonance_insertion_3", &
  "complex resonance history", &
  u, results)

```

```

<Resonance insertion: test declarations>+≡
    public :: resonance_insertion_3

<Resonance insertion: tests>+≡
    subroutine resonance_insertion_3 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(particle_set_t) :: pset
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        type(color_t) :: col
        class(rng_t), allocatable :: rng
        real(default) :: probability
        type(particle_t), dimension(:), allocatable :: prt_invalid
        integer, dimension(:), allocatable :: i_invalid
        integer :: i

        write (u, "(A)")  "* Test output: resonance_insertion_3"
        write (u, "(A)")  "* Purpose: resonance insertion with color mismatch"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM"), var_str ("SM.mdl"), &
             os_data, model)

        write (u, "(A)")  "* Initialize particle set"
        write (u, "(A)")

        call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 6, &
            pdg = [2, -2, 24, 5, 5, -5, -24, -5], model = model)

        call col%init_col_acl (1,0)
        call pset%set_color (1, col)

        call col%init_col_acl (0,2)
        call pset%set_color (2, col)

        call col%init_col_acl (0,0)
        call pset%set_color (3, col)

        call col%init_col_acl (1,0)
        call pset%set_color (4, col)

        call col%init_col_acl (3,0)
        call pset%set_color (5, col)
    end subroutine resonance_insertion_3

```

```

call col%init_col_acl (0,3)
call pset%set_color (6, col)

call col%init_col_acl (0,0)
call pset%set_color (7, col)

call col%init_col_acl (0,2)
call pset%set_color (8, col)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, 6, model, 6)
call res_history%add_resonance (res_info)
call res_info%init (12, 25, model, 6)
call res_history%add_resonance (res_info)
call res_info%init (60, -6, model, 6)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%init_selector ([1._default])

```

```

call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (0, .false.)

call evt_resonance%write (u)

write (u, "(A)")
call evt_resonance%find_prt_invalid_color (i_invalid, prt_invalid)
write (u, "(A)") "Particles with invalid color:"
select case (size (prt_invalid))
case (0)
    write (u, "(2x,A)") "[none]"
case default
    do i = 1, size (prt_invalid)
        write (u, "(1x,A,1x,I0)", advance="no") "Particle", i_invalid(i)
        call prt_invalid(i)%write (u)
    end do
end select

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: resonance_insertion_3"

end subroutine resonance_insertion_3

```

Resonance history selection

Another test with zero momenta: select one of several resonant channels using the selector component.

```

<Resonance insertion: execute tests>+≡
    call test (resonance_insertion_4, "resonance_insertion_4", &
        "resonance history selection", &
        u, results)

<Resonance insertion: test declarations>+≡
    public :: resonance_insertion_4

<Resonance insertion: tests>+≡
    subroutine resonance_insertion_4 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(particle_set_t) :: pset
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(evt_trivial_t), target :: evt_trivial

```

```

type(evt_resonance_t), target :: evt_resonance
type(color_t) :: col
class(rng_t), allocatable :: rng
real(default) :: probability
integer :: i

write (u, "(A)")  "* Test output: resonance_insertion_4"
write (u, "(A)")  "* Purpose: resonance history selection"
write (u, "(A)")

write (u, "(A)")  "* Initialize environment"
write (u, "(A)")

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
       os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 4, &
      pdg = [1, -1, 1, -2, -3, 4], model = model)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonance history set"
write (u, "(A)")

call res_history_set(1)%init ()

call res_info%init (3, -24, model, 4)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_info%init (12, 24, model, 4)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_info%init (12, 24, model, 4)
call res_history%add_resonance (res_info)
call res_info%init (15, 25, model, 4)
call res_history%add_resonance (res_info)
call res_history_set(1)%enter (res_history)

```

```

call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

do i = 1, 6
  write (u, "(A,1x,I0)")  "* Event #", i
  write (u, "(A)")

  call evt_resonance%prepare_new_event (1, 1)
  call evt_resonance%init_selector ([1._default, 2._default, 1._default])
  call evt_resonance%generate_weighted (probability)
  call evt_resonance%make_particle_set (0, .false.)

  call evt_resonance%write (u)
  write (u, "(A)")
end do

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_insertion_4"

end subroutine resonance_insertion_4

```

Resonance history selection

Another test with zero momenta: select either a resonant channel or no resonance.

```

(Resonance insertion: execute tests)+=
  call test (resonance_insertion_5, "resonance_insertion_5", &

```

```

        "resonance history on/off", &
        u, results)
<Resonance insertion: test declarations>+≡
    public :: resonance_insertion_5
<Resonance insertion: tests>+≡
    subroutine resonance_insertion_5 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(particle_set_t) :: pset
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        type(color_t) :: col
        class(rng_t), allocatable :: rng
        real(default) :: probability
        integer :: i

        write (u, "(A)")  "* Test output: resonance_insertion_5"
        write (u, "(A)")  "*   Purpose: resonance history selection including no resonance"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM"), var_str ("SM.mdl"), &
            os_data, model)

        write (u, "(A)")  "* Initialize particle set"
        write (u, "(A)")

        call pset%init_direct (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 4, &
            pdg = [1, -1, 1, -2, -3, 4], model = model)

        write (u, "(A)")  "* Fill trivial event transform"
        write (u, "(A)")

        call evt_trivial%reset ()
        call evt_trivial%set_particle_set (pset, 1, 1)

        write (u, "(A)")  "* Prepare resonance history set"
        write (u, "(A)")

        call res_history_set(1)%init ()

        call res_info%init (3, -24, model, 4)
        call res_history%add_resonance (res_info)

```



```

call res_history_set(1)%enter (res_history)
call res_history%clear ()

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)

write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

do i = 1, 2
  write (u, "(A,1x,I0)")  "* Event #", i
  write (u, "(A)")

  call evt_resonance%prepare_new_event (1, 1)
  call evt_resonance%init_selector ([1._default, 3._default], offset = -1)
  call evt_resonance%generate_weighted (probability)
  call evt_resonance%make_particle_set (0, .false.)

  call evt_resonance%write (u)
  write (u, "(A)")
end do

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_insertion_5"

end subroutine resonance_insertion_5

```

Resonance insertion with structured beams

Insert a resonance (W boson) into an event with beam and virtual particles.

(Resonance insertion: execute tests)+≡

```

call test (resonance_insertion_6, "resonance_insertion_6", &
  "resonance insertion with beam structure", &
  u, results)

```

```

<Resonance insertion: test declarations>+≡
    public :: resonance_insertion_6

<Resonance insertion: tests>+≡
    subroutine resonance_insertion_6 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(model_list_t) :: model_list
        type(particle_set_t) :: pset
        type(model_t), pointer :: model
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        class(rng_t), allocatable :: rng
        real(default) :: probability

        write (u, "(A)")  "* Test output: resonance_insertion_6"
        write (u, "(A)")  "*   Purpose: resonance insertion with structured beams"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM"), var_str ("SM.mdl"), &
             os_data, model)

        write (u, "(A)")  "* Initialize particle set"
        write (u, "(A)")

        call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
                               pdg = [11, -11, 11, -11, 22, 22, 13, -13], model = model)

        write (u, "(A)")  "* Fill trivial event transform"
        write (u, "(A)")

        call evt_trivial%reset ()
        call evt_trivial%set_particle_set (pset, 1, 1)
        call evt_trivial%write (u)
        call write_separator (u, 2)

        write (u, "(A)")
        write (u, "(A)")  "* Prepare resonance history set"
        write (u, "(A)")

        call res_history_set(1)%init ()

        call res_info%init (3, 23, model, 2)
        call res_history%add_resonance (res_info)
        call res_history_set(1)%enter (res_history)
        call res_history%clear ()

```

```

call res_history_set(1)%freeze ()

write (u, "(A)")  "* Initialize resonance insertion transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

allocate (rng_test_t :: rng)
call evt_resonance%import_rng (rng)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill resonance insertion transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%init_selector ([1._default])
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (0, .false.)

call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_resonance%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: resonance_insertion_6"

end subroutine resonance_insertion_6

```

32.4 Recoil kinematics

```

<recoil_kinematics.f90>≡
  <File header>

  module recoil_kinematics

    <Use kinds>
    use constants, only: twopi
    use lorentz, only: vector4_t

```

```

use lorentz, only: vector4_null
use lorentz, only: vector4_moving
use lorentz, only: vector3_moving
use lorentz, only: transverse_part
use lorentz, only: lorentz_transformation_t
use lorentz, only: inverse
use lorentz, only: boost
use lorentz, only: transformation
use lorentz, only: operator(+)
use lorentz, only: operator(-)
use lorentz, only: operator(*)
use lorentz, only: operator(**)
use lorentz, only: lambda

<Standard module head>

<Recoil kinematics: public>

<Recoil kinematics: parameters>

<Recoil kinematics: types>

contains

<Recoil kinematics: procedures>

end module recoil_kinematics

```

32.4.1 ϕ sampler

This is trivial. Generate an azimuthal angle, given a $(0,1)$ RNG parameter.

```

<Recoil kinematics: procedures>≡
  elemental subroutine generate_phi_recoil (r, phi)
    real(default), intent(in) :: r
    real(default), intent(out) :: phi

    phi = r * twopi

  end subroutine generate_phi_recoil

```

32.4.2 Q^2 sampler

The dynamics of factorization suggests to generate a flat Q^2 distribution from a (random) number, event by event.

At the lowest momentum transfer values, the particle (electron) mass sets a smooth cutoff. The formula can produce Q values below the electron mass, down to zero, but with a power distribution that eventually evolves into the expected logarithmic distribution for $Q^2 > m^2$.

We are talking about the absolute value here, so all Q^2 values are positive. For the actual momentum transfer, $q^2 = -Q^2$.

```

<Recoil kinematics: public>≡

```

```

public :: generate_q2_recoil
<Recoil kinematics: procedures>+≡
elemental subroutine generate_q2_recoil (s, x_bar, q2_max, m2, r, q2)
  real(default), intent(in) :: s
  real(default), intent(in) :: q2_max
  real(default), intent(in) :: x_bar
  real(default), intent(in) :: m2
  real(default), intent(in) :: r
  real(default), intent(out) :: q2

  real(default) :: q2_max_evt

  q2_max_evt = q2_max_event (s, x_bar, q2_max)

  q2 = m2 * (exp (r * log (1 + (q2_max_evt / m2))) - 1)

end subroutine generate_q2_recoil

```

The Q distribution is cut off from above by the kinematic limit, which depends on the energy that is available for the radiated photon, or by a user-defined cutoff – whichever is less. The kinematic limit fits the formulas for recoil momenta (see below), and it also implicitly enters the ISR collinear structure function, so the normalization of the distribution should be correct.

```

<Recoil kinematics: procedures>+≡
elemental function q2_max_event (s, x_bar, q2_max) result (q2)
  real(default), intent(in) :: s
  real(default), intent(in) :: x_bar
  real(default), intent(in) :: q2_max
  real(default) :: q2

  q2 = min (x_bar * s, q2_max)

end function q2_max_event

```

32.4.3 Kinematics functions

Given values for energies, $Q_{1,2}^2$, azimuthal angle, compute the matching polar angle of the radiating particle. The subroutine returns $\sin \theta$ and $\cos \theta$.

```

<Recoil kinematics: procedures>+≡
subroutine polar_angles (s, xb, rho, ee, q2, sin_th, cos_th, ok)
  real(default), intent(in) :: s
  real(default), intent(in) :: xb
  real(default), intent(in) :: rho
  real(default), dimension(2), intent(in) :: ee
  real(default), dimension(2), intent(in) :: q2
  real(default), dimension(2), intent(out) :: sin_th
  real(default), dimension(2), intent(out) :: cos_th
  logical, intent(out) :: ok

  real(default), dimension(2) :: sin2_th_2

```

```

sin2_th_2 = q2 / (ee * rho * xb * s)

if (all (sin2_th_2 <= 1)) then
  sin_th = 2 * sqrt (sin2_th_2 * (1 - sin2_th_2))
  cos_th = 1 - 2 * sin2_th_2
  ok = .true.
else
  sin_th = 0
  cos_th = 1
  ok = .false.
end if

end subroutine polar_angles

```

Compute the acollinearity parameter λ from azimuthal and polar angles. The result is a number between 0 and 1.

```

<Recoil kinematics: procedures>+≡
function lambda_factor (sin_th, cos_th, cphi) result (lambda)
  real(default), dimension(2), intent(in) :: sin_th
  real(default), dimension(2), intent(in) :: cos_th
  real(default), intent(in) :: cphi
  real(default) :: lambda

  lambda = (1 - cos_th(1) * cos_th(2) - cphi * sin_th(1) * sin_th(2)) / 2

end function lambda_factor

```

Compute the factor that rescales photon energies, such that the radiation angles match the kinematics parameters.

For small values of $\bar{x}/\cosh\eta$, we have to use the Taylor expansion if we do not want to lose precision. The optional argument allows for a unit test that compares exact and approximate.

```

<Recoil kinematics: procedures>+≡
function scale_factor (che, lambda, xb0, approximate) result (rho)
  real(default), intent(in) :: che
  real(default), intent(in) :: lambda
  real(default), intent(in) :: xb0
  logical, intent(in), optional :: approximate
  real(default) :: rho

  real(default), parameter :: &
    e0 = (100 * epsilon (1._default)) ** (0.3_default)
  logical :: approx

  if (present (approximate)) then
    approx = approximate
  else
    approx = (xb0/che) < e0
  end if

  if (approx) then
    rho = 1 - lambda * (xb0/(2*che)) * (1 + (1-lambda) * (xb0/che))
  else

```

```

      rho = (che / ((1-lambda)*xb0)) &
      * (1 - sqrt (1 - 2 * (1-lambda) * (xb0/che) &
      &      + (1-lambda) * (xb0 / che)**2))
    end if

end function scale_factor

```

The code snippet below is not used anywhere, but may be manually inserted in a unit test to numerically verify the approximation above.

```

<Recoil kinematics: extra test code>≡
  write (u, "(A)")
  write (u, "(A)") "*** Table: scale factor calculation"
  write (u, "(A)")

  lambda = 0.25_default
  write (u, FMT1) "lambda =", lambda

  che = 4._default
  write (u, FMT1) "che   =", che

  write (u, "(A)") "  x0      rho(exact)   rho(approx)   rho(chosen)"
  xb0 = 1._default
  do i = 1, 30
    xb0 = xb0 / 10
    write (u, FMT4)  xb0, &
      scale_factor (che, lambda, xb0, approximate=.false.), &
      scale_factor (che, lambda, xb0, approximate=.true.), &
      scale_factor (che, lambda, xb0)
  end do

```

Compute the current values for the $x_{1,2}$ parameters, given the updated scale factor ρ and the collinear parameters.

```

<Recoil kinematics: procedures>+≡
  subroutine scaled_x (rho, ee, xb0, x, xb)
    real(default), intent(in) :: rho
    real(default), dimension(2), intent(in) :: ee
    real(default), intent(in) :: xb0
    real(default), dimension(2), intent(out) :: x
    real(default), dimension(2), intent(out) :: xb

    xb = rho * ee * xb0
    x = 1 - xb

  end subroutine scaled_x

```

32.4.4 Iterative solution of kinematics constraints

Find a solution of the kinematics constraints. We know the parameters appropriate for collinear kinematics \sqrt{s} , $x_{1,2}^c$. We have picked values for the momentum transfer $Q_{1,2}$ and the azimuthal angles $\phi_{1,2}$. The solution consists of modified energy fractions $x_{1,2}$ and polar angles $\theta_{1,2}$.

If the computation fails, which can happen for large momentum transfer, the flag ok will indicate this.

<Recoil kinematics: public>+≡

public :: solve_recoil

<Recoil kinematics: procedures>+≡

subroutine solve_recoil (sqrts, xc, xcb, phi, q2, x, xb, cos_th, sin_th, ok)

```

    real(default), intent(in) :: sqrts
    real(default), dimension(2), intent(in) :: xc
    real(default), dimension(2), intent(in) :: xcb
    real(default), dimension(2), intent(in) :: phi
    real(default), dimension(2), intent(in) :: q2
    real(default), dimension(2), intent(out) :: x
    real(default), dimension(2), intent(out) :: xb
    real(default), dimension(2), intent(out) :: cos_th
    real(default), dimension(2), intent(out) :: sin_th
    logical, intent(out) :: ok

```

```

    real(default) :: s
    real(default), dimension(2) :: ee
    real(default), dimension(2) :: th
    real(default) :: xb0, cphi
    real(default) :: che, lambda
    real(default) :: rho_new, rho, rho_old
    real(default) :: dr_old, dr_new
    real(default), parameter :: dr_limit = 100 * epsilon (1._default)
    integer, parameter :: n_it_max = 20
    integer :: i

```

```

    ok = .true.

```

```

    s = sqrts**2
    ee = sqrt ([xcb(1)/xcb(2), xcb(2)/xcb(1)])
    che = sum (ee) / 2
    xb0 = sqrt (xcb(1) * xcb(2))
    cphi = cos (phi(1) - phi(2))

```

```

    rho_old = 10
    rho = 1
    th = 0
    sin_th = sin (th)
    cos_th = cos (th)
    lambda = lambda_factor (sin_th, cos_th, cphi)
    call scaled_x (rho, ee, xb0, x, xb)

```

```

    iterate_loop: do i = 1, n_it_max

```

```

        call polar_angles (s, xb0, rho, ee, q2, sin_th, cos_th, ok)
        if (.not. ok) return
        th = atan2 (sin_th, cos_th)

```

```

        lambda = lambda_factor (sin_th, cos_th, cphi)
        rho_new = scale_factor (che, lambda, xb0)
        call scaled_x (rho_new, ee, xb0, x, xb)

```



```

dr_old = abs (rho - rho_old)
dr_new = abs (rho_new - rho)

rho_old = rho
rho = rho_new

if (dr_new < dr_limit .or. dr_new >= dr_old) exit iterate_loop

end do iterate_loop

end subroutine solve_recoil

```

With all kinematics parameters known, construct actual four-vectors for the recoil momenta, the off-shell (spacelike) parton momenta, and on-shell projected parton momenta.

```

<Recoil kinematics: public>+≡
public :: recoil_momenta

<Recoil kinematics: procedures>+≡
subroutine recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, &
    km, qm, qo, ok)
    real(default), intent(in) :: sqrts
    real(default), dimension(2), intent(in) :: xc
    real(default), dimension(2), intent(in) :: xb
    real(default), dimension(2), intent(in) :: cos_th
    real(default), dimension(2), intent(in) :: sin_th
    real(default), dimension(2), intent(in) :: phi
    real(default), dimension(2), intent(in) :: mo
    type(vector4_t), dimension(2), intent(out) :: km
    type(vector4_t), dimension(2), intent(out) :: qm
    type(vector4_t), dimension(2), intent(out) :: qo
    logical, intent(out) :: ok

    type(vector4_t), dimension(2) :: pm
    type(lorentz_transformation_t) :: lt
    real(default) :: sqsh
    real(default) :: po4, po2
    real(default), dimension(2) :: p0, p3

    pm(1) = &
        vector4_moving (sqrts/2, &
            vector3_moving ([0._default, 0._default, sqrts/2]))
    pm(2) = &
        vector4_moving (sqrts/2, &
            vector3_moving ([0._default, 0._default, -sqrts/2]))

    km(1) = xb(1) * (sqrts/2) * vector4_moving ( &
        1._default, &
        vector3_moving ([ &
            & sin_th(1) * cos (phi(1)), &
            & sin_th(1) * sin (phi(1)), &
            & cos_th(1)]) &
        )

```

```

km(2) = xb(2) * (sqrts/2) * vector4_moving ( &
    1._default, &
    vector3_moving ([ &
        & -sin_th(2) * cos (phi(2)), &
        & -sin_th(2) * sin (phi(2)), &
        & -cos_th(2)] &
    )

qm(1) = pm(1) - km(1)
qm(2) = pm(2) - km(2)

sqsh = sqrt (xc(1)*xc(2)) * sqrts
lt = transformation (3, qm(1), qm(2), sqsh)

po4 = lambda (sqsh**2, mo(1)**2, mo(2)**2)
ok = po4 > 0
if (ok) then
    po2 = sqrt (po4)/4
    p0 = sqrt (po2 + mo**2)
    p3 = [sqrt (po2), -sqrt (po2)]
    qo = lt * vector4_moving (p0, p3, 3)
else
    qo = vector4_null
end if

end subroutine recoil_momenta

```

Compute the Lorentz transformation that we can use to transform any outgoing momenta into the new c.m. system of the incoming partons. Not relying on the previous calculations, we determine the transformation that transforms the original collinear partons into their c.m. system, and then transform this to the new c.m. system.

```

<Recoil kinematics: public>+≡
public :: recoil_transformation

<Recoil kinematics: procedures>+≡
subroutine recoil_transformation (sqrts, xc, qo, lt)
    real(default), intent(in) :: sqrts
    real(default), dimension(2), intent(in) :: xc
    type(vector4_t), dimension(2), intent(in) :: qo
    type(lorentz_transformation_t), intent(out) :: lt

    real(default) :: sqsh
    type(vector4_t), dimension(2) :: qc
    type(lorentz_transformation_t) :: ltc, lto

    qc(1) = xc(1) * vector4_moving (sqrts/2, sqrts/2, 3)
    qc(2) = xc(2) * vector4_moving (sqrts/2, -sqrts/2, 3)

    sqsh = sqrt (xc(1) * xc(2)) * sqrts
    ltc = transformation (3, qc(1), qc(2), sqsh)
    lto = transformation (3, qo(1), qo(2), sqsh)
    lt = lto * inverse (ltc)

```

```
end subroutine recoil_transformation
```

Compute the Lorentz boost that transforms the c.m. frame of the momenta into the lab frame where they are given. Also return their common invariant mass, \sqrt{s} .

If the initial momenta are not collinear, `ok` is set false.

```
<Recoil kinematics: public>+≡
  public :: initial_transformation

<Recoil kinematics: procedures>+≡
  subroutine initial_transformation (p, sqrts, lt, ok)
    type(vector4_t), dimension(2), intent(in) :: p
    real(default), intent(out) :: sqrts
    type(lorentz_transformation_t), intent(out) :: lt
    logical, intent(out) :: ok

    ok = all (transverse_part (p) == 0)

    sqrts = (p(1) + p(2)) ** 1
    lt = boost (p(1) + p(2), sqrts)

  end subroutine initial_transformation
```

32.4.5 Generate recoil event

Combine the above kinematics calculations. First generate azimuthal angles and momentum transfer, solve kinematics and compute momenta for the radiated photons and the on-shell projected, recoiling partons.

The `mo` masses are used for the on-shell projection of the partons after radiation. They may be equal to `m`, or set to zero.

If `ok` is false, the data point has failed and we should repeat the procedure for a new set of RNG parameters `r`.

```
<Recoil kinematics: public>+≡
  public :: generate_recoil

<Recoil kinematics: procedures>+≡
  subroutine generate_recoil (sqrts, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
    real(default), intent(in) :: sqrts
    real(default), intent(in), dimension(2) :: q_max
    real(default), intent(in), dimension(2) :: m
    real(default), intent(in), dimension(2) :: mo
    real(default), intent(in), dimension(2) :: xc
    real(default), intent(in), dimension(2) :: xcb
    real(default), intent(in), dimension(4) :: r
    type(vector4_t), dimension(2), intent(out) :: km
    type(vector4_t), dimension(2), intent(out) :: qm
    type(vector4_t), dimension(2), intent(out) :: qo
    logical, intent(out) :: ok

    real(default), dimension(2) :: q2
    real(default), dimension(2) :: phi
    real(default), dimension(2) :: x
```

```

real(default), dimension(2) :: xb
real(default), dimension(2) :: cos_th
real(default), dimension(2) :: sin_th

call generate_q2_recoil (sqrts**2, xcb, q_max**2, m**2, r(1:2), q2)
call generate_phi_recoil (r(3:4), phi)

call solve_recoil (sqrts, xc, xcb, phi, q2, x, xb, cos_th, sin_th, ok)
if (ok) then
    call recoil_momenta &
        (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
end if

end subroutine generate_recoil

```

32.4.6 Unit tests

Test module, followed by the corresponding implementation module.

```

<recoil_kinematics.ut.f90>≡
  <File header>

  module recoil_kinematics_ut
    use unit_tests
    use recoil_kinematics_uti

    <Standard module head>

    <Recoil kinematics: public test>

    contains

    <Recoil kinematics: test driver>

  end module recoil_kinematics_ut

<recoil_kinematics.uti.f90>≡
  <File header>

  module recoil_kinematics_uti

    <Use kinds>
    use constants, only: twopi
    use constants, only: degree
    use lorentz, only: vector4_t
    use lorentz, only: vector4_moving
    use lorentz, only: lorentz_transformation_t
    use lorentz, only: inverse
    use lorentz, only: operator(+)
    use lorentz, only: operator(*)
    use lorentz, only: operator(**)
    use lorentz, only: pacify

    use recoil_kinematics, only: solve_recoil

```

```

    use recoil_kinematics, only: recoil_momenta
    use recoil_kinematics, only: recoil_transformation
    use recoil_kinematics, only: initial_transformation
    use recoil_kinematics, only: generate_q2_recoil
    use recoil_kinematics, only: generate_recoil

```

⟨Standard module head⟩

⟨Recoil kinematics: test declarations⟩

contains

⟨Recoil kinematics: tests⟩

end module recoil_kinematics_util

API: driver for the unit tests below.

```

⟨Recoil kinematics: public test⟩≡
    public :: recoil_kinematics_test

⟨Recoil kinematics: test driver⟩≡
    subroutine recoil_kinematics_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    ⟨Recoil kinematics: execute tests⟩
    end subroutine recoil_kinematics_test

```

Recoil kinematics

For a set of input data, solve the kinematics constraints and generate momenta accordingly.

```

⟨Recoil kinematics: execute tests⟩≡
    call test (recoil_kinematics_1, "recoil_kinematics_1", &
        "iterative solution of non-collinear kinematics", &
        u, results)

⟨Recoil kinematics: test declarations⟩≡
    public :: recoil_kinematics_1

⟨Recoil kinematics: tests⟩≡
    subroutine recoil_kinematics_1 (u)
        integer, intent(in) :: u

        real(default) :: sqrts
        real(default), dimension(2) :: xc, xcb
        real(default), dimension(2) :: q
        real(default), dimension(2) :: phi
        real(default), dimension(2) :: mo
        real(default), dimension(2) :: cos_th, sin_th
        real(default), dimension(2) :: x
        real(default), dimension(2) :: xb
        type(vector4_t), dimension(2) :: km
        type(vector4_t), dimension(2) :: qm

```

```

type(vector4_t), dimension(2) :: qo
integer :: i
logical :: ok

character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
character(*), parameter :: FMT2 = "(1x,A,9(1x,F10.5))"
character(*), parameter :: FMT4 = "(3x,ES8.1,9(1x,ES19.12))"

write (u, "(A)")  "* Test output: recoil_kinematics_1"
write (u, "(A)")  "* Purpose: compute kinematics for various input data"
write (u, "(A)")

sqrt_s = 100
write (u, FMT1) "sqrt_s =", sqrt_s

write (u, "(A)")
write (u, "(A)") "*** collinear data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = 0
mo = 0

call show_data
call solve_recoil (sqrt_s, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results

call recoil_momenta (sqrt_s, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** moderate data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 0.05_default] * sqrt_s

call show_data
call solve_recoil (sqrt_s, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results
call recoil_momenta (sqrt_s, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** semi-soft data set"
write (u, "(A)")

xcb= [0.1_default, 0.0001_default]
xc = 1 - xcb
phi = [0.1_default, 0.2_default] * twopi

```

```

q = [0.2_default, 0.00001_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** hard-soft data set"
write (u, "(A)")

xcb= [0.1_default, 1.e-30_default]
xc = 1 - xcb
phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 1.e-35_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** hard data set"
write (u, "(A)")

xc = [0.2_default, 0.4_default]
xcb = 1 - xc
phi = [0.1_default, 0.8_default] * twopi
q = [0.74_default, 0.3_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call show_results

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)") "*** failing data set"
write (u, "(A)")

xc = [0.2_default, 0.4_default]
xcb = 1 - xc
phi = [0.1_default, 0.8_default] * twopi
q = [0.9_default, 0.3_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
if (.not. ok) then
    write (u, "(A)")

```

```

        write (u, "(A)") "Failed as expected."
    end if

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: recoil_kinematics_1"

contains

subroutine show_data
    write (u, FMT1) "sqs_h =", sqrt (xc(1) * xc(2)) * sqrts
    write (u, FMT1) "xc    =", xc
    write (u, FMT1) "xcb   =", xcb
    write (u, FMT1) "Q     =", Q
    write (u, FMT1) "phi/D =", phi / degree
end subroutine show_data

subroutine show_results
    write (u, "(A)")
    write (u, "(A)") "Result:"
    write (u, FMT1) "th/D  =", atan2 (sin_th, cos_th) / degree
    write (u, FMT1) "x     =", x
    write (u, "(A)")
end subroutine show_results

subroutine show_momenta
    type(vector4_t) :: qm0, qo0
    real(default), parameter :: tol = 1.e-7_default
    call pacify (km, tol)
    call pacify (qm, tol)
    call pacify (qo, tol)
    write (u, "(A)") "Momenta: k"
    call km(1)%write (u, testflag=.true.)
    call km(2)%write (u, testflag=.true.)
    write (u, FMT1) "k^2 =", abs (km(1)**2), abs (km(2)**2)
    write (u, "(A)")
    write (u, "(A)") "Momenta: q"
    call qm(1)%write (u, testflag=.true.)
    call qm(2)%write (u, testflag=.true.)
    write (u, "(A)")
    write (u, "(A)") "Momenta: q(os)"
    call qo(1)%write (u, testflag=.true.)
    call qo(2)%write (u, testflag=.true.)
    write (u, "(A)")
    write (u, "(A)") "Check: parton momentum sum: q vs q(os)"
    qm0 = qm(1) + qm(2)
    call qm0%write (u, testflag=.true.)
    qo0 = qo(1) + qo(2)
    call qo0%write (u, testflag=.true.)
    write (u, "(A)")
    write (u, "(A)") "* Check: momentum transfer (off-shell/on-shell)"
    write (u, FMT2) "|q| =", abs (qm(1)**1), abs (qm(2)**1)
    write (u, FMT2) "Q   =", q
    write (u, FMT2) "|qo|=", abs (qo(1)**1), abs (qo(2)**1)
    write (u, "(A)")

```



```

        write (u, "(A)") "* Check: sqrts, sqrts_hat"
        write (u, FMT1) "|p| =", (km(1)+km(2)+qm(1)+qm(2))**1, (qm(1)+qm(2))**1
        write (u, FMT1) "sqs =", sqrts, sqrt (product (xc)) * sqrts
        write (u, FMT1) "|po|=", abs ((km(1)+km(2)+qo(1)+qo(2))**1), abs ((qo(1)+qo(2))**1)
    end subroutine show_momenta

end subroutine recoil_kinematics_1

```

Recoil Q distribution

Sample the Q distribution for equidistant bins in the input variable.

```

<Recoil kinematics: execute tests>+≡
    call test (recoil_kinematics_2, "recoil_kinematics_2", &
        "Q distribution", &
        u, results)

<Recoil kinematics: test declarations>+≡
    public :: recoil_kinematics_2

<Recoil kinematics: tests>+≡
    subroutine recoil_kinematics_2 (u)
        integer, intent(in) :: u

        real(default) :: sqrts
        real(default) :: q_max
        real(default) :: m
        real(default) :: x_bar
        real(default) :: r
        real(default) :: q2, q2_old
        integer :: i
        integer :: n_bin

        character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
        character(*), parameter :: FMT3 = "(2x,9(1x,F10.5))"

        write (u, "(A)") "* Test output: recoil_kinematics_2"
        write (u, "(A)") "* Purpose: compute Q distribution"
        write (u, "(A)")

        n_bin = 20

        write (u, "(A)") "* No Q cutoff, xbar = 1"
        write (u, "(A)")

        sqrts = 100
        q_max = sqrts
        m = 0.511e-3_default
        x_bar = 1._default
        call show_table

        write (u, "(A)")
        write (u, "(A)") "* With Q cutoff, xbar = 1"
        write (u, "(A)")

```

```

q_max = 10
call show_table

write (u, "(A)")
write (u, "(A)") "* No Q cutoff, xbar = 0.01"
write (u, "(A)")

q_max = sqrts
x_bar = 0.01_default
call show_table

write (u, "(A)")
write (u, "(A)") "* Test output end: recoil_kinematics_2"

contains

subroutine show_table
  write (u, FMT1) "sqrts =", sqrts
  write (u, FMT1) "q_max =", q_max
  write (u, FMT1) "m      =", m
  write (u, FMT1) "x_bar =", x_bar
  write (u, "(A)")
  write (u, "(1x,A)") "Table:  r          |Q|      |Q_i/Q_(i-1)|"
  q2_old = 0
  do i = 0, n_bin
    r = real (i, default) / n_bin
    call generate_q2_recoil (sqrts**2, x_bar, q_max**2, m**2, r, q2)
    if (q2_old > 0) then
      write (u, FMT3) r, sqrt (q2), sqrt (q2 / q2_old)
    else
      write (u, FMT3) r, sqrt (q2)
    end if
    q2_old = q2
  end do
end subroutine show_table

end subroutine recoil_kinematics_2

```

Generate recoil event

Combine Q^2 sampling with momentum generation.

```

<Recoil kinematics: execute tests>+≡
  call test (recoil_kinematics_3, "recoil_kinematics_3", &
    "generate recoil event", &
    u, results)

<Recoil kinematics: test declarations>+≡
  public :: recoil_kinematics_3

<Recoil kinematics: tests>+≡
  subroutine recoil_kinematics_3 (u)
    integer, intent(in) :: u

    real(default) :: sqrts

```

```

real(default), dimension(2) :: q_max
real(default), dimension(2) :: m, mo
real(default), dimension(2) :: xc, xcb
real(default), dimension(4) :: r
type(vector4_t), dimension(2) :: km
type(vector4_t), dimension(2) :: qm
type(vector4_t), dimension(2) :: qo
logical :: ok

character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
character(*), parameter :: FMT2 = "(1x,A,9(1x,F10.5))"

write (u, "(A)")  "* Test output: recoil_kinematics_3"
write (u, "(A)")  "* Purpose: generate momenta from RNG parameters"
write (u, "(A)")

write (u, "(A)")  "*** collinear data set"
write (u, "(A)")

sqrt_s = 100
q_max = sqrt_s
m      = 0.511e-3_default
mo     = 0

xc = [0.6_default, 0.9_default]
xcb = 1 - xc

r = [0._default, 0._default, 0._default, 0._default]

call show_data
call generate_recoil (sqrt_s, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)")  "*** moderate data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc

r = [0.8_default, 0.2_default, 0.1_default, 0.2_default]

call show_data
call generate_recoil (sqrt_s, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
call show_momenta

write (u, "(A)")
write (u, "(A)")  "*** failing data set"
write (u, "(A)")

xc = [0.2_default, 0.4_default]
xcb = 1 - xc

r = [0.9999_default, 0.3_default, 0.1_default, 0.8_default]

```

```

call show_data
call generate_recoil (sqrts, q_max, m, mo, xc, xcb, r, km, qm, qo, ok)
if (.not. ok) then
    write (u, "(A)")
    write (u, "(A)") "Failed as expected."
else
    call show_momenta
end if

contains

subroutine show_data
    write (u, FMT1) "sqrts =", sqrts
    write (u, FMT1) "q_max =", q_max
    write (u, FMT1) "m      =", m
    write (u, FMT1) "xc     =", xc
    write (u, FMT1) "xcb    =", xcb
    write (u, FMT1) "r      =", r
end subroutine show_data

subroutine show_momenta
    real(default), parameter :: tol = 1.e-7_default
    call pacify (km, tol)
    call pacify (qo, tol)
    write (u, "(A)")
    write (u, "(A)") "* Momenta: k"
    call km(1)%write (u, testflag=.true.)
    call km(2)%write (u, testflag=.true.)
    write (u, FMT1) "k^2 =", abs (km(1)**2), abs (km(2)**2)
    write (u, "(A)")
    write (u, "(A)") "* Momenta: q(os)"
    call qo(1)%write (u, testflag=.true.)
    call qo(2)%write (u, testflag=.true.)
    write (u, FMT1) "q^2 =", abs (qo(1)**2), abs (qo(2)**2)
    write (u, "(A)")
    write (u, "(A)") "* Check: momentum transfer (off-shell/on-shell)"
    write (u, FMT2) "Q    =", q_check (1), q_check (2)
    write (u, FMT2) "|q| =", abs (qm(1)**1), abs (qm(2)**1)
    write (u, "(A)")
    write (u, "(A)") "* Check: sqrts, sqrts_hat"
    write (u, FMT1) "sqrs =", sqrts, sqrt (product (xc)) * sqrts
    write (u, FMT1) "|po| =", abs ((km(1)+km(2)+qo(1)+qo(2))**1), abs ((qo(1)+qo(2))**1)
end subroutine show_momenta

function q_check (i) result (q)
    integer, intent(in) :: i
    real(default) :: q
    real(default) :: q2
    call generate_q2_recoil (sqrts**2, xcb(i), q_max(i)**2, m(i)**2, r(i), q2)
    q = sqrt (q2)
end function q_check

end subroutine recoil_kinematics_3

```

Transformation after recoil

Given a solution to recoil kinematics, compute the Lorentz transformation that transforms the old collinear parton momenta into the new parton momenta.

```
<Recoil kinematics: execute tests>+≡
  call test (recoil_kinematics_4, "recoil_kinematics_4", &
    "reference frame", &
    u, results)

<Recoil kinematics: test declarations>+≡
  public :: recoil_kinematics_4

<Recoil kinematics: tests>+≡
  subroutine recoil_kinematics_4 (u)
    integer, intent(in) :: u

    real(default) :: sqrts
    real(default), dimension(2) :: xc, xcb
    real(default), dimension(2) :: q
    real(default), dimension(2) :: phi
    real(default), dimension(2) :: cos_th, sin_th
    real(default), dimension(2) :: mo
    real(default), dimension(2) :: x
    real(default), dimension(2) :: xb
    type(vector4_t), dimension(2) :: km
    type(vector4_t), dimension(2) :: qm
    type(vector4_t), dimension(2) :: qo
    type(lorentz_transformation_t) :: lt
    logical :: ok

    character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
    character(*), parameter :: FMT2 = "(1x,A,9(1x,F10.5))"

    write (u, "(A)")  "* Test output: recoil_kinematics_4"
    write (u, "(A)")  "* Purpose: check Lorentz transformation for recoil"
    write (u, "(A)")

    sqrts = 100
    write (u, FMT1) "sqrts =", sqrts

    write (u, "(A)")
    write (u, "(A)") "*** collinear data set"
    write (u, "(A)")

    xc = [0.6_default, 0.9_default]
    xcb = 1 - xc
    phi = [0.1_default, 0.2_default] * twopi
    q = 0
    mo = 0

    call show_data
    call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
```

```

call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call recoil_transformation (sqrts, xc, qo, lt)
call show_transformation

write (u, "(A)")
write (u, "(A)") "*** moderate data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 0.05_default] * sqrts

call show_data
call solve_recoil (sqrts, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call recoil_momenta (sqrts, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call recoil_transformation (sqrts, xc, qo, lt)
call show_transformation

write (u, "(A)")
write (u, "(A)") "* Test output end: recoil_kinematics_4"

contains

subroutine show_data
  write (u, FMT1) "sqs_h =", sqrt (xc(1) * xc(2)) * sqrts
  write (u, FMT1) "xc   =", xc
  write (u, FMT1) "xcb   =", xcb
  write (u, FMT1) "Q     =", Q
  write (u, FMT1) "phi/D =", phi / degree
end subroutine show_data

subroutine show_transformation
  type(vector4_t), dimension(2) :: qc
  type(vector4_t), dimension(2) :: qct
  real(default), parameter :: tol = 1.e-7_default
  qc(1) = xc(1) * vector4_moving (sqrts/2, sqrts/2, 3)
  qc(2) = xc(2) * vector4_moving (sqrts/2, -sqrts/2, 3)
  qct = lt * qc
  call pacify (qct, tol)
  write (u, "(A)")
  write (u, "(A)") "Momenta: q(os)"
  call qo(1)%write (u, testflag=.true.)
  call qo(2)%write (u, testflag=.true.)
  write (u, "(A)")
  write (u, "(A)") "Momenta: LT * qc"
  call qct(1)%write (u, testflag=.true.)
  call qct(2)%write (u, testflag=.true.)
end subroutine show_transformation

end subroutine recoil_kinematics_4

```

Transformation before recoil

Given a pair of incoming 'beam' partons (i.e., before ISR splitting), compute the transformation that transforms their common c.m. frame into the lab frame.

```
<Recoil kinematics: execute tests>+≡
    call test (recoil_kinematics_5, "recoil_kinematics_5", &
               "initial reference frame", &
               u, results)

<Recoil kinematics: test declarations>+≡
    public :: recoil_kinematics_5

<Recoil kinematics: tests>+≡
    subroutine recoil_kinematics_5 (u)
        integer, intent(in) :: u

        real(default) :: sqrts
        real(default) :: sqrtsi
        real(default), dimension(2) :: x
        type(vector4_t), dimension(2) :: p
        type(vector4_t), dimension(2) :: pi
        type(vector4_t), dimension(2) :: p0
        type(lorentz_transformation_t) :: lt
        logical :: ok

        character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
        character(*), parameter :: FMT2 = "(1x,A,9(1x,F10.5))"

        write (u, "(A)")  "*" Test output: recoil_kinematics_5"
        write (u, "(A)")  "*" Purpose: determine initial Lorentz transformation"
        write (u, "(A)")

        sqrts = 100
        write (u, FMT1) "sqrts =", sqrts

        x = [0.6_default, 0.9_default]

        p(1) = x(1) * vector4_moving (sqrts/2, sqrts/2, 3)
        p(2) = x(2) * vector4_moving (sqrts/2, -sqrts/2, 3)

        call show_data
        call initial_transformation (p, sqrtsi, lt, ok)

        pi(1) = vector4_moving (sqrtsi/2, sqrtsi/2, 3)
        pi(2) = vector4_moving (sqrtsi/2, -sqrtsi/2, 3)

        p0 = inverse (lt) * p

        call show_momenta

        write (u, "(A)")
        write (u, "(A)")  "*" Test output end: recoil_kinematics_5"

contains
```

```

subroutine show_data
  write (u, FMT1) "sqrts =", sqrts
  write (u, FMT1) "x      =", x
end subroutine show_data

subroutine show_momenta
  real(default), parameter :: tol = 1.e-7_default
  write (u, "(A)")
  write (u, "(A)") "* Momenta: p_in(c.m.)"
  call pi(1)%write (u, testflag=.true.)
  call pi(2)%write (u, testflag=.true.)
  write (u, "(A)")
  write (u, "(A)") "* Momenta: inv(LT) * p_in(lab)"
  call p0(1)%write (u, testflag=.true.)
  call p0(2)%write (u, testflag=.true.)
end subroutine show_momenta

end subroutine recoil_kinematics_5

```

Transformation after recoil with on-shell momenta

Given a solution to recoil kinematics, compute the Lorentz transformation that transforms the old collinear parton momenta into the new parton momenta.

Compare the results for massless and massive on-shell projection.

```

<Recoil kinematics: execute tests>+≡
  call test (recoil_kinematics_6, "recoil_kinematics_6", &
    "massless/massive on-shell projection", &
    u, results)

<Recoil kinematics: test declarations>+≡
  public :: recoil_kinematics_6

<Recoil kinematics: tests>+≡
  subroutine recoil_kinematics_6 (u)
    integer, intent(in) :: u

    real(default) :: sqrts
    real(default), dimension(2) :: xc, xcb
    real(default), dimension(2) :: q
    real(default), dimension(2) :: phi
    real(default), dimension(2) :: cos_th, sin_th
    real(default), dimension(2) :: x
    real(default), dimension(2) :: xb
    real(default), dimension(2) :: mo, z
    type(vector4_t), dimension(2) :: km
    type(vector4_t), dimension(2) :: qm
    type(vector4_t), dimension(2) :: qo
    type(lorentz_transformation_t) :: lt
    logical :: ok

    character(*), parameter :: FMT1 = "(1x,A,9(1x,F15.10))"
    character(*), parameter :: FMT2 = "(1x,A,9(1x,F11.6))"

```



```

write (u, "(A)")  "* Test output: recoil_kinematics_6"
write (u, "(A)")  "* Purpose: check effect of mass in on-shell projection"
write (u, "(A)")

sqrt_s = 10
write (u, FMT1)  "sqrt_s =", sqrt_s
z = 0
mo = 0.511e-3
write (u, FMT1)  "mass =", mo

write (u, "(A)")
write (u, "(A)")  "*** collinear data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = 0

call show_data
call solve_recoil (sqrt_s, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call recoil_momenta (sqrt_s, xc, xb, cos_th, sin_th, phi, z, km, qm, qo, ok)
call recoil_transformation (sqrt_s, xc, qo, lt)
write (u, "(A)")
write (u, "(A)")  "Massless projection:"
call show_momenta

call recoil_momenta (sqrt_s, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call recoil_transformation (sqrt_s, xc, qo, lt)
write (u, "(A)")
write (u, "(A)")  "Massive projection:"
call show_momenta

write (u, "(A)")
write (u, "(A)")  "*** moderate data set"
write (u, "(A)")

xc = [0.6_default, 0.9_default]
xcb = 1 - xc
phi = [0.1_default, 0.2_default] * twopi
q = [0.2_default, 0.05_default] * sqrt_s

call show_data
call solve_recoil (sqrt_s, xc, xcb, phi, q**2, x, xb, cos_th, sin_th, ok)
call recoil_momenta (sqrt_s, xc, xb, cos_th, sin_th, phi, z, km, qm, qo, ok)
call recoil_transformation (sqrt_s, xc, qo, lt)
write (u, "(A)")
write (u, "(A)")  "Massless projection:"
call show_momenta

call recoil_momenta (sqrt_s, xc, xb, cos_th, sin_th, phi, mo, km, qm, qo, ok)
call recoil_transformation (sqrt_s, xc, qo, lt)
write (u, "(A)")

```

```

write (u, "(A)") "Massive projection:"
call show_momenta

write (u, "(A)")
write (u, "(A)")  "** Test output end: recoil_kinematics_6"

contains

subroutine show_data
  write (u, FMT1) "sqs_h =", sqrt (xc(1) * xc(2)) * sqrts
  write (u, FMT1) "xc    =", xc
  write (u, FMT1) "xcb   =", xcb
  write (u, FMT1) "Q     =", Q
  write (u, FMT1) "phi/D =", phi / degree
end subroutine show_data

subroutine show_momenta
  write (u, "(A)") "Momenta: q(os)"
  call qo(1)%write (u, testflag=.true.)
  write (u, FMT2)  "m = ", abs (qo(1)**1)
  call qo(2)%write (u, testflag=.true.)
  write (u, FMT2)  "m = ", abs (qo(2)**1)
end subroutine show_momenta

end subroutine recoil_kinematics_6

```

32.5 Transverse momentum for the ISR and EPA approximations

The ISR and EPA handler takes an event with a single radiated collinear particle (photon for ISR, beam particle for EPA) for each beam, respectively, and inserts transverse momentum for both. The four-particle kinematics allows us to generate Q^2 and azimuthal angles independently, without violating energy-momentum conservation. The Q^2 distribution is logarithmic, as required by the effective particle approximation, and reflected in the inclusive ISR/EPA structure functions. We also conserve the invariant mass of the partonic system after radiation. The total transverse-momentum kick is applied in form of a Lorentz transformation to the elementary process, both in- and out-particles. In fact, the incoming partons (beam particle for ISR, photon for EPA) which would be virtual space-like in the exact kinematics configuration, are replaced by on-shell incoming partons, such that energy, momentum, and invariant mass \sqrt{s} are conserved.

Regarding kinematics, we treat all particles as massless. The beam-particle mass only appears as the parameter `isr_mass` or `epa_mass`, respectively, and cuts off the logarithmic distribution. The upper cutoff is `isr_q_max` (`epa_q_max`), which defaults to the available energy \sqrt{s} .

The only differences between ISR and EPA, in this context, are the particle types, and an extra \bar{x} factor in the lower cutoff for EPA, see below.

(`isr_epa_handler.f90`) \equiv

```

<File header>

module isr_epa_handler

<Use kinds>
<Use strings>
  use diagnostics, only: msg_fatal
  use diagnostics, only: msg_bug
  use io_units
  use format_defs, only: FMT_12, FMT_19
  use format_utils, only: write_separator
  use format_utils, only: pac_fmt
  use physics_defs, only: PHOTON
  use lorentz, only: vector4_t
  use lorentz, only: energy
  use lorentz, only: lorentz_transformation_t
  use lorentz, only: identity
  use lorentz, only: inverse
  use lorentz, only: operator(*)
  use sm_qcd
  use flavors, only: flavor_t
  use particles, only: particle_t
  use model_data
  use models
  use rng_base, only: rng_t
  use event_transforms
  use recoil_kinematics, only: initial_transformation
  use recoil_kinematics, only: generate_recoil
  use recoil_kinematics, only: recoil_transformation

<Standard module head>

<ISR/EPA handler: public>

<ISR/EPA handler: parameters>

<ISR/EPA handler: types>

contains

<ISR/EPA handler: procedures>

end module isr_epa_handler

```

32.5.1 Event transform type

Convention: **beam** are the incoming partons before ISR – not necessarily the actual beams, need not be in c.m. frame. **radiated** are the radiated particles (photon for ISR), and **parton** are the remainders which initiate the elementary process. These particles are copied verbatim from the event record, and must be collinear.

The kinematical parameters are **sqrts** = invariant mass of the **beam** particles, **q_max** and **m** determining the Q^2 distribution, and **xc/xcb** as the energy

fraction (complement) of the partons, relative to the beams.

Transformations: `lti` is the Lorentz transformation that would boost `pi` (c.m. frame) back to the original `beam` momenta (lab frame). `lto` is the recoil transformation, transforming the partons after ISR from the collinear frame to the recoiling frame. `lt` is the combination of both, which is to be applied to all particles after the hard interaction.

Momenta: `pi` are the beams transformed to their common c.m. frame. `ki` and `qi` are the photon/parton momenta in the `pi` c.m. frame. `km` and `qm` are the photon/parton momenta with the Q distribution applied, and finally `qo` are the partons `qm` projected on-shell.

```

<ISR/EPA handler: public>≡
    public :: evt_isr_epa_t

<ISR/EPA handler: types>≡
    type, extends (evt_t) :: evt_isr_epa_t
        private
            integer :: mode = ISR_TRIVIAL_COLLINEAR
            logical :: isr_active = .false.
            logical :: epa_active = .false.
            real(default) :: isr_q_max = 0
            real(default) :: epa_q_max = 0
            real(default) :: isr_mass = 0
            real(default) :: epa_mass = 0
            logical :: isr_keep_mass = .true.
            real(default) :: sqrts = 0
            integer, dimension(2) :: rad_mode = BEAM_RAD_NONE
            real(default), dimension(2) :: q_max = 0
            real(default), dimension(2) :: m = 0
            real(default), dimension(2) :: xc = 0
            real(default), dimension(2) :: xcb = 0
            type(lorentz_transformation_t) :: lti = identity
            type(lorentz_transformation_t) :: lto = identity
            type(lorentz_transformation_t) :: lt = identity
            integer, dimension(2) :: i_beam = 0
            type(particle_t), dimension(2) :: beam
            type(vector4_t), dimension(2) :: pi
            integer, dimension(2) :: i_radiated = 0
            type(particle_t), dimension(2) :: radiated
            type(vector4_t), dimension(2) :: ki
            type(vector4_t), dimension(2) :: km
            integer, dimension(2) :: i_parton = 0
            type(particle_t), dimension(2) :: parton
            type(vector4_t), dimension(2) :: qi
            type(vector4_t), dimension(2) :: qm
            type(vector4_t), dimension(2) :: qo
        contains
            <ISR/EPA handler: evt_isr: TBP>
    end type evt_isr_epa_t

```

32.5.2 ISR/EPA distinction

```

<ISR/EPA handler: parameters>≡

```

```

integer, parameter, public :: BEAM_RAD_NONE = 0
integer, parameter, public :: BEAM_RAD_ISR = 1
integer, parameter, public :: BEAM_RAD_EPA = 2

```

```

<ISR/EPA handler: procedures>≡
function rad_mode_string (mode) result (string)
  type(string_t) :: string
  integer, intent(in) :: mode
  select case (mode)
    case (BEAM_RAD_NONE); string = "---"
    case (BEAM_RAD_ISR); string = "ISR"
    case (BEAM_RAD_EPA); string = "EPA"
    case default; string = "???"
  end select
end function rad_mode_string

```

32.5.3 Photon insertion modes

```

<ISR/EPA handler: parameters>+≡
integer, parameter, public :: ISR_TRIVIAL_COLLINEAR = 0
integer, parameter, public :: ISR_PAIR_RECOIL = 1

```

```

<ISR/EPA handler: evt isr: TBP>≡
procedure :: get_mode_string => evt_isr_epa_get_mode_string

```

```

<ISR/EPA handler: procedures>+≡
function evt_isr_epa_get_mode_string (evt) result (string)
  type(string_t) :: string
  class(evt_isr_epa_t), intent(in) :: evt
  select case (evt%mode)
    case (ISR_TRIVIAL_COLLINEAR)
      string = "trivial, collinear"
    case (ISR_PAIR_RECOIL)
      string = "pair recoil"
    case default
      string = "[undefined]"
  end select
end function evt_isr_epa_get_mode_string

```

Set the numerical mode ID from a user-level string representation.

```

<ISR/EPA handler: evt isr: TBP>+≡
procedure :: set_mode_string => evt_isr_epa_set_mode_string

```

```

<ISR/EPA handler: procedures>+≡
subroutine evt_isr_epa_set_mode_string (evt, string)
  class(evt_isr_epa_t), intent(inout) :: evt
  type(string_t), intent(in) :: string
  select case (char (string))
    case ("trivial")
      evt%mode = ISR_TRIVIAL_COLLINEAR
    case ("recoil")
      evt%mode = ISR_PAIR_RECOIL
  end select
end subroutine

```

```

    case default
        call msg_fatal ("ISR handler: mode '" // char (string) &
            // "' is undefined")
    end select
end subroutine evt_isr_epa_set_mode_string

```

32.5.4 Output

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: write_name => evt_isr_epa_write_name

<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_write_name (evt, unit)
        class(evt_isr_epa_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Event transform: ISR/EPA handler"
    end subroutine evt_isr_epa_write_name

```

The overall recoil-handling mode.

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: write_mode => evt_isr_epa_write_mode

<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_write_mode (evt, unit)
        class(evt_isr_epa_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A,1x,I0,':',1x,A)") "Insertion mode =", evt%mode, &
            char (evt%get_mode_string ())
    end subroutine evt_isr_epa_write_mode

```

The input data for ISR and EPA, respectively.

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: write_input => evt_isr_epa_write_input

<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_write_input (evt, unit, testflag)
        class(evt_isr_epa_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: testflag
        character(len=7) :: fmt
        integer :: u
        u = given_output_unit (unit)
        call pac_fmt (fmt, FMT_19, FMT_12, testflag)
        if (evt%isr_active) then
            write (u, "(3x,A,1x," // fmt // ")") "ISR: Q_max =", evt%isr_q_max
            write (u, "(3x,A,1x," // fmt // ")") "      m      =", evt%isr_mass
            write (u, "(3x,A,1x,L1)") "      keep m=", evt%isr_keep_mass
        else
            write (u, "(3x,A)") "ISR: [inactive]"
        end if
    end subroutine evt_isr_epa_write_input

```

```

end if
if (evt%epa_active) then
  write (u, "(3x,A,1x," // fmt // ")") "EPA: Q_max =", evt%epa_q_max
  write (u, "(3x,A,1x," // fmt // ")") "      m      =", evt%epa_mass
else
  write (u, "(3x,A)") "EPA: [inactive]"
end if
end subroutine evt_isr_epa_write_input

```

The trivial mode does not depend on any data, since it does nothing to the event.

```

<ISR/EPA handler: evt_isr: TBP>+≡
  procedure :: write_data => evt_isr_epa_write_data
<ISR/EPA handler: procedures>+≡
  subroutine evt_isr_epa_write_data (evt, unit, testflag)
    class(evt_isr_epa_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    character(len=7), parameter :: FMTL_19 = "A3,16x"
    character(len=7), parameter :: FMTL_12 = "A3,9x"
    character(len=7) :: fmt, fmtl
    integer :: u
    u = given_output_unit (unit)
    call pac_fmt (fmt, FMT_19, FMT_12, testflag)
    call pac_fmt (fmtl, FMTL_19, FMTL_12, testflag)
    select case (evt%mode)
    case (ISR_PAIR_RECOIL)
      write (u, "(1x,A)") "Event:"
      write (u, "(3x,A,2(1x," // ffmtl // ")") &
        "mode = ", &
        char (rad_mode_string (evt%rad_mode(1))), &
        char (rad_mode_string (evt%rad_mode(2)))
      write (u, "(3x,A,2(1x," // ffmt // ")") "Q_max =", evt%q_max
      write (u, "(3x,A,2(1x," // ffmt // ")") "m      =", evt%m
      write (u, "(3x,A,2(1x," // ffmt // ")") "x      =", evt%xc
      write (u, "(3x,A,2(1x," // ffmt // ")") "xb     =", evt%xcb
      write (u, "(3x,A,1x," // ffmt // ")") "sqrts =", evt%sqrts
      call write_separator (u)
      write (u, "(A)") "Lorentz boost (partons before radiation &
        &c.m. -> lab) ="
      call evt%lti%write (u, testflag)
      write (u, "(A)") "Lorentz transformation (collinear partons &
        &-> partons with recoil in c.m.) ="
      call evt%lto%write (u, testflag)
      write (u, "(A)") "Combined transformation (partons &
        &-> partons with recoil in lab frame) ="
      call evt%lt%write (u, testflag)
    end select
  end subroutine evt_isr_epa_write_data

```

Output method.

```

<ISR/EPA handler: evt_isr: TBP>+≡
  procedure :: write => evt_isr_epa_write

```

```

<ISR/EPA handler: procedures>+=
subroutine evt_isr_epa_write (evt, unit, verbose, more_verbose, testflag)
  class(evt_isr_epa_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose, more_verbose, testflag
  logical :: show_mass
  integer :: u, i
  u = given_output_unit (unit)
  if (present (testflag)) then
    show_mass = .not. testflag
  else
    show_mass = .true.
  end if
  call write_separator (u, 2)
  call evt%write_name (u)
  call write_separator (u, 2)
  call evt%write_mode (u)
  call evt%write_input (u, testflag=testflag)
  call evt%write_data (u, testflag=testflag)
  call write_separator (u)
  call evt%base_write (u, testflag = testflag, show_set = .false.)
  if (all (evt%i_beam > 0)) then
    call write_separator (u)
    write (u, "(A,2(1x,I0))") "Partons before radiation:", evt%i_beam
    do i = 1, 2
      call evt%beam(i)%write (u, testflag=testflag)
    end do
    call write_separator (u)
    write (u, "(A)") "... boosted to c.m.:"
    do i = 1, 2
      call evt%pi(i)%write (u, show_mass=show_mass, testflag=testflag)
    end do
  end if
  if (all (evt%i_radiated > 0)) then
    call write_separator (u)
    write (u, "(A,2(1x,I0))") "Radiated particles, collinear:", &
      evt%i_radiated
    do i = 1, 2
      call evt%radiated(i)%write (u, testflag=testflag)
    end do
    call write_separator (u)
    write (u, "(A)") "... boosted to c.m.:"
    do i = 1, 2
      call evt%ki(i)%write (u, show_mass=show_mass, testflag=testflag)
    end do
    call write_separator (u)
    write (u, "(A)") "... with kT:"
    do i = 1, 2
      call evt%km(i)%write (u, show_mass=show_mass, testflag=testflag)
    end do
  end if
  if (all (evt%i_parton > 0)) then
    call write_separator (u)
    write (u, "(A,2(1x,I0))") "Partons after radiation, collinear:", &

```



```

        evt%i_parton
    do i = 1, 2
        call evt%parton(i)%write (u, testflag=testflag)
    end do
    call write_separator (u)
    write (u, "(A)") "... boosted to c.m.:"
    do i = 1, 2
        call evt%qi(i)%write (u, show_mass=show_mass, testflag=testflag)
    end do
    call write_separator (u)
    write (u, "(A)") "... with qT, off-shell:"
    do i = 1, 2
        call evt%qm(i)%write (u, show_mass=show_mass, testflag=testflag)
    end do
    call write_separator (u)
    write (u, "(A)") "... projected on-shell:"
    do i = 1, 2
        call evt%qo(i)%write (u, show_mass=show_mass, testflag=testflag)
    end do
    call write_separator (u)
end if
if (evt%particle_set_exists) &
    call evt%particle_set%write &
    (u, summary = .true., compressed = .true., testflag = testflag)
call write_separator (u)
end subroutine evt_isr_epa_write

```

32.5.5 Initialization

Manually import a random-number generator object. This should be done only for testing purposes. The standard procedure is to **connect** a process to an event transform; this will create an appropriate **rng** from the RNG factory in the process object.

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: import_rng => evt_isr_epa_import_rng

<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_import_rng (evt, rng)
        class(evt_isr_epa_t), intent(inout) :: evt
        class(rng_t), allocatable, intent(inout) :: rng
        call move_alloc (from = rng, to = evt%rng)
    end subroutine evt_isr_epa_import_rng

```

Set constant kinematics limits and initialize for ISR. Note that **sqrts** is used only as the fallback value for **q_max**. The actual **sqrts** value for the transform object is inferred from the incoming particles, event by event.

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: set_data_isr => evt_isr_epa_set_data_isr

<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_set_data_isr (evt, sqrts, q_max, m, keep_mass)
        class(evt_isr_epa_t), intent(inout) :: evt

```

```

real(default), intent(in) :: sqrts
real(default), intent(in) :: q_max
real(default), intent(in) :: m
logical, intent(in) :: keep_mass
if (sqrts <= 0) then
  call msg_fatal ("ISR handler: sqrts value must be positive")
end if
if (q_max <= 0 .or. q_max > sqrts) then
  evt%isr_q_max = sqrts
else
  evt%isr_q_max = q_max
end if
if (m > 0) then
  evt%isr_mass = m
else
  call msg_fatal ("ISR handler: ISR_mass value must be positive")
end if
evt%isr_active = .true.
evt%isr_keep_mass = keep_mass
end subroutine evt_isr_epa_set_data_isr

```

Set constant kinematics limits and initialize for EPA. Note that `sqrts` is used only as the fallback value for `q_max`. The actual `sqrts` value for the transform object is inferred from the incoming particles, event by event.

(ISR/EPA handler: evt_isr: TBP)+≡

```

procedure :: set_data_epa => evt_isr_epa_set_data_epa

```

(ISR/EPA handler: procedures)+≡

```

subroutine evt_isr_epa_set_data_epa (evt, sqrts, q_max, m)
  class(evt_isr_epa_t), intent(inout) :: evt
  real(default), intent(in) :: sqrts
  real(default), intent(in) :: q_max
  real(default), intent(in) :: m
  if (sqrts <= 0) then
    call msg_fatal ("EPA handler: sqrts value must be positive")
  end if
  if (q_max <= 0 .or. q_max > sqrts) then
    evt%epa_q_max = sqrts
  else
    evt%epa_q_max = q_max
  end if
  if (m > 0) then
    evt%epa_mass = m
  else
    call msg_fatal ("EPA handler: EPA_mass value must be positive")
  end if
  evt%epa_active = .true.
end subroutine evt_isr_epa_set_data_epa

```

32.5.6 Fetch event data

Identify the radiated particles and the recoil momenta in the particle set. Without much sophistication, start from the end and find particles with the “remnant” status. Their parents should point to the recoiling parton. If successful, set the particle indices in the `evt` object, for further processing.

```

<ISR/EPA handler: evt isr: TBP>+≡
  procedure, private :: identify_radiated

<ISR/EPA handler: procedures>+≡
  subroutine identify_radiated (evt)
    class(evt_isr_epa_t), intent(inout) :: evt
    integer :: i, k
    k = 2
    FIND_LAST_RADIATED: do i = evt%particle_set%get_n_tot (), 1, -1
      associate (prt => evt%particle_set%prt(i))
        if (prt%is_beam_remnant ()) then
          evt%i_radiated(k) = i
          evt%radiated(k) = prt
          k = k - 1
          if (k == 0) exit FIND_LAST_RADIATED
        end if
      end associate
    end do FIND_LAST_RADIATED
    if (k /= 0) call err_count
  contains
    subroutine err_count
      call evt%particle_set%write ()
      call msg_fatal ("ISR/EPA handler: &
        &event does not contain two radiated particles")
    end subroutine err_count
  end subroutine identify_radiated

```

When the radiated particles are known, we can fetch their parent particles and ask for the other child, the incoming parton.

```

<ISR/EPA handler: evt isr: TBP>+≡
  procedure, private :: identify_partons

<ISR/EPA handler: procedures>+≡
  subroutine identify_partons (evt)
    class(evt_isr_epa_t), intent(inout) :: evt
    integer, dimension(:), allocatable :: parent, child
    integer :: i, j
    if (all (evt%i_radiated > 0)) then
      do i = 1, 2
        parent = evt%radiated(i)%get_parents ()
        if (size (parent) /= 1) call err_mismatch
        evt%i_beam(i) = parent(1)
        evt%beam(i) = evt%particle_set%prt(parent(1))
        associate (prt => evt%beam(i))
          child = prt%get_children ()
          if (size (child) /= 2) call err_mismatch
          do j = 1, 2
            if (child(j) /= evt%i_radiated(i)) then

```

```

        evt%i_parton(i) = child(j)
        evt%parton(i) = evt%particle_set%prt(child(j))
    end if
end do
end associate
end do
end if
contains
    subroutine err_mismatch
        call evt%particle_set%write ()
        call msg_bug ("ISR/EPA handler: mismatch in parent-child relations")
    end subroutine err_mismatch
end subroutine identify_partons

```

Check whether the radiated particle is a photon, or the incoming parton is a photon. Then set the ISR/EPA switch appropriately, for each beam.

(ISR/EPA handler: evt isr: TBP)+≡

```

    procedure :: check_radiation => evt_isr_epa_check_radiation

```

(ISR/EPA handler: procedures)+≡

```

    subroutine evt_isr_epa_check_radiation (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
        type(flavor_t) :: flv
        integer :: i
        do i = 1, 2
            flv = evt%radiated(i)%get_flv ()
            if (flv%get_pdg () == PHOTON) then
                if (evt%isr_active) then
                    evt%rad_mode(i) = BEAM_RAD_ISR
                else
                    call err_isr_init
                end if
            else
                flv = evt%parton(i)%get_flv ()
                if (flv%get_pdg () == PHOTON) then
                    if (evt%epa_active) then
                        evt%rad_mode(i) = BEAM_RAD_EPA
                    else
                        call err_epa_init
                    end if
                else
                    call err_no_photon
                end if
            end if
        end do
    contains
        subroutine err_isr_init
            call evt%particle_set%write ()
            call msg_fatal ("ISR/EPA handler: &
                &event contains radiated photon, but ISR is not initialized")
        end subroutine err_isr_init
        subroutine err_epa_init
            call evt%particle_set%write ()
            call msg_fatal ("ISR/EPA handler: &

```

```

        &event contains incoming photon, but EPA is not initialized")
end subroutine err_epa_init
subroutine err_no_photon
    call evt%particle_set%write ()
    call msg_fatal ("ISR/EPA handler: &
        &event does not appear to be ISR or EPA - missing photon")
end subroutine err_no_photon
end subroutine evt_isr_epa_check_radiation

```

Internally set the appropriate parameters (ISR/EPA) for the two beams in the recoil mode.

```

<ISR/EPA handler: evt isr: TBP>+≡
    procedure :: set_recoil_parameters => evt_isr_epa_set_recoil_parameters

<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_set_recoil_parameters (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
        integer :: i
        do i = 1, 2
            select case (evt%rad_mode(i))
            case (BEAM_RAD_ISR)
                evt%q_max(i) = evt%isr_q_max
                evt%m(i) = evt%isr_mass
            case (BEAM_RAD_EPA)
                evt%q_max(i) = evt%epa_q_max
                evt%m(i) = evt%epa_mass
            end select
        end do
    end subroutine evt_isr_epa_set_recoil_parameters

```

Boost the particles that participate in ISR to their proper c.m. frame, copying the momenta to \mathbf{p}_i , \mathbf{k}_i , \mathbf{q}_i . Also assign `sqrts` properly.

```

<ISR/EPA handler: evt isr: TBP>+≡
    procedure, private :: boost_to_cm

<ISR/EPA handler: procedures>+≡
    subroutine boost_to_cm (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
        type(vector4_t), dimension(2) :: p
        type(vector4_t), dimension(2) :: k
        type(vector4_t), dimension(2) :: q
        logical :: ok
        p = evt%beam%get_momentum ()
        k = evt%radiated%get_momentum ()
        q = evt%parton%get_momentum ()
        call initial_transformation (p, evt%sqrts, evt%lti, ok)
        if (.not. ok) call err_non_collinear
        evt%pi = inverse (evt%lti) * p
        evt%ki = inverse (evt%lti) * k
        evt%qi = inverse (evt%lti) * q
    contains
        subroutine err_non_collinear
            call evt%particle_set%write ()
            call msg_fatal ("ISR/EPA handler: &

```

```

        &partons before radiation are not collinear")
    end subroutine err_non_collinear
end subroutine boost_to_cm

```

We can infer the x and \bar{x} values of the event by looking at the energy fractions of the radiated particles and incoming partons, respectively, relative to their parents. Of course, we must assume that they are all collinear, and that energy is conserved.

```

<ISR/EPA handler: evt isr: TBP>+≡
    procedure, private :: infer_x

<ISR/EPA handler: procedures>+≡
    subroutine infer_x (evt)
        class(evt_isr_epa_t), intent(inout) :: evt
        real(default) :: E_parent, E_radiated, E_parton
        integer :: i
        if (all (evt%i_radiated > 0)) then
            do i = 1, 2
                E_parent = energy (evt%pi(i))
                E_radiated = energy (evt%ki(i))
                E_parton = energy (evt%qi(i))
                if (E_parent > 0) then
                    evt%xc(i) = E_parton / E_parent
                    evt%xcb(i) = E_radiated / E_parent
                else
                    call err_energy
                end if
            end do
        end if
contains
        subroutine err_energy
            call evt%particle_set%write ()
            call msg_bug ("ISR/EPA handler: non-positive energy in splitting")
        end subroutine err_energy
    end subroutine infer_x

```

32.5.7 Two-parton recoil

For transforming partons into recoil momenta, we make use of the routines in the `recoil_kinematics` module. In addition to the collinear momenta, we use the x energy fractions, and four numbers from the RNG.

There is one subtle difference w.r.t. ISR case: the EPA mass parameter is multiplied by the energy fraction x , separately for each beam. This is the effective lower Q cutoff.

For certain kinematics, close to the Q_{\max} endpoint, this may fail, and `ok` is set to false. In that case, we should generate new recoil momenta for the same event. This is handled by the generic unweighting procedure.

```

<ISR/EPA handler: evt isr: TBP>+≡
    procedure, private :: generate_recoil => evt_generate_recoil

```

```

<ISR/EPA handler: procedures>+≡
subroutine evt_generate_recoil (evt, ok)
  class(evt_isr_epa_t), intent(inout) :: evt
  logical, intent(out) :: ok
  real(default), dimension(4) :: r
  real(default), dimension(2) :: m, mo
  integer :: i
  call evt%rng%generate (r)
  m = 0
  mo = 0
  do i = 1, 2
    select case (evt%rad_mode(i))
    case (BEAM_RAD_ISR)
      m(i) = evt%m(i)
      if (evt%isr_keep_mass) mo(i) = m(i)
    case (BEAM_RAD_EPA)
      m(i) = evt%xc(i) * evt%m(i)
    end select
  end do
  call generate_recoil (evt%sqrts, evt%q_max, m, mo, evt%xc, evt%xcb, r, &
    evt%km, evt%qm, evt%qo, ok)
end subroutine evt_generate_recoil

```

Replace the collinear radiated (incoming) parton momenta by the momenta that we have generated, respectively. Recall that the recoil has been applied in the c.m. system of the partons before ISR, so we apply the stored Lorentz transformation to boost them to the lab frame.

```

<ISR/EPA handler: evt isr: TBP>+≡
procedure, private :: replace_radiated
procedure, private :: replace_partons

<ISR/EPA handler: procedures>+≡
subroutine replace_radiated (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
  integer :: i
  do i = 1, 2
    associate (prt => evt%particle_set%prt(evt%i_radiated(i)))
      call prt%set_momentum (evt%lti * evt%km(i))
    end associate
  end do
end subroutine replace_radiated

subroutine replace_partons (evt)
  class(evt_isr_epa_t), intent(inout) :: evt
  integer :: i
  do i = 1, 2
    associate (prt => evt%particle_set%prt(evt%i_parton(i)))
      call prt%set_momentum (evt%lti * evt%qo(i))
    end associate
  end do
end subroutine replace_partons

```

32.5.8 Transform the event

Knowing the new incoming partons for the elementary process, we can make use of another procedure in `recoil_kinematics` to determine the Lorentz transformation that transforms the collinear frame into the frame with transverse momentum. We apply this transformation, recursively, to all particles that originate from those incoming partons in the original particle set.

We have to allow for the pre-ISR partons being not in their common c.m. frame. Taking into account non-commutativity, we actually have to first transform the outgoing particles to that c.m. frame, then apply the recoil transformation, then boost back to the lab frame.

The `mask` keep track of particles that we transform, just in case the parent-child tree is multiply connected.

```

<ISR/EPA handler: evt isr: TBP>+≡
  procedure :: transform_outgoing => evt_transform_outgoing

<ISR/EPA handler: procedures>+≡
  subroutine evt_transform_outgoing (evt)
    class(evt_isr_epa_t), intent(inout) :: evt
    logical, dimension(:), allocatable :: mask
    call recoil_transformation (evt%sqrts, evt%xc, evt%qo, evt%lto)
    evt%lt = evt%lti * evt%lto * inverse (evt%lti)
    allocate (mask (evt%particle_set%get_n_tot ()), source=.false.)
    call transform_children (evt%i_parton(1))
  contains
    recursive subroutine transform_children (i)
      integer, intent(in) :: i
      integer :: j, n_child, c
      integer, dimension(:), allocatable :: child
      child = evt%particle_set%prt(i)%get_children ()
      do j = 1, size (child)
        c = child(j)
        if (.not. mask(c)) then
          associate (prt => evt%particle_set%prt(c))
            call prt%set_momentum (evt%lt * prt%get_momentum ())
            mask(c) = .true.
            call transform_children (c)
          end associate
        end if
      end do
    end subroutine transform_children
  end subroutine evt_transform_outgoing

```

32.5.9 Implemented methods

Here we take the particle set from the previous event transform and copy it, then generate the transverse momentum for the radiated particles and for the incoming partons. If this fails (rarely, for large p_T), return zero for the probability, to trigger another try.

NOTE: The boost for the initial partonic system, if not in the c.m. frame, has not been implemented yet.

```

<ISR/EPA handler: evt isr: TBP>+≡

```



```

    procedure :: generate_weighted => &
        evt_isr_epa_generate_weighted
<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_generate_weighted (evt, probability)
        class(evt_isr_epa_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
        logical :: valid
        call evt%particle_set%final ()
        evt%particle_set = evt%previous%particle_set
        evt%particle_set_exists = .true.
        select case (evt%mode)
        case (ISR_TRIVIAL_COLLINEAR)
            probability = 1
            valid = .true.
        case (ISR_PAIR_RECOIL)
            call evt%identify_radiated ()
            call evt%identify_partons ()
            call evt%check_radiation ()
            call evt%set_recoil_parameters ()
            call evt%boost_to_cm ()
            call evt%infer_x ()
            call evt%generate_recoil (valid)
            if (valid) then
                probability = 1
            else
                probability = 0
            end if
        case default
            call msg_bug ("ISR/EPA handler: generate weighted: unsupported mode")
        end select
        evt%particle_set_exists = .false.
    end subroutine evt_isr_epa_generate_weighted

```

Insert the generated radiated particles and incoming partons with p_T in their respective places.

The factorization parameters are irrelevant.

```

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: make_particle_set => &
        evt_isr_epa_make_particle_set
<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_make_particle_set &
        (evt, factorization_mode, keep_correlations, r)
        class(evt_isr_epa_t), intent(inout) :: evt
        integer, intent(in) :: factorization_mode
        logical, intent(in) :: keep_correlations
        real(default), dimension(:), intent(in), optional :: r
        select case (evt%mode)
        case (ISR_TRIVIAL_COLLINEAR)
        case (ISR_PAIR_RECOIL)
            call evt%replace_radiated ()
            call evt%replace_partons ()
            call evt%transform_outgoing ()

```

```

        case default
            call msg_bug ("ISR/EPA handler: make particle set: unsupported mode")
        end select
        evt%particle_set_exists = .true.
    end subroutine evt_isr_epa_make_particle_set

<ISR/EPA handler: evt_isr: TBP>+≡
    procedure :: prepare_new_event => &
        evt_isr_epa_prepare_new_event

<ISR/EPA handler: procedures>+≡
    subroutine evt_isr_epa_prepare_new_event (evt, i_mci, i_term)
        class(evt_isr_epa_t), intent(inout) :: evt
        integer, intent(in) :: i_mci, i_term
        call evt%reset ()
    end subroutine evt_isr_epa_prepare_new_event

```

32.5.10 Unit tests: ISR

Test module, followed by the corresponding implementation module.

This test module differs from most of the other test modules, since it contains two test subroutines: one for ISR and one for EPA below.

```

<isr_epa_handler_ut.f90>≡
    <File header>

    module isr_epa_handler_ut
        use unit_tests
        use isr_epa_handler_util

    <Standard module head>

    <ISR/EPA handler: public test>

    contains

    <ISR/EPA handler: test driver>

    end module isr_epa_handler_ut

<isr_epa_handler_util.f90>≡
    <File header>

    module isr_epa_handler_util

    <Use kinds>
    <Use strings>
        use format_utils, only: write_separator
        use os_interface
        use lorentz, only: vector4_t, vector4_moving, operator(*)
        use rng_base, only: rng_t
        use models, only: syntax_model_file_init, syntax_model_file_final
        use models, only: model_list_t, model_t

```

```

    use particles, only: particle_set_t

    use event_transforms
    use isr_epa_handler, only: evt_isr_epa_t

    use rng_base_ut, only: rng_test_t

    <Standard module head>

    <ISR/EPA handler: test declarations>

    contains

    <ISR/EPA handler: tests>

    end module isr_epa_handler_util

API: driver for the unit tests below.
<ISR/EPA handler: public test>≡
    public :: isr_handler_test
<ISR/EPA handler: test driver>≡
    subroutine isr_handler_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <ISR/EPA handler: execute ISR tests>
    end subroutine isr_handler_test

```

Trivial case

Handle photons resulting from ISR radiation. This test is for the trivial case where the event is kept collinear.

```

<ISR/EPA handler: execute ISR tests>≡
    call test (isr_handler_1, "isr_handler_1", &
        "collinear case, no modification", &
        u, results)

<ISR/EPA handler: test declarations>≡
    public :: isr_handler_1

<ISR/EPA handler: tests>≡
    subroutine isr_handler_1 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(particle_set_t) :: pset
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(evt_trivial_t), target :: evt_trivial
        type(evt_isr_epa_t), target :: evt_isr_epa
        type(vector4_t), dimension(8) :: p
        real(default) :: sqrts
        real(default), dimension(2) :: x, xb
        real(default) :: probability
    end subroutine isr_handler_1

```

```

write (u, "(A)")  "* Test output: isr_handler_1"
write (u, "(A)")  "* Purpose: apply photon handler trivially (no-op)"
write (u, "(A)")

write (u, "(A)")  "* Initialize environment"
write (u, "(A)")

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
       os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
      pdg = [11, -11, 11, -11, 22, 22, 13, -13], model = model)

sqrts = 100._default
x = [0.6_default, 0.9_default]
xb= 1 - x

p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize ISR handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill ISR handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)

```

```

call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)") "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: isr_handler_1"

end subroutine isr_handler_1

```

Photon pair with recoil

Handle photons resulting from ISR radiation. This test invokes the two-photon recoil mechanism. Both photons acquire transverse momentum, the parton momenta recoil, such that total energy-momentum is conserved, and all outgoing photons and partons are on-shell (massless).

```

<ISR/EPA handler: execute ISR tests>+≡
  call test (isr_handler_2, "isr_handler_2", &
    "two-photon recoil", &
    u, results)

<ISR/EPA handler: test declarations>+≡
  public :: isr_handler_2

<ISR/EPA handler: tests>+≡
  subroutine isr_handler_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x, xb
    class(rng_t), allocatable :: rng
    real(default) :: probability

    write (u, "(A)")  "* Test output: isr_handler_2"
    write (u, "(A)")  "* Purpose: apply photon handler with two-photon recoil"
    write (u, "(A)")

```

```

write (u, "(A)")  "* Initialize environment"
write (u, "(A)")

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
       os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
      pdg = [11, -11, 11, -11, 22, 22, 13, -13], model = model)

sqrts = 100._default
x = [0.6_default, 0.9_default]
xb= 1 - x

p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize ISR handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%set_mode_string (var_str ("recoil"))
call evt_isr_epa%set_data_isr ( &
      sqrts = sqrts, &
      q_max = sqrts, &
      m = 511.e-3_default, &
      keep_mass = .false. &
      )

allocate (rng_test_t :: rng)
call rng%init (3) ! default would produce pi for azimuthal angle
call evt_isr_epa%import_rng (rng)

```

```

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill ISR handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: isr_handler_2"

end subroutine isr_handler_2

```

Boosted beams

Handle photons resulting from ISR radiation. This test invokes the two-photon recoil mechanism, in the case that the partons before ISR are not in their c.m. frame (but collinear).

```

<ISR/EPA handler: execute ISR tests>+≡
  call test (isr_handler_3, "isr_handler_3", &
    "two-photon recoil with boost", &
    u, results)

```

```

<ISR/EPA handler: test declarations>+≡
  public :: isr_handler_3

```

```

<ISR/EPA handler: tests>+≡
  subroutine isr_handler_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x0
    real(default), dimension(2) :: x, xb
  end subroutine isr_handler_3

```

```

class(rng_t), allocatable :: rng
real(default) :: probability

write (u, "(A)")  "* Test output: isr_handler_3"
write (u, "(A)")  "*   Purpose: apply photon handler for boosted beams &
                    &and two-photon recoil"
write (u, "(A)")

write (u, "(A)")  "* Initialize environment"
write (u, "(A)")

call syntax_model_file_init ()
call os_data%init ()
call model_list%read_model &
    (var_str ("SM"), var_str ("SM.mdl"), &
    os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
    pdg = [11, -11, 11, -11, 22, 22, 13, -13], model = model)

write (u, "(A)")  "* Event data"
write (u, "(A)")

sqrts = 100._default
write (u, "(A,2(1x,F12.7))") "sqrts   =", sqrts

x0 = [0.9_default, 0.4_default]
write (u, "(A,2(1x,F12.7))") "x0       =", x0

write (u, "(A)")
write (u, "(A,2(1x,F12.7))") "sqs_hat =", sqrts * sqrt (product (x0))

x = [0.6_default, 0.9_default]
xb = 1 - x
write (u, "(A,2(1x,F12.7))") "x       =", x

write (u, "(A)")
write (u, "(A,2(1x,F12.7))") "x0 * x  =", x0 * x

p(1) = x0(1) * vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = x0(2) * vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")
write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

```



```

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize ISR handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%set_mode_string (var_str ("recoil"))
call evt_isr_epa%set_data_isr ( &
    sqrts = sqrts, &
    q_max = sqrts, &
    m = 511.e-3_default, &
    keep_mass = .false. &
)

allocate (rng_test_t :: rng)
call rng%init (3) ! default would produce pi for azimuthal angle
call evt_isr_epa%import_rng (rng)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill ISR handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: isr_handler_3"

end subroutine isr_handler_3

```

32.5.11 Unit tests: EPA

API: Extra driver for the unit tests below.

```
<ISR/EPA handler: public test>+=  
    public :: epa_handler_test  
  
<ISR/EPA handler: test driver>+=  
    subroutine epa_handler_test (u, results)  
        integer, intent(in) :: u  
        type(test_results_t), intent(inout) :: results  
<ISR/EPA handler: execute EPA tests>  
    end subroutine epa_handler_test
```

Trivial case

Handle events resulting from the EPA approximation. This test is for the trivial case where the event is kept collinear.

```
<ISR/EPA handler: execute EPA tests>=  
    call test (epa_handler_1, "epa_handler_1", &  
        "collinear case, no modification", &  
        u, results)  
  
<ISR/EPA handler: test declarations>+=  
    public :: epa_handler_1  
  
<ISR/EPA handler: tests>+=  
    subroutine epa_handler_1 (u)  
        integer, intent(in) :: u  
        type(os_data_t) :: os_data  
        type(particle_set_t) :: pset  
        type(model_list_t) :: model_list  
        type(model_t), pointer :: model  
        type(evt_trivial_t), target :: evt_trivial  
        type(evt_isr_epa_t), target :: evt_isr_epa  
        type(vector4_t), dimension(8) :: p  
        real(default) :: sqrts  
        real(default), dimension(2) :: x, xb  
        real(default) :: probability  
  
        write (u, "(A)")  "* Test output: epa_handler_1"  
        write (u, "(A)")  "*   Purpose: apply beam handler trivially (no-op)"  
        write (u, "(A)")  
  
        write (u, "(A)")  "* Initialize environment"  
        write (u, "(A)")  
  
        call syntax_model_file_init ()  
        call os_data%init ()  
        call model_list%read_model &  
            (var_str ("SM"), var_str ("SM.mdl"), &  
            os_data, model)  
  
        write (u, "(A)")  "* Initialize particle set"  
        write (u, "(A)")
```

```

call pset%init_direct &
  (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
   pdg = [11, -11, 22, 22, 11, -11, 13, -13], &
   model = model)

sqrts = 100._default
x = [0.6_default, 0.9_default]
xb= 1 - x

p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize EPA handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%write (u)

write (u, "(A)")
write (u, "(A)")  "* Fill EPA handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: epa_handler_1"

end subroutine epa_handler_1

```

Beam pair with recoil

Handle beams resulting from the EPA approximation. This test invokes the two-beam recoil mechanism. Both beam remnants acquire transverse momentum, the photon momenta recoil, such that total energy-momentum is conserved, and all outgoing beam remnants and photons are on-shell (massless).

```

<ISR/EPA handler: execute EPA tests>+≡
  call test (epa_handler_2, "epa_handler_2", &
    "two-beam recoil", &
    u, results)

<ISR/EPA handler: test declarations>+≡
  public :: epa_handler_2

<ISR/EPA handler: tests>+≡
  subroutine epa_handler_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x, xb
    class(rng_t), allocatable :: rng
    real(default) :: probability

    write (u, "(A)")  "* Test output: epa_handler_2"
    write (u, "(A)")  "* Purpose: apply beam handler with two-beam recoil"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &
      os_data, model)

    write (u, "(A)")  "* Initialize particle set"
    write (u, "(A)")

    call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
      pdg = [11, -11, 22, 22, 11, -11, 13, -13], model = model)

```

```

sqrts = 100._default
x = [0.6_default, 0.9_default]
xb= 1 - x

p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize EPA handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%set_mode_string (var_str ("recoil"))
call evt_isr_epa%set_data_epa ( &
    sqrts = sqrts, &
    q_max = sqrts, &
    m = 511.e-3_default &
)

allocate (rng_test_t :: rng)
call rng%init (3) ! default would produce pi for azimuthal angle
call evt_isr_epa%import_rng (rng)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill EPA handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

```

```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: epa_handler_2"

end subroutine epa_handler_2

```

Boosted beams

Handle radiated beam remnants resulting from EPA radiation. This test invokes the two-beam recoil mechanism, in the case that the partons before EPA are not in their c.m. frame (but collinear).

```

<ISR/EPA handler: execute EPA tests>+=
  call test (epa_handler_3, "epa_handler_3", &
    "two-beam recoil with boost", &
    u, results)

<ISR/EPA handler: test declarations>+=
  public :: epa_handler_3

<ISR/EPA handler: tests>+=
  subroutine epa_handler_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(particle_set_t) :: pset
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(evt_trivial_t), target :: evt_trivial
    type(evt_isr_epa_t), target :: evt_isr_epa
    type(vector4_t), dimension(8) :: p
    real(default) :: sqrts
    real(default), dimension(2) :: x0
    real(default), dimension(2) :: x, xb
    class(rng_t), allocatable :: rng
    real(default) :: probability

    write (u, "(A)")  "* Test output: epa_handler_3"
    write (u, "(A)")  "* Purpose: apply beam handler for boosted beams &
      &and two-beam recoil"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call syntax_model_file_init ()
    call os_data%init ()
    call model_list%read_model &
      (var_str ("SM"), var_str ("SM.mdl"), &

```

```

os_data, model)

write (u, "(A)")  "* Initialize particle set"
write (u, "(A)")

call pset%init_direct (n_beam = 2, n_in = 2, n_rem = 2, n_vir = 0, n_out = 2, &
    pdg = [11, -11, 22, 22, 11, -11, 13, -13], model = model)

write (u, "(A)")  "* Event data"
write (u, "(A)")

sqrts = 100._default
write (u, "(A,2(1x,F12.7))")  "sqrts   =", sqrts

x0 = [0.9_default, 0.4_default]
write (u, "(A,2(1x,F12.7))")  "x0       =", x0

write (u, "(A)")
write (u, "(A,2(1x,F12.7))")  "sqs_hat =", sqrts * sqrt (product (x0))

x = [0.6_default, 0.9_default]
xb= 1 - x
write (u, "(A,2(1x,F12.7))")  "x       =", x

write (u, "(A)")
write (u, "(A,2(1x,F12.7))")  "x0 * x  =", x0 * x

p(1) = x0(1) * vector4_moving (sqrts/2, sqrts/2, 3)
p(2) = x0(2) * vector4_moving (sqrts/2,-sqrts/2, 3)
p(3:4) = x * p(1:2)
p(5:6) = xb * p(1:2)
p(7:8) = p(3:4)

call pset%set_momentum (p, on_shell = .false.)

write (u, "(A)")
write (u, "(A)")  "* Fill trivial event transform"
write (u, "(A)")

call evt_trivial%reset ()
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)
call write_separator (u, 2)

write (u, "(A)")
write (u, "(A)")  "* Initialize EPA handler transform"
write (u, "(A)")

evt_trivial%next => evt_isr_epa
evt_isr_epa%previous => evt_trivial

call evt_isr_epa%set_mode_string (var_str ("recoil"))
call evt_isr_epa%set_data_epa ( &
    sqrts = sqrts, &

```

```

        q_max = sqrt(s, &
        m = 511.e-3_default &
        )

allocate (rng_test_t :: rng)
call rng%init (3) ! default would produce pi for azimuthal angle
call evt_isr_epa%import_rng (rng)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill EPA handler transform"
write (u, "(A)")

call evt_isr_epa%prepare_new_event (1, 1)
call evt_isr_epa%generate_weighted (probability)
call evt_isr_epa%make_particle_set (0, .false.)

call evt_isr_epa%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A,1x,F8.5)")  "Event probability =", probability

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_isr_epa%final ()
call evt_trivial%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: epa_handler_3"

end subroutine epa_handler_3

```

32.6 Decays

```

<decays.f90>≡
  <File header>

  module decays

    <Use kinds>
    <Use strings>
    use io_units
    use format_utils, only: write_indent, write_separator
    use format_defs, only: FMT_15
    use numeric_utils
    use diagnostics
    use flavors
    use helicities
    use quantum_numbers

```



```

    use interactions
    use evaluators
    use variables, only: var_list_t
    use model_data
    use rng_base
    use selectors
    use parton_states
    use process, only: process_t
    use instances, only: process_instance_t, pacify
    use process_stacks
    use event_transforms

    <Standard module head>

    <Decays: public>

    <Decays: types>

    <Decays: interfaces>

contains

    <Decays: procedures>

end module decays

```

32.6.1 Final-State Particle Configuration

A final-state particle may be either stable or unstable. Here is an empty abstract type as the parent of both, with holds just the flavor information.

```

<Decays: types>≡
    type, abstract :: any_config_t
    private
    contains
    <Decays: any config: TBP>
    end type any_config_t

```

Finalizer, depends on the implementation.

```

<Decays: any config: TBP>≡
    procedure (any_config_final), deferred :: final

<Decays: interfaces>≡
    interface
    subroutine any_config_final (object)
    import
        class(any_config_t), intent(inout) :: object
    end subroutine any_config_final
    end interface

```

The output is also deferred:

```

<Decays: any config: TBP>+≡
    procedure (any_config_write), deferred :: write

```

```

<Decays: interfaces>+≡
  interface
    subroutine any_config_write (object, unit, indent, verbose)
      import
      class(any_config_t), intent(in) :: object
      integer, intent(in), optional :: unit, indent
      logical, intent(in), optional :: verbose
    end subroutine any_config_write
  end interface

```

This is a container for a stable or unstable particle configurator. We need this wrapper for preparing arrays that mix stable and unstable particles.

```

<Decays: types>+≡
  type :: particle_config_t
  private
    class(any_config_t), allocatable :: c
  end type particle_config_t

```

32.6.2 Final-State Particle

In theory, for the particle instance we only need to consider the unstable case. However, it is more straightforward to treat configuration and instance on the same footing, and to introduce a wrapper for particle objects as above.

```

<Decays: types>+≡
  type, abstract :: any_t
  private
    contains
    <Decays: any: TBP>
  end type any_t

```

Finalizer, depends on the implementation.

```

<Decays: any: TBP>≡
  procedure (any_final), deferred :: final
<Decays: interfaces>+≡
  interface
    subroutine any_final (object)
      import
      class(any_t), intent(inout) :: object
    end subroutine any_final
  end interface

```

The output is also deferred:

```

<Decays: any: TBP>+≡
  procedure (any_write), deferred :: write
<Decays: interfaces>+≡
  interface
    subroutine any_write (object, unit, indent)
      import
      class(any_t), intent(in) :: object

```

```

        integer, intent(in), optional :: unit, indent
    end subroutine any_write
end interface

```

This is a container for a stable or unstable outgoing particle. We need this wrapper for preparing arrays that mix stable and unstable particles.

```

<Decays: types>+≡
    type :: particle_out_t
    private
    class(any_t), allocatable :: c
end type particle_out_t

```

32.6.3 Decay Term Configuration

A decay term is a distinct final state, corresponding to a process term. Each decay process may give rise to several terms with, possibly, differing flavor content.

```

<Decays: types>+≡
    type :: decay_term_config_t
    private
    type(particle_config_t), dimension(:), allocatable :: prt
    contains
    <Decays: decay term config: TBP>
end type decay_term_config_t

```

Finalizer, recursive.

```

<Decays: decay term config: TBP>≡
    procedure :: final => decay_term_config_final

<Decays: procedures>≡
    recursive subroutine decay_term_config_final (object)
    class(decay_term_config_t), intent(inout) :: object
    integer :: i
    if (allocated (object%prt)) then
        do i = 1, size (object%prt)
            if (allocated (object%prt(i)%c)) call object%prt(i)%c%final ()
        end do
    end if
end subroutine decay_term_config_final

```

Output, with optional indentation

```

<Decays: decay term config: TBP>+≡
    procedure :: write => decay_term_config_write

<Decays: procedures>+≡
    recursive subroutine decay_term_config_write (object, unit, indent, verbose)
    class(decay_term_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: i, j, u, ind
    logical :: verb

```

```

u = given_output_unit (unit)
ind = 0; if (present (indent)) ind = indent
verb = .true.; if (present (verbose)) verb = verbose
call write_indent (u, ind)
write (u, "(1x,A)", advance="no") "Final state:"
do i = 1, size (object%prt)
  select type (prt_config => object%prt(i)%c)
  type is (stable_config_t)
    write (u, "(1x,A)", advance="no") &
      char (prt_config%flv(1)%get_name ())
    do j = 2, size (prt_config%flv)
      write (u, "(:',A)", advance="no") &
        char (prt_config%flv(j)%get_name ())
    end do
  type is (unstable_config_t)
    write (u, "(1x,A)", advance="no") &
      char (prt_config%flv%get_name ())
  end select
end do
write (u, *)
if (verb) then
  do i = 1, size (object%prt)
    call object%prt(i)%c%write (u, ind)
  end do
end if
end subroutine decay_term_config_write

```

Initialize, given a set of flavors. For each flavor, we must indicate whether the particle is stable. The second index of the flavor array runs over alternatives for each decay product; alternatives are allowed only if the decay product is itself stable.

```

<Decays: decay term config: TBP>+≡
  procedure :: init => decay_term_config_init

<Decays: procedures>+≡
  recursive subroutine decay_term_config_init &
    (term, flv, stable, model, process_stack, var_list)
    class(decay_term_config_t), intent(out) :: term
    type(flavor_t), dimension(:,:), intent(in) :: flv
    logical, dimension(:), intent(in) :: stable
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    type(var_list_t), intent(in), optional :: var_list
    type(string_t), dimension(:), allocatable :: decay
    integer :: i
    allocate (term%prt (size (flv, 1)))
    do i = 1, size (flv, 1)
      associate (prt => term%prt(i))
        if (stable(i)) then
          allocate (stable_config_t :: prt%c)
        else
          allocate (unstable_config_t :: prt%c)
        end if
        select type (prt_config => prt%c)

```

```

type is (stable_config_t)
  call prt_config%init (flv(i,:))
type is (unstable_config_t)
  if (all (flv(i,:) == flv(i,1))) then
    call prt_config%init (flv(i,1))
    call flv(i,1)%get_decays (decay)
    call prt_config%init_decays &
      (decay, model, process_stack, var_list)
  else
    call prt_config%write ()
    call msg_fatal ("Decay configuration: &
      &unstable product must be unique")
  end if
end select
end associate
end do
end subroutine decay_term_config_init

```

Recursively compute widths and branching ratios for all unstable particles.

```

<Decays: decay term config: TBP>+≡
  procedure :: compute => decay_term_config_compute

<Decays: procedures>+≡
  recursive subroutine decay_term_config_compute (term)
    class(decay_term_config_t), intent(inout) :: term
    integer :: i
    do i = 1, size (term%prt)
      select type (unstable_config => term%prt(i)%c)
        type is (unstable_config_t)
          call unstable_config%compute ()
        end select
      end do
    end do
  end subroutine decay_term_config_compute

```

32.6.4 Decay Term

A decay term instance is selected when we generate an event for the associated process instance. When evaluated, it triggers further decays down the chain.

Only unstable products are allocated as child particles.

```

<Decays: types>+≡
  type :: decay_term_t
  private
    type(decay_term_config_t), pointer :: config => null ()
    type(particle_out_t), dimension(:), allocatable :: particle_out
  contains
    <Decays: decay term: TBP>
  end type decay_term_t

```

Finalizer.

```

<Decays: decay term: TBP>≡
  procedure :: final => decay_term_final

```

```

<Decays: procedures>+≡
recursive subroutine decay_term_final (object)
  class(decay_term_t), intent(inout) :: object
  integer :: i
  if (allocated (object%particle_out)) then
    do i = 1, size (object%particle_out)
      call object%particle_out(i)%c%final ()
    end do
  end if
end subroutine decay_term_final

```

Output.

```

<Decays: decay term: TBP>+≡
  procedure :: write => decay_term_write

<Decays: procedures>+≡
recursive subroutine decay_term_write (object, unit, indent)
  class(decay_term_t), intent(in) :: object
  integer, intent(in), optional :: unit, indent
  integer :: i, u, ind
  u = given_output_unit (unit)
  ind = 0; if (present (indent)) ind = indent
  call object%config%write (u, ind, verbose = .false.)
  do i = 1, size (object%particle_out)
    call object%particle_out(i)%c%write (u, ind)
  end do
end subroutine decay_term_write

```

Recursively write the embedded process instances.

```

<Decays: decay term: TBP>+≡
  procedure :: write_process_instances => decay_term_write_process_instances

<Decays: procedures>+≡
recursive subroutine decay_term_write_process_instances (term, unit, verbose)
  class(decay_term_t), intent(in) :: term
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose
  integer :: i
  do i = 1, size (term%particle_out)
    select type (unstable => term%particle_out(i)%c)
      type is (unstable_t)
        call unstable%write_process_instances (unit, verbose)
    end select
  end do
end subroutine decay_term_write_process_instances

```

Initialization, using the configuration object. We allocate particle objects in parallel to the particle configuration objects which we use to initialize them, one at a time.

```

<Decays: decay term: TBP>+≡
  procedure :: init => decay_term_init

```

```

<Decays: procedures>+≡
recursive subroutine decay_term_init (term, config)
  class(decay_term_t), intent(out) :: term
  type(decay_term_config_t), intent(in), target :: config
  integer :: i
  term%config => config
  allocate (term%particle_out (size (config%prt)))
  do i = 1, size (config%prt)
    select type (prt_config => config%prt(i)%c)
    type is (stable_config_t)
      allocate (stable_t :: term%particle_out(i)%c)
      select type (stable => term%particle_out(i)%c)
      type is (stable_t)
        call stable%init (prt_config)
      end select
    type is (unstable_config_t)
      allocate (unstable_t :: term%particle_out(i)%c)
      select type (unstable => term%particle_out(i)%c)
      type is (unstable_t)
        call unstable%init (prt_config)
      end select
    end select
  end do
end subroutine decay_term_init

```

Implement a RNG instance, spawned by the process object.

```

<Decays: decay term: TBP>+≡
  procedure :: make_rng => decay_term_make_rng

<Decays: procedures>+≡
subroutine decay_term_make_rng (term, process)
  class(decay_term_t), intent(inout) :: term
  type(process_t), intent(inout) :: process
  class(rng_t), allocatable :: rng
  integer :: i
  do i = 1, size (term%particle_out)
    select type (unstable => term%particle_out(i)%c)
    type is (unstable_t)
      call process%make_rng (rng)
      call unstable%import_rng (rng)
    end select
  end do
end subroutine decay_term_make_rng

```

Link the interactions for unstable decay products to the interaction of the parent process.

```

<Decays: decay term: TBP>+≡
  procedure :: link_interactions => decay_term_link_interactions

<Decays: procedures>+≡
recursive subroutine decay_term_link_interactions (term, trace)
  class(decay_term_t), intent(inout) :: term
  type(interaction_t), intent(in), target :: trace
  integer :: i

```

```

do i = 1, size (term%particle_out)
  select type (unstable => term%particle_out(i)%c)
    type is (unstable_t)
      call unstable%link_interactions (i, trace)
    end select
  end do
end subroutine decay_term_link_interactions

```

Recursively generate a decay chain, for each of the unstable particles in the final state.

```

<Decays: decay term: TBP>+≡
  procedure :: select_chain => decay_term_select_chain

<Decays: procedures>+≡
  recursive subroutine decay_term_select_chain (term)
    class(decay_term_t), intent(inout) :: term
    integer :: i
    do i = 1, size (term%particle_out)
      select type (unstable => term%particle_out(i)%c)
        type is (unstable_t)
          call unstable%select_chain ()
        end select
      end do
    end subroutine decay_term_select_chain

```

Recursively generate a decay event, for each of the unstable particles in the final state.

```

<Decays: decay term: TBP>+≡
  procedure :: generate => decay_term_generate

<Decays: procedures>+≡
  recursive subroutine decay_term_generate (term)
    class(decay_term_t), intent(inout) :: term
    integer :: i
    do i = 1, size (term%particle_out)
      select type (unstable => term%particle_out(i)%c)
        type is (unstable_t)
          call unstable%generate ()
        end select
      end do
    end subroutine decay_term_generate

```

32.6.5 Decay Root Configuration

At the root of a decay chain, there is a parent process. The decay root stores a pointer to the parent process and the set of decay configurations.

```

<Decays: public>≡
  public :: decay_root_config_t

```



```

<Decays: types>+=
  type :: decay_root_config_t
  private
    type(string_t) :: process_id
    type(process_t), pointer :: process => null ()
    class(model_data_t), pointer :: model => null ()
    type(decay_term_config_t), dimension(:), allocatable :: term_config
  contains
    <Decays: decay root config: TBP>
  end type decay_root_config_t

```

The finalizer is recursive since there may be cascade decays.

```

<Decays: decay root config: TBP>=
  procedure :: final => decay_root_config_final

<Decays: procedures>+=
  recursive subroutine decay_root_config_final (object)
    class(decay_root_config_t), intent(inout) :: object
    integer :: i
    if (allocated (object%term_config)) then
      do i = 1, size (object%term_config)
        call object%term_config(i)%final ()
      end do
    end if
  end subroutine decay_root_config_final

```

The output routine is also recursive, and it contains an adjustable indentation.

```

<Decays: decay root config: TBP>+=
  procedure :: write => decay_root_config_write
  procedure :: write_header => decay_root_config_write_header
  procedure :: write_terms => decay_root_config_write_terms

<Decays: procedures>+=
  recursive subroutine decay_root_config_write (object, unit, indent, verbose)
    class(decay_root_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(1x,A)") "Final-state decay tree:"
    call object%write_header (unit, indent)
    call object%write_terms (unit, indent, verbose)
  end subroutine decay_root_config_write

  subroutine decay_root_config_write_header (object, unit, indent)
    class(decay_root_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    if (associated (object%process)) then

```

```

        write (u, 3) "process ID      =", char (object%process_id), "*"
    else
        write (u, 3) "process ID      =", char (object%process_id)
    end if
3   format (3x,A,2(1x,A))
end subroutine decay_root_config_write_header

recursive subroutine decay_root_config_write_terms &
    (object, unit, indent, verbose)
    class(decay_root_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: i, u, ind
    logical :: verb
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    verb = .true.; if (present (verbose)) verb = verbose
    if (verb .and. allocated (object%term_config)) then
        do i = 1, size (object%term_config)
            call object%term_config(i)%write (u, ind + 1)
        end do
    end if
end subroutine decay_root_config_write_terms

```

Initialize for a named process and (optionally) a pre-determined number of terms.

<Decays: decay root config: TBP>+≡

```
procedure :: init => decay_root_config_init
```

<Decays: procedures>+≡

```

subroutine decay_root_config_init (decay, model, process_id, n_terms)
    class(decay_root_config_t), intent(out) :: decay
    class(model_data_t), intent(in), target :: model
    type(string_t), intent(in) :: process_id
    integer, intent(in), optional :: n_terms
    decay%model => model
    decay%process_id = process_id
    if (present (n_terms)) then
        allocate (decay%term_config (n_terms))
    end if
end subroutine decay_root_config_init

```

Declare a decay term, given an array of flavors.

<Decays: decay root config: TBP>+≡

```
procedure :: init_term => decay_root_config_init_term
```

<Decays: procedures>+≡

```

recursive subroutine decay_root_config_init_term &
    (decay, i, flv, stable, model, process_stack, var_list)
    class(decay_root_config_t), intent(inout) :: decay
    integer, intent(in) :: i
    type(flavor_t), dimension(:, :), intent(in) :: flv
    logical, dimension(:), intent(in) :: stable
    class(model_data_t), intent(in), target :: model

```

```

    type(process_stack_t), intent(in), optional :: process_stack
    type(var_list_t), intent(in), optional, target :: var_list
    call decay%term_config(i)%init (flv, stable, model, process_stack, var_list)
end subroutine decay_root_config_init_term

```

Connect the decay root configuration with a process object (which should represent the parent process). This includes initialization, therefore intent(out).

The flavor state is retrieved from the process term object. However, we have to be careful: the flavor object points to the model instance that is stored in the process object. This model instance may not contain the current setting for unstable particles and decay. Therefore, we assign the model directly.

If the `process_instance` argument is provided, we use this for the flavor state. This applies to the decay root only, where the process can be entangled with a beam setup, and the latter contains beam remnants as further outgoing particles. These must be included in the set of outgoing flavors, since the decay application is also done on the connected state.

Infer stability from the particle properties, using the first row in the set of flavor states. For unstable particles, we look for decays, recursively, available from the process stack (if present).

For the unstable particles, we have to check whether their masses match between the production and the decay. Fortunately, both versions are available for comparison.

The optional `var_list` argument may override integral/error values for decay processes.

```

<Decays: decay root config: TBP>+=
  procedure :: connect => decay_root_config_connect

<Decays: procedures>+=
  recursive subroutine decay_root_config_connect &
    (decay, process, model, process_stack, process_instance, var_list)
    class(decay_root_config_t), intent(out) :: decay
    type(process_t), intent(in), target :: process
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    type(process_instance_t), intent(in), optional, target :: process_instance
    type(var_list_t), intent(in), optional, target :: var_list
    type(connected_state_t), pointer :: connected_state
    type(interaction_t), pointer :: int
    type(flavor_t), dimension(:, :), allocatable :: flv
    logical, dimension(:), allocatable :: stable
    real(default), dimension(:), allocatable :: m_prod, m_dec
    integer :: i
    call decay%init (model, process%get_id (), process%get_n_terms ())
    do i = 1, size (decay%term_config)
      if (present (process_instance)) then
        connected_state => process_instance%get_connected_state_ptr (i)
        int => connected_state%get_matrix_int_ptr ()
        call interaction_get_flv_out (int, flv)
      else
        call process%get_term_flv_out (i, flv)
      end if
      allocate (m_prod (size (flv(:, 1)%get_mass ())))

```

```

    m_prod = flv(:,1)%get_mass ()
    call flv%set_model (model)
    allocate (m_dec (size (flv(:,1)%get_mass ())))
    m_dec = flv(:,1)%get_mass ()
    allocate (stable (size (flv, 1)))
    stable = flv(:,1)%is_stable ()
    call check_masses ()
    call decay%init_term (i, flv, stable, model, process_stack, var_list)
    deallocate (flv, stable, m_prod, m_dec)
end do
decay%process => process
contains
subroutine check_masses ()
    integer :: i
    logical :: ok
    ok = .true.
    do i = 1, size (m_prod)
        if (.not. stable(i)) then
            if (.not. nearly_equal (m_prod(i), m_dec(i))) then
                write (msg_buffer, "(A,A,A)" "particle '", &
                    char (flv(i,1)%get_name ()), "':"
                call msg_message
                write (msg_buffer, &
                    "(2x,A,1x," // FMT_15 // ",3x,A,1x," // FMT_15 // ")") &
                    "m_prod =", m_prod(i), "m_dec =", m_dec(i)
                call msg_message
                ok = .false.
            end if
        end if
    end do
    if (.not. ok) call msg_fatal &
        ("Particle mass mismatch between production and decay")
end subroutine check_masses
end subroutine decay_root_config_connect

```

Recursively compute widths, errors, and branching ratios.

```

<Decays: decay root config: TBP>+≡
    procedure :: compute => decay_root_config_compute

<Decays: procedures>+≡
    recursive subroutine decay_root_config_compute (decay)
        class(decay_root_config_t), intent(inout) :: decay
        integer :: i
        do i = 1, size (decay%term_config)
            call decay%term_config(i)%compute ()
        end do
    end subroutine decay_root_config_compute

```

32.6.6 Decay Root Instance

This is the common parent type for decay and decay root. The process instance points to the parent process. The model pointer is separate because particle

settings may be updated w.r.t. the parent process object.

```

<Decays: types>+≡
  type, abstract :: decay_gen_t
  private
    type(decay_term_t), dimension(:), allocatable :: term
    type(process_instance_t), pointer :: process_instance => null ()
    integer :: selected_mci = 0
    integer :: selected_term = 0
  contains
    <Decays: decay gen: TBP>
  end type decay_gen_t

```

The decay root represents the parent process. When an event is generated, the generator selects the term to which the decay chain applies (if possible).

The process instance is just a pointer.

```

<Decays: public>+≡
  public :: decay_root_t

<Decays: types>+≡
  type, extends (decay_gen_t) :: decay_root_t
  private
    type(decay_root_config_t), pointer :: config => null ()
  contains
    <Decays: decay root: TBP>
  end type decay_root_t

```

The finalizer has to recursively finalize the terms, but we can skip the process instance which is not explicitly allocated.

```

<Decays: decay gen: TBP>≡
  procedure :: base_final => decay_gen_final

<Decays: procedures>+≡
  recursive subroutine decay_gen_final (object)
    class(decay_gen_t), intent(inout) :: object
    integer :: i
    if (allocated (object%term)) then
      do i = 1, size (object%term)
        call object%term(i)%final ()
      end do
    end if
  end subroutine decay_gen_final

```

No extra finalization for the decay root.

```

<Decays: decay root: TBP>≡
  procedure :: final => decay_root_final

<Decays: procedures>+≡
  subroutine decay_root_final (object)
    class(decay_root_t), intent(inout) :: object
    call object%base_final ()
  end subroutine decay_root_final

```

Output.

```

<Decays: decay root: TBP>+≡
  procedure :: write => decay_root_write

<Decays: procedures>+≡
  subroutine decay_root_write (object, unit)
    class(decay_root_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    if (associated (object%config)) then
      call object%config%write (unit, verbose = .false.)
    else
      write (u, "(1x,A)") "Final-state decay tree: [not configured]"
    end if
    if (object%selected_mci > 0) then
      write (u, "(3x,A,I0)") "Selected MCI      = ", object%selected_mci
    else
      write (u, "(3x,A)") "Selected MCI      = [undefined]"
    end if
    if (object%selected_term > 0) then
      write (u, "(3x,A,I0)") "Selected term    = ", object%selected_term
      call object%term(object%selected_term)%write (u, 1)
    else
      write (u, "(3x,A)") "Selected term    = [undefined]"
    end if
  end subroutine decay_root_write

```

Write the process instances, recursively.

```

<Decays: decay gen: TBP>+≡
  procedure :: write_process_instances => decay_gen_write_process_instances

<Decays: procedures>+≡
  recursive subroutine decay_gen_write_process_instances (decay, unit, verbose)
    class(decay_gen_t), intent(in) :: decay
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    logical :: verb
    verb = .true.; if (present (verbose)) verb = verbose
    if (associated (decay%process_instance)) then
      if (verb) then
        call decay%process_instance%write (unit)
      else
        call decay%process_instance%write_header (unit)
      end if
    end if
    if (decay%selected_term > 0) then
      call decay%term(decay%selected_term)%write_process_instances (unit, verb)
    end if
  end subroutine decay_gen_write_process_instances

```

Generic initializer. All can be done recursively.

```

<Decays: decay gen: TBP>+≡
  procedure :: base_init => decay_gen_init

```

```

<Decays: procedures>+≡
recursive subroutine decay_gen_init (decay, term_config)
  class(decay_gen_t), intent(out) :: decay
  type(decay_term_config_t), dimension(:), intent(in), target :: term_config
  integer :: i
  allocate (decay%term (size (term_config)))
  do i = 1, size (decay%term)
    call decay%term(i)%init (term_config(i))
  end do
end subroutine decay_gen_init

```

Specific initializer. We assign the configuration object, which should correspond to a completely initialized decay configuration tree. We also connect to an existing process instance. Then, we recursively link the child interactions to the parent process.

```

<Decays: decay root: TBP>+≡
  procedure :: init => decay_root_init

<Decays: procedures>+≡
  subroutine decay_root_init (decay_root, config, process_instance)
    class(decay_root_t), intent(out) :: decay_root
    type(decay_root_config_t), intent(in), target :: config
    type(process_instance_t), intent(in), target :: process_instance
    call decay_root%base_init (config%term_config)
    decay_root%config => config
    decay_root%process_instance => process_instance
    call decay_root%make_term_rng (config%process)
    call decay_root%link_term_interactions ()
  end subroutine decay_root_init

```

Explicitly set/get mci and term indices. (Used in unit test.)

```

<Decays: decay gen: TBP>+≡
  procedure :: set_mci => decay_gen_set_mci
  procedure :: set_term => decay_gen_set_term
  procedure :: get_mci => decay_gen_get_mci
  procedure :: get_term => decay_gen_get_term

<Decays: procedures>+≡
  subroutine decay_gen_set_mci (decay, i)
    class(decay_gen_t), intent(inout) :: decay
    integer, intent(in) :: i
    decay%selected_mci = i
  end subroutine decay_gen_set_mci

  subroutine decay_gen_set_term (decay, i)
    class(decay_gen_t), intent(inout) :: decay
    integer, intent(in) :: i
    decay%selected_term = i
  end subroutine decay_gen_set_term

  function decay_gen_get_mci (decay) result (i)
    class(decay_gen_t), intent(inout) :: decay
    integer :: i
    i = decay%selected_mci
  end function decay_gen_get_mci

```

```

end function decay_gen_get_mci

function decay_gen_get_term (decay) result (i)
  class(decay_gen_t), intent(inout) :: decay
  integer :: i
  i = decay%selected_term
end function decay_gen_get_term

```

Implement random-number generators for unstable decay selection in all terms. This is not recursive.

We also make use of the fact that `process` is a pointer; the (state of the RNG factory inside the) target process will be modified by the rng-spawning method, but not the pointer.

```

<Decays: decay gen: TBP>+≡
  procedure :: make_term_rng => decay_gen_make_term_rng

<Decays: procedures>+≡
  subroutine decay_gen_make_term_rng (decay, process)
    class(decay_gen_t), intent(inout) :: decay
    type(process_t), intent(in), pointer :: process
    integer :: i
    do i = 1, size (decay%term)
      call decay%term(i)%make_rng (process)
    end do
  end subroutine decay_gen_make_term_rng

```

Recursively link interactions of the enclosed decay terms to the corresponding terms in the current process instance.

```

<Decays: decay gen: TBP>+≡
  procedure :: link_term_interactions => decay_gen_link_term_interactions

<Decays: procedures>+≡
  recursive subroutine decay_gen_link_term_interactions (decay)
    class(decay_gen_t), intent(inout) :: decay
    integer :: i
    type(interaction_t), pointer :: trace
    associate (instance => decay%process_instance)
      do i = 1, size (decay%term)
        trace => instance%get_trace_int_ptr (i)
        call decay%term(i)%link_interactions (trace)
      end do
    end associate
  end subroutine decay_gen_link_term_interactions

```

Select a decay chain: decay modes and process components.

```

<Decays: decay root: TBP>+≡
  procedure :: select_chain => decay_root_select_chain

<Decays: procedures>+≡
  subroutine decay_root_select_chain (decay_root)
    class(decay_root_t), intent(inout) :: decay_root
    if (decay_root%selected_term > 0) then
      call decay_root%term(decay_root%selected_term)%select_chain ()
    end if
  end subroutine decay_root_select_chain

```



```

else
  call msg_bug ("Decays: no term selected for parent process")
end if
end subroutine decay_root_select_chain

```

Generate a decay tree, i.e., for the selected term in the parent process, recursively generate a decay event for all unstable particles.

Factor out the trace of the connected state of the parent process. This trace should not be taken into account for unweighting the decay chain, since it was already used for unweighting the parent event, or it determines the overall event weight.

```

⟨Decays: decay root: TBP⟩+≡
  procedure :: generate => decay_root_generate

⟨Decays: procedures⟩+≡
  subroutine decay_root_generate (decay_root)
    class(decay_root_t), intent(inout) :: decay_root
    type(connected_state_t), pointer :: connected_state
    if (decay_root%selected_term > 0) then
      connected_state => decay_root%process_instance%get_connected_state_ptr &
        (decay_root%selected_term)
      call connected_state%normalize_matrix_by_trace ()
      call decay_root%term(decay_root%selected_term)%generate ()
    else
      call msg_bug ("Decays: no term selected for parent process")
    end if
  end subroutine decay_root_generate

```

32.6.7 Decay Configuration

A decay configuration describes a distinct decay mode of a particle. Each decay mode may include several terms, which correspond to the terms in the associated process. In addition to the base type, the decay configuration object contains the integral of the parent process and the selector for the MCI group inside this process.

The flavor component should be identical to the flavor component of the parent particle (`unstable` object).

```

⟨Decays: types⟩+≡
  type, extends (decay_root_config_t) :: decay_config_t
  private
  type(flavor_t) :: flv
  real(default) :: weight = 0
  real(default) :: integral = 0
  real(default) :: abs_error = 0
  real(default) :: rel_error = 0
  type(selector_t) :: mci_selector
  contains
  ⟨Decays: decay config: TBP⟩
end type decay_config_t

```

The output routine extends the decay-root writer by listing numerical component values.

```

<Decays: decay config: TBP>≡
  procedure :: write => decay_config_write

<Decays: procedures>+≡
  recursive subroutine decay_config_write (object, unit, indent, verbose)
    class(decay_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(1x,A)") "Decay:"
    call object%write_header (unit, indent)
    call write_indent (u, ind)
    write (u, 2) "branching ratio =", object%weight * 100
    call write_indent (u, ind)
    write (u, 1) "partial width   =", object%integral
    call write_indent (u, ind)
    write (u, 1) "error (abs)      =", object%abs_error
    call write_indent (u, ind)
    write (u, 1) "error (rel)       =", object%rel_error
1   format (3x,A,ES19.12)
2   format (3x,A,F11.6,1x,'%')
    call object%write_terms (unit, indent, verbose)
  end subroutine decay_config_write

```

Connect a decay configuration with a process object (which should represent the decay). This includes initialization, therefore intent(out). We first connect the process itself, then do initializations that are specific for this decay.

Infer stability from the particle properties, using the first row in the set of flavor states. Once we can deal with predetermined decay chains, they should be used instead.

If there is an optional `var_list`, check if the stored values for the decay partial width and error have been overridden there.

```

<Decays: decay config: TBP>+≡
  procedure :: connect => decay_config_connect

<Decays: procedures>+≡
  recursive subroutine decay_config_connect &
    (decay, process, model, process_stack, process_instance, var_list)
    class(decay_config_t), intent(out) :: decay
    type(process_t), intent(in), target :: process
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    type(process_instance_t), intent(in), optional, target :: process_instance
    type(var_list_t), intent(in), optional, target :: var_list
    real(default), dimension(:), allocatable :: integral_mci
    type(string_t) :: process_id
    integer :: i, n_mci
    call decay%decay_root_config_t%connect &
      (process, model, process_stack, var_list=var_list)

```

```

process_id = process%get_id ()
if (process%lab_is_cm ()) then
    call msg_fatal ("Decay process " // char (process_id) &
        // ": unusable because rest frame is fixed.")
end if
decay%integral = process%get_integral ()
decay%abs_error = process%get_error ()
if (present (var_list)) then
    call update (decay%integral, "integral(" // process_id // ")")
    call update (decay%abs_error, "error(" // process_id // ")")
end if
n_mci = process%get_n_mci ()
allocate (integral_mci (n_mci))
do i = 1, n_mci
    integral_mci(i) = process%get_integral_mci (i)
end do
call decay%mci_selector%init (integral_mci)
contains
subroutine update (var, var_name)
    real(default), intent(inout) :: var
    type(string_t), intent(in) :: var_name
    if (var_list%contains (var_name)) then
        var = var_list%get_rval (var_name)
    end if
end subroutine update
end subroutine decay_config_connect

```

Set the flavor entry, which repeats the flavor of the parent unstable particle.

```

<Decays: decay config: TBP>+≡
    procedure :: set_flv => decay_config_set_flv

<Decays: procedures>+≡
    subroutine decay_config_set_flv (decay, flv)
        class(decay_config_t), intent(inout) :: decay
        type(flavor_t), intent(in) :: flv
        decay%flv = flv
    end subroutine decay_config_set_flv

```

Compute embedded branchings and the relative error. This method does not apply to the decay root.

```

<Decays: decay config: TBP>+≡
    procedure :: compute => decay_config_compute

<Decays: procedures>+≡
    recursive subroutine decay_config_compute (decay)
        class(decay_config_t), intent(inout) :: decay
        call decay%decay_root_config_t%compute ()
        if (.not. vanishes (decay%integral)) then
            decay%rel_error = decay%abs_error / decay%integral
        else
            decay%rel_error = 0
        end if
    end subroutine decay_config_compute

```

32.6.8 Decay Instance

The decay contains a collection of terms. One of them is selected when the decay is evaluated. This is similar to the decay root, but we implement it independently.

The process instance object is allocated via a pointer, so it automatically behaves as a target.

```
<Decays: types>+≡
  type, extends (decay_gen_t) :: decay_t
  private
    type(decay_config_t), pointer :: config => null ()
    class(rng_t), allocatable :: rng
  contains
    <Decays: decay: TBP>
  end type decay_t
```

The finalizer is recursive.

```
<Decays: decay: TBP>≡
  procedure :: final => decay_final

<Decays: procedures>+≡
  recursive subroutine decay_final (object)
    class(decay_t), intent(inout) :: object
    integer :: i
    call object%base_final ()
    do i = 1, object%config%process%get_n_mci ()
      call object%process_instance%final_simulation (i)
    end do
    call object%process_instance%final ()
    deallocate (object%process_instance)
  end subroutine decay_final
```

Output.

```
<Decays: decay: TBP>+≡
  procedure :: write => decay_write

<Decays: procedures>+≡
  recursive subroutine decay_write (object, unit, indent, recursive)
    class(decay_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent, recursive
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call object%config%write (unit, indent, verbose = .false.)
    if (allocated (object%rng)) then
      call object%rng%write (u, ind + 1)
    end if
    call write_indent (u, ind)
    if (object%selected_mci > 0) then
      write (u, "(3x,A,I0)") "Selected MCI    = ", object%selected_mci
    else
      write (u, "(3x,A)") "Selected MCI    = [undefined]"
    end if
    call write_indent (u, ind)
```

```

    if (object%selected_term > 0) then
      write (u, "(3x,A,I0)") "Selected term  = ", object%selected_term
      call object%term(object%selected_term)%write (u, ind + 1)
    else
      write (u, "(3x,A)") "Selected term  = [undefined]"
    end if
  end subroutine decay_write

```

Initializer. Base initialization is done recursively. Then, we prepare the current process instance and allocate a random-number generator for term selection. For all unstable particles, we also allocate a r.n.g. as spawned by the current process.

```

<Decays: decay: TBP>+≡
  procedure :: init => decay_init

<Decays: procedures>+≡
  recursive subroutine decay_init (decay, config)
    class(decay_t), intent(out) :: decay
    type(decay_config_t), intent(in), target :: config
    integer :: i
    call decay%base_init (config%term_config)
    decay%config => config
    allocate (decay%process_instance)
    call decay%process_instance%init (decay%config%process)
    call decay%process_instance%setup_event_data (decay%config%model)
    do i = 1, decay%config%process%get_n_mci ()
      call decay%process_instance%init_simulation (i)
    end do
    call decay%config%process%make_rng (decay%rng)
    call decay%make_term_rng (decay%config%process)
  end subroutine decay_init

```

Link interactions to the parent process. `i_prt` is the index of the current outgoing particle in the parent interaction, for which we take the trace evaluator. We link it to the beam particle in the beam interaction of the decay process instance. Then, repeat the procedure for the outgoing particles.

```

<Decays: decay: TBP>+≡
  procedure :: link_interactions => decay_link_interactions

<Decays: procedures>+≡
  recursive subroutine decay_link_interactions (decay, i_prt, trace)
    class(decay_t), intent(inout) :: decay
    integer, intent(in) :: i_prt
    type(interaction_t), intent(in), target :: trace
    type(interaction_t), pointer :: beam_int
    integer :: n_in, n_vir
    beam_int => decay%process_instance%get_beam_int_ptr ()
    n_in = trace%get_n_in ()
    n_vir = trace%get_n_vir ()
    call beam_int%set_source_link (1, trace, &
      n_in + n_vir + i_prt)
    call decay%link_term_interactions ()
  end subroutine decay_link_interactions

```

Determine a decay chain. For each unstable particle we select one of the possible decay modes, and for each decay process we select one of the possible decay MCI components, calling the random-number generators. We do not generate momenta, yet.

```

<Decays: decay: TBP>+≡
  procedure :: select_chain => decay_select_chain

<Decays: procedures>+≡
  recursive subroutine decay_select_chain (decay)
    class(decay_t), intent(inout) :: decay
    real(default) :: x
    integer :: i
    call decay%rng%generate (x)
    decay%selected_mci = decay%config%mci_selector%select (x)
    call decay%process_instance%choose_mci (decay%selected_mci)
    decay%selected_term = decay%process_instance%select_i_term ()
    do i = 1, size (decay%term)
      call decay%term(i)%select_chain ()
    end do
  end subroutine decay_select_chain

```

Generate a decay. We first receive the beam momenta from the parent process (assuming that this is properly linked), then call the associated process object for a new event.

Factor out the trace of the helicity density matrix of the isolated state (the one that will be used for the decay chain). The trace is taken into account for unweighting the individual decay event and should therefore be ignored for unweighting the correlated decay chain afterwards.

```

<Decays: decay: TBP>+≡
  procedure :: generate => decay_generate

<Decays: procedures>+≡
  recursive subroutine decay_generate (decay)
    class(decay_t), intent(inout) :: decay
    type(isolated_state_t), pointer :: isolated_state
    integer :: i
    call decay%process_instance%receive_beam_momenta ()
    call decay%process_instance%generate_unweighted_event (decay%selected_mci)
    if (signal_is_pending ()) return
    call decay%process_instance%evaluate_event_data ()
    isolated_state => &
      decay%process_instance%get_isolated_state_ptr (decay%selected_term)
    call isolated_state%normalize_matrix_by_trace ()
    do i = 1, size (decay%term)
      call decay%term(i)%generate ()
      if (signal_is_pending ()) return
    end do
  end subroutine decay_generate

```

32.6.9 Stable Particles

This is a stable particle. The flavor can be ambiguous (e.g., partons).

```

<Decays: types>+=
  type, extends (any_config_t) :: stable_config_t
  private
    type(flavor_t), dimension(:), allocatable :: flv
  contains
    <Decays: stable config: TBP>
  end type stable_config_t

```

The finalizer is empty:

```

<Decays: stable config: TBP>=
  procedure :: final => stable_config_final

<Decays: procedures>+=
  subroutine stable_config_final (object)
    class(stable_config_t), intent(inout) :: object
  end subroutine stable_config_final

```

Output.

```

<Decays: stable config: TBP>+=
  procedure :: write => stable_config_write

<Decays: procedures>+=
  recursive subroutine stable_config_write (object, unit, indent, verbose)
    class(stable_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: u, i, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call write_indent (u, ind)
    write (u, "(1x,'+',1x,A)", advance = "no") "Stable:"
    write (u, "(1x,A)", advance = "no") char (object%flv(1)%get_name ())
    do i = 2, size (object%flv)
      write (u, "(:',A)", advance = "no") &
        char (object%flv(i)%get_name ())
    end do
    write (u, *)
  end subroutine stable_config_write

```

Initializer. We are presented with an array of flavors, but there may be double entries which we remove, so we store only the distinct flavors.

```

<Decays: stable config: TBP>+=
  procedure :: init => stable_config_init

<Decays: procedures>+=
  subroutine stable_config_init (config, flv)
    class(stable_config_t), intent(out) :: config
    type(flavor_t), dimension(:), intent(in) :: flv
    integer, dimension (size (flv)) :: pdg
    logical, dimension (size (flv)) :: mask
    integer :: i
    pdg = flv%get_pdg ()
    mask(1) = .true.
    forall (i = 2 : size (pdg))

```

```

        mask(i) = all (pdg(i) /= pdg(1:i-1))
    end forall
    allocate (config%flv (count (mask)))
    config%flv = pack (flv, mask)
end subroutine stable_config_init

```

Here is the corresponding object instance. Except for the pointer to the configuration, there is no content.

```

<Decays: types>+≡
    type, extends (any_t) :: stable_t
    private
        type(stable_config_t), pointer :: config => null ()
    contains
        <Decays: stable: TBP>
    end type stable_t

```

The finalizer does nothing.

```

<Decays: stable: TBP>≡
    procedure :: final => stable_final

<Decays: procedures>+≡
    subroutine stable_final (object)
        class(stable_t), intent(inout) :: object
    end subroutine stable_final

```

We can delegate output to the configuration object.

```

<Decays: stable: TBP>+≡
    procedure :: write => stable_write

<Decays: procedures>+≡
    subroutine stable_write (object, unit, indent)
        class(stable_t), intent(in) :: object
        integer, intent(in), optional :: unit, indent
        call object%config%write (unit, indent)
    end subroutine stable_write

```

Initializer: just assign the configuration.

```

<Decays: stable: TBP>+≡
    procedure :: init => stable_init

<Decays: procedures>+≡
    subroutine stable_init (stable, config)
        class(stable_t), intent(out) :: stable
        type(stable_config_t), intent(in), target :: config
        stable%config => config
    end subroutine stable_init

```

32.6.10 Unstable Particles

A branching configuration enables us to select among distinct decay modes of a particle. We store the particle flavor (with its implicit link to a model), an array of decay configurations, and a selector object.

The total width, absolute and relative error are stored as `integral`, `abs_error`, and `rel_error`, respectively.

The flavor must be unique in this case.

```

<Decays: public>+≡
    public :: unstable_config_t

<Decays: types>+≡
    type, extends (any_config_t) :: unstable_config_t
    private
    type(flavor_t) :: flv
    real(default) :: integral = 0
    real(default) :: abs_error = 0
    real(default) :: rel_error = 0
    type(selector_t) :: selector
    type(decay_config_t), dimension(:), allocatable :: decay_config
    contains
    <Decays: unstable config: TBP>
    end type unstable_config_t

```

Finalizer. The branching configuration can be a recursive structure.

```

<Decays: unstable config: TBP>≡
    procedure :: final => unstable_config_final

<Decays: procedures>+≡
    recursive subroutine unstable_config_final (object)
    class(unstable_config_t), intent(inout) :: object
    integer :: i
    if (allocated (object%decay_config)) then
        do i = 1, size (object%decay_config)
            call object%decay_config(i)%final ()
        end do
    end if
    end subroutine unstable_config_final

```

Output. Since this may be recursive, we include indentation.

```

<Decays: unstable config: TBP>+≡
    procedure :: write => unstable_config_write

<Decays: procedures>+≡
    recursive subroutine unstable_config_write (object, unit, indent, verbose)
    class(unstable_config_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    logical, intent(in), optional :: verbose
    integer :: u, i, ind
    logical :: verb
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    verb = .true.; if (present (verbose)) verb = verbose
    call write_indent (u, ind)
    write (u, "(1x,'+',1x,A,1x,A)") "Unstable:", &
        char (object%flv%get_name ())
    call write_indent (u, ind)
    write (u, 1) "total width =", object%integral
    call write_indent (u, ind)

```

```

        write (u, 1) "error (abs) =", object%abs_error
        call write_indent (u, ind)
        write (u, 1) "error (rel) =", object%rel_error
1    format (5x,A,ES19.12)
        if (verb .and. allocated (object%decay_config)) then
            do i = 1, size (object%decay_config)
                call object%decay_config(i)%write (u, ind + 1)
            end do
        end if
    end subroutine unstable_config_write

```

Initializer. For the unstable particle, the flavor is unique.

```

<Decays: unstable config: TBP>+≡
    procedure :: init => unstable_config_init

<Decays: procedures>+≡
    subroutine unstable_config_init (unstable, flv, set_decays, model)
        class(unstable_config_t), intent(out) :: unstable
        type(flavor_t), intent(in) :: flv
        logical, intent(in), optional :: set_decays
        class(model_data_t), intent(in), optional, target :: model
        type(string_t), dimension(:), allocatable :: decay
        unstable%flv = flv
        if (present (set_decays)) then
            call unstable%flv%get_decays (decay)
            call unstable%init_decays (decay, model)
        end if
    end subroutine unstable_config_init

```

Further initialization: determine the number of decay modes. We can assume that the flavor of the particle has been set already.

If the process stack is given, we can delve recursively into actually assigning decay processes. Otherwise, we just initialize with decay process names.

```

<Decays: unstable config: TBP>+≡
    procedure :: init_decays => unstable_config_init_decays

<Decays: procedures>+≡
    recursive subroutine unstable_config_init_decays &
        (unstable, decay_id, model, process_stack, var_list)
        class(unstable_config_t), intent(inout) :: unstable
        type(string_t), dimension(:), intent(in) :: decay_id
        class(model_data_t), intent(in), target :: model
        type(process_stack_t), intent(in), optional :: process_stack
        type(var_list_t), intent(in), optional :: var_list
        integer :: i
        allocate (unstable%decay_config (size (decay_id)))
        do i = 1, size (decay_id)
            associate (decay => unstable%decay_config(i))
                if (present (process_stack)) then
                    call decay%connect (process_stack%get_process_ptr (decay_id(i)), &
                        model, process_stack, var_list=var_list)
                else
                    call decay%init (model, decay_id(i))
                end if
            end associate
        end do
    end subroutine unstable_config_init_decays

```

```

        call decay%set_flg (unstable%flv)
    end associate
end do
end subroutine unstable_config_init_decays

```

Explicitly connect a specific decay with a process. This is used only in unit tests.

```

<Decays: unstable config: TBP>+≡
    procedure :: connect_decay => unstable_config_connect_decay

<Decays: procedures>+≡
    subroutine unstable_config_connect_decay (unstable, i, process, model)
        class(unstable_config_t), intent(inout) :: unstable
        integer, intent(in) :: i
        type(process_t), intent(in), target :: process
        class(model_data_t), intent(in), target :: model
        associate (decay => unstable%decay_config(i))
            call decay%connect (process, model)
        end associate
    end subroutine unstable_config_connect_decay

```

Compute the total width and branching ratios, initializing the decay selector.

```

<Decays: unstable config: TBP>+≡
    procedure :: compute => unstable_config_compute

<Decays: procedures>+≡
    recursive subroutine unstable_config_compute (unstable)
        class(unstable_config_t), intent(inout) :: unstable
        integer :: i
        do i = 1, size (unstable%decay_config)
            call unstable%decay_config(i)%compute ()
        end do
        unstable%integral = sum (unstable%decay_config%integral)
        if (unstable%integral <= 0) then
            call unstable%write ()
            call msg_fatal ("Decay configuration: computed total width is zero")
        end if
        unstable%abs_error = sqrt (sum (unstable%decay_config%abs_error ** 2))
        unstable%rel_error = unstable%abs_error / unstable%integral
        call unstable%selector%init (unstable%decay_config%integral)
        do i = 1, size (unstable%decay_config)
            unstable%decay_config(i)%weight &
                = unstable%selector%get_weight (i)
        end do
    end subroutine unstable_config_compute

```

Now we define the instance of an unstable particle.

```

<Decays: public>+≡
    public :: unstable_t

<Decays: types>+≡
    type, extends (any_t) :: unstable_t
        private

```

```

    type(unstable_config_t), pointer :: config => null ()
    class(rng_t), allocatable :: rng
    integer :: selected_decay = 0
    type(decay_t), dimension(:), allocatable :: decay
contains
  <Decays: unstable: TBP>
end type unstable_t

```

Recursive finalizer.

```

<Decays: unstable: TBP>≡
  procedure :: final => unstable_final
<Decays: procedures>+≡
  recursive subroutine unstable_final (object)
    class(unstable_t), intent(inout) :: object
    integer :: i
    if (allocated (object%decay)) then
      do i = 1, size (object%decay)
        call object%decay(i)%final ()
      end do
    end if
  end subroutine unstable_final

```

Output.

```

<Decays: unstable: TBP>+≡
  procedure :: write => unstable_write
<Decays: procedures>+≡
  recursive subroutine unstable_write (object, unit, indent)
    class(unstable_t), intent(in) :: object
    integer, intent(in), optional :: unit, indent
    integer :: u, ind
    u = given_output_unit (unit)
    ind = 0; if (present (indent)) ind = indent
    call object%config%write (u, ind, verbose=.false.)
    if (allocated (object%rng)) then
      call object%rng%write (u, ind + 2)
    end if
    call write_indent (u, ind)
    if (object%selected_decay > 0) then
      write (u, "(5x,A,I0)") "Sel. decay = ", object%selected_decay
      call object%decay(object%selected_decay)%write (u, ind + 1)
    else
      write (u, "(5x,A)") "Sel. decay = [undefined]"
    end if
  end subroutine unstable_write

```

Write the embedded process instances.

```

<Decays: unstable: TBP>+≡
  procedure :: write_process_instances => unstable_write_process_instances
<Decays: procedures>+≡
  recursive subroutine unstable_write_process_instances &
    (unstable, unit, verbose)

```

```

class(unstable_t), intent(in) :: unstable
integer, intent(in), optional :: unit
logical, intent(in), optional :: verbose
if (unstable%selected_decay > 0) then
    call unstable%decay(unstable%selected_decay)% &
        write_process_instances (unit, verbose)
end if
end subroutine unstable_write_process_instances

```

Initialization, using the configuration object.

```

<Decays: unstable: TBP>+≡
    procedure :: init => unstable_init

<Decays: procedures>+≡
    recursive subroutine unstable_init (unstable, config)
        class(unstable_t), intent(out) :: unstable
        type(unstable_config_t), intent(in), target :: config
        integer :: i
        unstable%config => config
        allocate (unstable%decay (size (config%decay_config)))
        do i = 1, size (config%decay_config)
            call unstable%decay(i)%init (config%decay_config(i))
        end do
    end subroutine unstable_init

```

Recursively link interactions to the parent process. `i_prt` is the index of the current outgoing particle in the parent interaction.

```

<Decays: unstable: TBP>+≡
    procedure :: link_interactions => unstable_link_interactions

<Decays: procedures>+≡
    recursive subroutine unstable_link_interactions (unstable, i_prt, trace)
        class(unstable_t), intent(inout) :: unstable
        integer, intent(in) :: i_prt
        type(interaction_t), intent(in), target :: trace
        integer :: i
        do i = 1, size (unstable%decay)
            call unstable%decay(i)%link_interactions (i_prt, trace)
        end do
    end subroutine unstable_link_interactions

```

Import the random-number generator state.

```

<Decays: unstable: TBP>+≡
    procedure :: import_rng => unstable_import_rng

<Decays: procedures>+≡
    subroutine unstable_import_rng (unstable, rng)
        class(unstable_t), intent(inout) :: unstable
        class(rng_t), intent(inout), allocatable :: rng
        call move_alloc (from = rng, to = unstable%rng)
    end subroutine unstable_import_rng

```

Generate a decay chain. First select a decay mode, then call the `select_chain` method of the selected mode.

```

<Decays: unstable: TBP>+≡
  procedure :: select_chain => unstable_select_chain

<Decays: procedures>+≡
  recursive subroutine unstable_select_chain (unstable)
    class(unstable_t), intent(inout) :: unstable
    real(default) :: x
    call unstable%rng%generate (x)
    unstable%selected_decay = unstable%config%selector%select (x)
    call unstable%decay(unstable%selected_decay)%select_chain ()
  end subroutine unstable_select_chain

```

Generate a decay event.

```

<Decays: unstable: TBP>+≡
  procedure :: generate => unstable_generate

<Decays: procedures>+≡
  recursive subroutine unstable_generate (unstable)
    class(unstable_t), intent(inout) :: unstable
    call unstable%decay(unstable%selected_decay)%generate ()
  end subroutine unstable_generate

```

32.6.11 Decay Chain

While the decay configuration tree and the decay tree are static entities (during a simulation run), the decay chain is dynamically generated for each event. The reason is that with the possibility of several decay modes for each particle, and several terms for each process, the total number of distinct decay chains is not under control.

Each entry in the decay chain is a connected parton state. The origin of the chain is a connected state in the parent process (not part of the chain itself). For each decay, mode and term chosen, we convolute this with the isolated (!) state of the current decay, to generate a new connected state. We accumulate this chain by recursively traversing the allocated decay tree. Whenever a particle decays, it becomes virtual and is replaced by its decay product, while all other particles stay in the parton state as spectators.

Technically, we implement the decay chain as a stack structure and include information from the associated decay object for easier debugging. This is a decay chain entry:

```

<Decays: types>+≡
  type, extends (connected_state_t) :: decay_chain_entry_t
  private
  integer :: index = 0
  type(decay_config_t), pointer :: config => null ()
  integer :: selected_mci = 0
  integer :: selected_term = 0
  type(decay_chain_entry_t), pointer :: previous => null ()
  end type decay_chain_entry_t

```

This is the complete chain; we need just a pointer to the last entry. We also include a pointer to the master process instance, which serves as the seed for the decay chain.

The evaluator `correlated_trace` traces over all quantum numbers for the final spin-correlated (but color-summed) evaluator of the decay chain. This allows us to compute the probability for a momentum configuration, given that all individual density matrices (of the initial process and the subsequent decays) have been normalized to one.

Note: This trace is summed over color, so color is treated exactly when computing spin correlations. However, we do not keep non-diagonal color correlations. When an event is accepted, we compute probabilities for all color states and can choose one of them.

```

<Decays: public>+≡
    public :: decay_chain_t

<Decays: types>+≡
    type :: decay_chain_t
        private
            type(process_instance_t), pointer :: process_instance => null ()
            integer :: selected_term = 0
            type(evaluator_t) :: correlated_trace
            type(decay_chain_entry_t), pointer :: last => null ()
        contains
            <Decays: decay_chain: TBP>
        end type decay_chain_t

```

The finalizer recursively deletes and deallocates the entries.

```

<Decays: decay_chain: TBP>≡
    procedure :: final => decay_chain_final

<Decays: procedures>+≡
    subroutine decay_chain_final (object)
        class(decay_chain_t), intent(inout) :: object
        type(decay_chain_entry_t), pointer :: entry
        do while (associated (object%last))
            entry => object%last
            object%last => entry%previous
            call entry%final ()
            deallocate (entry)
        end do
        call object%correlated_trace%final ()
    end subroutine decay_chain_final

```

Doing output recursively allows us to display the chain in chronological order.

```

<Decays: decay_chain: TBP>+≡
    procedure :: write => decay_chain_write

<Decays: procedures>+≡
    subroutine decay_chain_write (object, unit)
        class(decay_chain_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
    end subroutine decay_chain_write

```

```

call write_separator (u, 2)
write (u, "(1x,A)") "Decay chain:"
call write_entries (object%last)
call write_separator (u, 2)
write (u, "(1x,A)") "Evaluator (correlated trace of the decay chain):"
call write_separator (u)
call object%correlated_trace%write (u)
call write_separator (u, 2)
contains
recursive subroutine write_entries (entry)
  type(decay_chain_entry_t), intent(in), pointer :: entry
  if (associated (entry)) then
    call write_entries (entry%previous)
    call write_separator (u, 2)
    write (u, "(1x,A,I0)") "Decay #", entry%index
    call entry%config%write_header (u)
    write (u, "(3x,A,I0)") "Selected MCI    = ", entry%selected_mci
    write (u, "(3x,A,I0)") "Selected term  = ", entry%selected_term
    call entry%config%term_config(entry%selected_term)%write (u, indent=1)
    call entry%write (u)
  end if
end subroutine write_entries
end subroutine decay_chain_write

```

Build a decay chain, recursively following the selected decays and terms in a decay tree. Before start, we finalize the chain, deleting any previous contents.

```

<Decays: decay chain: TBP>+≡
  procedure :: build => decay_chain_build

<Decays: procedures>+≡
  subroutine decay_chain_build (chain, decay_root)
    class(decay_chain_t), intent(inout), target :: chain
    type(decay_root_t), intent(in) :: decay_root
    type(quantum_numbers_mask_t), dimension(:), allocatable :: qn_mask
    type(interaction_t), pointer :: int_last_decay
    call chain%final ()
    if (decay_root%selected_term > 0) then
      chain%process_instance => decay_root%process_instance
      chain%selected_term = decay_root%selected_term
      call chain%build_term_entries (decay_root%term(decay_root%selected_term))
    end if
    int_last_decay => chain%last%get_matrix_int_ptr ()
    allocate (qn_mask (int_last_decay%get_n_tot ()))
    call qn_mask%init (mask_f = .true., mask_c = .true., mask_h = .true.)
    call chain%correlated_trace%init_qn_sum (int_last_decay, qn_mask)
  end subroutine decay_chain_build

```

Build the entries that correspond to a decay term. We have to scan all unstable particles.

```

<Decays: decay chain: TBP>+≡
  procedure :: build_term_entries => decay_chain_build_term_entries

<Decays: procedures>+≡
  recursive subroutine decay_chain_build_term_entries (chain, term)

```



```

class(decay_chain_t), intent(inout) :: chain
type(decay_term_t), intent(in) :: term
integer :: i
do i = 1, size (term%particle_out)
  select type (unstable => term%particle_out(i)%c)
  type is (unstable_t)
    if (unstable%selected_decay > 0) then
      call chain%build_decay_entries &
        (unstable%decay(unstable%selected_decay))
    end if
  end select
end do
end subroutine decay_chain_build_term_entries

```

Build the entries that correspond to a specific decay. The decay term should have been determined, so we allocate a decay chain entry and fill it, then proceed to child decays.

For the first entry, we convolute the connected state of the parent process instance with the isolated state of the current decay (which does not contain an extra beam entry for the parent). For subsequent entries, we take the previous entry as first factor.

In principle, each chain entry (as a parton state) is capable of holding a subevent object and associated expressions. We currently do not make use of that feature.

Before generating the decays, factor out the trace of the helicity density matrix of the parent parton state. This trace has been used for unweighting the original event (unweighted case) or it determines the overall weight, so it should not be taken into account in the decay chain generation.

```

<Decays: decay chain: TBP>+≡
  procedure :: build_decay_entries => decay_chain_build_decay_entries

<Decays: procedures>+≡
  recursive subroutine decay_chain_build_decay_entries (chain, decay)
    class(decay_chain_t), intent(inout) :: chain
    type(decay_t), intent(in) :: decay
    type(decay_chain_entry_t), pointer :: entry
    type(connected_state_t), pointer :: previous_state
    type(isolated_state_t), pointer :: current_decay
    type(helicity_t) :: hel
    type(quantum_numbers_t) :: qn_filter_conn
    allocate (entry)
    if (associated (chain%last)) then
      entry%previous => chain%last
      entry%index = entry%previous%index + 1
      previous_state => entry%previous%connected_state_t
    else
      entry%index = 1
      previous_state => &
        chain%process_instance%get_connected_state_ptr (chain%selected_term)
    end if
    entry%config => decay%config
    entry%selected_mci = decay%selected_mci
    entry%selected_term = decay%selected_term
  end subroutine

```

```

current_decay => decay%process_instance%get_isolated_state_ptr &
    (decay%selected_term)
call entry%setup_connected_trace &
    (current_decay, previous_state%get_trace_int_ptr (), resonant=.true.)
if (entry%config%flv%has_decay_helicity ()) then
    call hel%init (entry%config%flv%get_decay_helicity ())
    call qn_filter_conn%init (hel)
    call entry%setup_connected_matrix &
        (current_decay, previous_state%get_matrix_int_ptr (), &
        resonant=.true., qn_filter_conn = qn_filter_conn)
    call entry%setup_connected_flows &
        (current_decay, previous_state%get_flows_int_ptr (), &
        resonant=.true., qn_filter_conn = qn_filter_conn)
else
    call entry%setup_connected_matrix &
        (current_decay, previous_state%get_matrix_int_ptr (), &
        resonant=.true.)
    call entry%setup_connected_flows &
        (current_decay, previous_state%get_flows_int_ptr (), &
        resonant=.true.)
end if
chain%last => entry
call chain%build_term_entries (decay%term(decay%selected_term))
end subroutine decay_chain_build_decay_entries

```

Recursively fill the decay chain with momenta and evaluate the matrix elements. Since all evaluators should have correct source entries at this point, momenta are automatically retrieved from the appropriate process instance.

Like we did above for the parent process, factor out the trace for each subsequent decay (the helicity density matrix in the isolated state, which is taken for the convolution).

```

<Decays: decay chain: TBP>+≡
    procedure :: evaluate => decay_chain_evaluate

<Decays: procedures>+≡
    subroutine decay_chain_evaluate (chain)
        class(decay_chain_t), intent(inout) :: chain
        call evaluate (chain%last)
        call chain%correlated_trace%receive_momenta ()
        call chain%correlated_trace%evaluate ()
    contains
        recursive subroutine evaluate (entry)
            type(decay_chain_entry_t), intent(inout), pointer :: entry
            if (associated (entry)) then
                call evaluate (entry%previous)
                call entry%receive_kinematics ()
                call entry%evaluate_trace ()
                call entry%evaluate_event_data ()
            end if
        end subroutine evaluate
    end subroutine decay_chain_evaluate

```

Return the probability of a decay chain. This is given as the trace of the density

matrix with intermediate helicity correlations, normalized by the product of the uncorrelated density matrix traces. This works only if an event has been evaluated and the `correlated_trace` evaluator is filled. By definition, this evaluator has only one matrix element, and this must be real.

```

<Decays: decay chain: TBP>+≡
  procedure :: get_probability => decay_chain_get_probability

<Decays: procedures>+≡
  function decay_chain_get_probability (chain) result (x)
    class(decay_chain_t), intent(in) :: chain
    real(default) :: x
    x = real (chain%correlated_trace%get_matrix_element (1))
  end function decay_chain_get_probability

```

32.6.12 Decay as Event Transform

The `evt_decay` object combines decay configuration, decay tree, and chain in a single object, as an implementation of the `evt` (event transform) abstract type.

The `var_list` may be a pointer to the user variable list, which could contain overridden parameters for the decay processes.

```

<Decays: public>+≡
  public :: evt_decay_t

<Decays: types>+≡
  type, extends (evt_t) :: evt_decay_t
    private
    type(decay_root_config_t) :: decay_root_config
    type(decay_root_t) :: decay_root
    type(decay_chain_t) :: decay_chain
    type(var_list_t), pointer :: var_list => null ()
  contains
    <Decays: evt decay: TBP>
  end type evt_decay_t

<Decays: evt decay: TBP>≡
  procedure :: write_name => evt_decay_write_name

<Decays: procedures>+≡
  subroutine evt_decay_write_name (evt, unit)
    class(evt_decay_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: partonic decays"
  end subroutine evt_decay_write_name

```

Output. We display the currently selected decay tree, which includes configuration data, and the decay chain, i.e., the evaluators.

```

<Decays: evt decay: TBP>+≡
  procedure :: write => evt_decay_write

```

```

<Decays: procedures>+≡
subroutine evt_decay_write (evt, unit, verbose, more_verbose, testflag)
  class(evt_decay_t), intent(in) :: evt
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: verbose, more_verbose, testflag
  logical :: verb, verb2
  integer :: u
  u = given_output_unit (unit)
  verb = .true.; if (present (verbose)) verb = verbose
  verb2 = .false.; if (present (more_verbose)) verb2 = more_verbose
  call write_separator (u, 2)
  call evt%write_name (u)
  call write_separator (u, 2)
  call evt%base_write (u, testflag = testflag)
  if (associated (evt%var_list)) then
    call write_separator (u)
    write (u, "(1x,A)" "Variable list for simulation: &
      &[associated, not shown]"
  end if
  if (verb) then
    call write_separator (u)
    call evt%decay_root%write (u)
    if (verb2) then
      call evt%decay_chain%write (u)
      call evt%decay_root%write_process_instances (u, verb)
    end if
  else
    call write_separator (u, 2)
  end if
end subroutine evt_decay_write

```

Set the pointer to a user variable list.

```

<Decays: evt decay: TBP>+≡
  procedure :: set_var_list => evt_decay_set_var_list

<Decays: procedures>+≡
subroutine evt_decay_set_var_list (evt, var_list)
  class(evt_decay_t), intent(inout) :: evt
  type(var_list_t), intent(in), target :: var_list
  evt%var_list => var_list
end subroutine evt_decay_set_var_list

```

Connect with a process instance and process. This initializes the decay configuration. The process stack is used to look for process objects that implement daughter decays.

When all processes are assigned, configure the decay tree instance, using the decay tree configuration. First obtain the branching ratios, then allocate the decay tree. This is done once for all events.

```

<Decays: evt decay: TBP>+≡
  procedure :: connect => evt_decay_connect

<Decays: procedures>+≡
subroutine evt_decay_connect (evt, process_instance, model, process_stack)

```

```

class(evt_decay_t), intent(inout), target :: evt
type(process_instance_t), intent(in), target :: process_instance
class(model_data_t), intent(in), target :: model
type(process_stack_t), intent(in), optional :: process_stack
call evt%base_connect (process_instance, model)
if (associated (evt%var_list)) then
    call evt%decay_root_config%connect (process_instance%process, &
        model, process_stack, process_instance, evt%var_list)
else
    call evt%decay_root_config%connect (process_instance%process, &
        model, process_stack, process_instance)
end if
call evt%decay_root_config%compute ()
call evt%decay_root%init (evt%decay_root_config, evt%process_instance)
end subroutine evt_decay_connect

```

Prepare a new event: Select a decay chain and build the corresponding chain object.

```

<Decays: evt decay: TBP>+≡
    procedure :: prepare_new_event => evt_decay_prepare_new_event

<Decays: procedures>+≡
    subroutine evt_decay_prepare_new_event (evt, i_mci, i_term)
        class(evt_decay_t), intent(inout) :: evt
        integer, intent(in) :: i_mci, i_term
        call evt%reset ()
        evt%decay_root%selected_mci = i_mci
        evt%decay_root%selected_term = i_term
        call evt%decay_root%select_chain ()
        call evt%decay_chain%build (evt%decay_root)
    end subroutine evt_decay_prepare_new_event

```

Generate a weighted event and assign the resulting weight (probability). We use a chain initialized by the preceding subroutine, fill it with momenta and evaluate.

```

<Decays: evt decay: TBP>+≡
    procedure :: generate_weighted => evt_decay_generate_weighted

<Decays: procedures>+≡
    subroutine evt_decay_generate_weighted (evt, probability)
        class(evt_decay_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
        call evt%decay_root%generate ()
        if (signal_is_pending ()) return
        call evt%decay_chain%evaluate ()
        probability = evt%decay_chain%get_probability ()
    end subroutine evt_decay_generate_weighted

```

To create a usable event, we have to transform the interaction into a particle set; this requires factorization for the correlated density matrix, according to the factorization mode.

```

<Decays: evt decay: TBP>+≡
    procedure :: make_particle_set => evt_decay_make_particle_set

```

```

<Decays: procedures>+≡
  subroutine evt_decay_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_decay_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode
    logical, intent(in) :: keep_correlations
    real(default), dimension(:), intent(in), optional :: r
    type(interaction_t), pointer :: int_matrix, int_flows
    type(decay_chain_entry_t), pointer :: last_entry
    last_entry => evt%decay_chain%last
    int_matrix => last_entry%get_matrix_int_ptr ()
    int_flows => last_entry%get_flows_int_ptr ()
    call evt%factorize_interactions (int_matrix, int_flows, &
      factorization_mode, keep_correlations, r)
    call evt%tag_incoming ()
  end subroutine evt_decay_make_particle_set

```

Auxiliary

Eliminate numerical noise for the associated process instances.

```

<Decays: public>+≡
  public :: pacify

<Decays: interfaces>+≡
  interface pacify
    module procedure pacify_decay
    module procedure pacify_decay_gen
    module procedure pacify_term
    module procedure pacify_unstable
  end interface pacify

<Decays: procedures>+≡
  subroutine pacify_decay (evt)
    class(evt_decay_t), intent(inout) :: evt
    call pacify_decay_gen (evt%decay_root)
  end subroutine pacify_decay

  recursive subroutine pacify_decay_gen (decay)
    class(decay_gen_t), intent(inout) :: decay
    if (associated (decay%process_instance)) then
      call pacify (decay%process_instance)
    end if
    if (decay%selected_term > 0) then
      call pacify_term (decay%term(decay%selected_term))
    end if
  end subroutine pacify_decay_gen

  recursive subroutine pacify_term (term)
    class(decay_term_t), intent(inout) :: term
    integer :: i
    do i = 1, size (term%particle_out)
      select type (unstable => term%particle_out(i)%c)
        type is (unstable_t); call pacify_unstable (unstable)
      end select
    end do
  end subroutine pacify_term

```

```

end do
end subroutine pacify_term

recursive subroutine pacify_unstable (unstable)
  class(unstable_t), intent(inout) :: unstable
  if (unstable%selected_decay > 0) then
    call pacify_decay_gen (unstable%decay(unstable%selected_decay))
  end if
end subroutine pacify_unstable

```

Prepare specific configurations for use in unit tests.

```

<Decays: unstable config: TBP>+=
  procedure :: init_test_case1
  procedure :: init_test_case2

<Decays: procedures>+=
  subroutine init_test_case1 (unstable, i, flv, integral, relerr, model)
    class(unstable_config_t), intent(inout) :: unstable
    integer, intent(in) :: i
    type(flavor_t), dimension(:,:), intent(in) :: flv
    real(default), intent(in) :: integral
    real(default), intent(in) :: relerr
    class(model_data_t), intent(in), target :: model
    associate (decay => unstable%decay_config(i))
      allocate (decay%term_config (1))
      call decay%init_term (1, flv, stable = [.true., .true.], model=model)
      decay%integral = integral
      decay%abs_error = integral * relerr
    end associate
  end subroutine init_test_case1

  subroutine init_test_case2 (unstable, flv1, flv21, flv22, model)
    class(unstable_config_t), intent(inout) :: unstable
    type(flavor_t), dimension(:,:), intent(in) :: flv1, flv21, flv22
    class(model_data_t), intent(in), target :: model
    associate (decay => unstable%decay_config(1))
      decay%integral = 1.e-3_default
      decay%abs_error = decay%integral * .01_default

      allocate (decay%term_config (1))
      call decay%init_term (1, flv1, stable = [.false., .true.], model=model)

      select type (w => decay%term_config(1)%prt(1)%c)
      type is (unstable_config_t)

        associate (w_decay => w%decay_config(1))
          w_decay%integral = 2._default
          allocate (w_decay%term_config (1))
          call w_decay%init_term (1, flv21, stable = [.true., .true.], &
            model=model)
        end associate
      associate (w_decay => w%decay_config(2))
        w_decay%integral = 1._default
        allocate (w_decay%term_config (1))

```

```

        call w_decay%init_term (1, flv22, stable = [.true., .true.], &
            model=model)
    end associate
    call w%compute ()

    end select
end associate
end subroutine init_test_case2

```

32.6.13 Unit tests

Test module, followed by the corresponding implementation module.

<decays_ut.f90>≡

<File header>

```

module decays_ut
    use unit_tests
    use decays_util

```

<Standard module head>

<Decays: public test>

<Decays: public test auxiliary>

contains

<Decays: test driver>

```

end module decays_ut

```

<decays_util.f90>≡

<File header>

```

module decays_util

```

<Use kinds>

<Use strings>

```

    use os_interface
    use sm_qcd
    use model_data
    use models
    use state_matrices, only: FM_IGNORE_HELICITY
    use interactions, only: reset_interaction_counter
    use flavors
    use process_libraries
    use rng_base
    use mci_base
    use mci_midpoint
    use phs_base
    use phs_single
    use prc_core
    use prc_test, only: prc_test_create_library

```



```

    use process, only: process_t
    use instances, only: process_instance_t
    use process_stacks

    use decays

    use rng_base_ut, only: rng_test_t, rng_test_factory_t

    <Standard module head>

    <Decays: public test auxiliary>

    <Decays: test declarations>

    contains

    <Decays: tests>

    <Decays: test auxiliary>

    end module decays_utl

```

API: driver for the unit tests below.

```

    <Decays: public test>≡
        public :: decays_test

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

```

Testbed

As a variation of the `prepare_test_process` routine used elsewhere, we define here a routine that creates two processes (scattering $ss \rightarrow ss$ and decay $s \rightarrow f\bar{f}$), compiles and integrates them and prepares for event generation.

```

    <Decays: public test auxiliary>≡
        public :: prepare_testbed

    <Decays: test auxiliary>≡
        subroutine prepare_testbed &
            (lib, process_stack, prefix, os_data, &
             scattering, decay, decay_rest_frame)
            type(process_library_t), intent(out), target :: lib
            type(process_stack_t), intent(out) :: process_stack
            type(string_t), intent(in) :: prefix
            type(os_data_t), intent(in) :: os_data
            logical, intent(in) :: scattering, decay
            logical, intent(in), optional :: decay_rest_frame

            type(model_t), target :: model

```

```

type(model_t), target :: model_copy
type(string_t) :: libname, procname1, procname2
type(process_entry_t), pointer :: process
type(process_instance_t), allocatable, target :: process_instance
class(phs_config_t), allocatable :: phs_config_template
type(field_data_t), pointer :: field_data
real(default) :: sqrts

libname = prefix // "_lib"
procname1 = prefix // "_p"
procname2 = prefix // "_d"

call model%init_test ()
call model%set_par (var_str ("ff"), 0.4_default)
call model%set_par (var_str ("mf"), &
    model%get_real (var_str ("ff")) * model%get_real (var_str ("ms")))

if (scattering .and. decay) then
    field_data => model%get_field_ptr (25)
    call field_data%set (p_is_stable = .false.)
end if

call prc_test_create_library (libname, lib, &
    scattering = .true., decay = .true., &
    procname1 = procname1, procname2 = procname2)

call reset_interaction_counter ()

allocate (phs_single_config_t :: phs_config_template)

if (scattering) then

    call model_copy%init (model%get_name (), &
        model%get_n_real (), &
        model%get_n_complex (), &
        model%get_n_field (), &
        model%get_n_vtx ())
    call model_copy%copy_from (model)

    allocate (process)
    call process%init (procname1, lib, os_data, model_copy)
    call process%setup_test_cores ()
    call process%init_components (phs_config_template)
    sqrts = 1000
    call process%setup_beams_sqrts (sqrts, i_core = 1)
    call process%configure_phs ()
    call process%setup_mci (dispatch_mci_test_midpoint)
    call process%setup_terms ()

    allocate (process_instance)
    call process_instance%init (process%process_t)
    call process_instance%integrate (1, n_it = 1, n_calls = 100)
    call process_instance%final_integration (1)
    call process_instance%final ()

```

```

        deallocate (process_instance)

        call process%prepare_simulation (1)
        call process_stack%push (process)
    end if

    if (decay) then
        call model_copy%init (model%get_name (), &
            model%get_n_real (), &
            model%get_n_complex (), &
            model%get_n_field (), &
            model%get_n_vtx ())
        call model_copy%copy_from (model)

        allocate (process)
        call process%init (procname2, lib, os_data, model_copy)
        call process%setup_test_cores ()
        call process%init_components (phs_config_template)
        if (present (decay_rest_frame)) then
            call process%setup_beams_decay (rest_frame = decay_rest_frame, i_core = 1)
        else
            call process%setup_beams_decay (rest_frame = .not. scattering, i_core = 1)
        end if
        call process%configure_phs ()
        call process%setup_mci (dispatch_mci_test_midpoint)
        call process%setup_terms ()

        allocate (process_instance)
        call process_instance%init (process%process_t)
        call process_instance%integrate (1, n_it=1, n_calls=100)
        call process%final_integration (1)
        call process_instance%final ()
        deallocate (process_instance)

        call process%prepare_simulation (1)
        call process_stack%push (process)
    end if

    call model%final ()
    call model_copy%final ()

end subroutine prepare_testbed

```

MCI record prepared for midpoint integrator.

(Decays: test auxiliary)+≡

```

subroutine dispatch_mci_test_midpoint (mci, var_list, process_id, is_nlo)
    use variables, only: var_list_t
    class(mci_t), allocatable, intent(out) :: mci
    type(var_list_t), intent(in) :: var_list
    type(string_t), intent(in) :: process_id
    logical, intent(in), optional :: is_nlo
    allocate (mci_midpoint_t :: mci)
end subroutine dispatch_mci_test_midpoint

```

Simple decay configuration

We define a branching configuration with two decay modes. We set the integral values by hand, so we do not need to evaluate processes, yet.

```
<Decays: execute tests>≡
  call test (decays_1, "decays_1", &
    "branching and decay configuration", &
    u, results)

<Decays: test declarations>≡
  public :: decays_1

<Decays: tests>≡
  subroutine decays_1 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t) :: flv_h
    type(flavor_t), dimension(2,1) :: flv_hbb, flv_hgg
    type(unstable_config_t), allocatable :: unstable

    write (u, "(A)")  "* Test output: decays_1"
    write (u, "(A)")  "* Purpose: Set up branching and decay configuration"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment"
    write (u, "(A)")

    call os_data%init ()
    call model%init_sm_test ()

    call flv_h%init (25, model)
    call flv_hbb(:,1)%init ([5, -5], model)
    call flv_hgg(:,1)%init ([22, 22], model)

    write (u, "(A)")  "* Set up branching and decay"
    write (u, "(A)")

    allocate (unstable)
    call unstable%init (flv_h)
    call unstable%init_decays ([var_str ("h_bb"), var_str ("h_gg")], model)

    call unstable%init_test_case1 &
      (1, flv_hbb, 1.234e-3_default, .02_default, model)

    call unstable%init_test_case1 &
      (2, flv_hgg, 3.085e-4_default, .08_default, model)

    call unstable%compute ()
    call unstable%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Cleanup"
```

```

call unstable%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: decays_1"

end subroutine decays_1

```

Cascade decay configuration

We define a branching configuration with one decay, which is followed by another branching.

```

<Decays: execute tests> +=
  call test (decays_2, "decays_2", &
    "cascade decay configuration", &
    u, results)

<Decays: test declarations> +=
  public :: decays_2

<Decays: tests> +=
  subroutine decays_2 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    type(model_data_t), target :: model
    type(flavor_t) :: flv_h, flv_wp, flv_wm
    type(flavor_t), dimension(2,1) :: flv_hww, flv_wud, flv_wen
    type(unstable_config_t), allocatable :: unstable

    write (u, "(A)")  "** Test output: decays_2"
    write (u, "(A)")  "** Purpose: Set up cascade branching"
    write (u, "(A)")

    write (u, "(A)")  "** Initialize environment"
    write (u, "(A)")

    call os_data%init ()
    call model%init_sm_test ()

    call model%set_unstable (25, [var_str ("h_ww")])
    call model%set_unstable (24, [var_str ("w_ud"), var_str ("w_en")])

    call flv_h%init (25, model)
    call flv_hww(:,1)%init ([24, -24], model)
    call flv_wp%init (24, model)
    call flv_wm%init (-24, model)
    call flv_wud(:,1)%init ([2, -1], model)
    call flv_wen(:,1)%init ([-11, 12], model)

    write (u, "(A)")  "** Set up branching and decay"
    write (u, "(A)")

```

```

allocate (unstable)
call unstable%init (flv_h, set_decays=.true., model=model)

call unstable%init_test_case2 (flv_hww, flv_wud, flv_wen, model)

call unstable%compute ()
call unstable%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call unstable%final ()
call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_2"

end subroutine decays_2

```

Decay and Process Object

We define a branching configuration with one decay and connect this with an actual process object.

```

<Decays: execute tests>+=
  call test (decays_3, "decays_3", &
    "associate process", &
    u, results)

<Decays: test declarations>+=
  public :: decays_3

<Decays: tests>+=
  subroutine decays_3 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    class(model_data_t), pointer :: model
    type(process_library_t), target :: lib
    type(string_t) :: prefix
    type(string_t) :: procname2
    type(process_stack_t) :: process_stack
    type(process_t), pointer :: process
    type(unstable_config_t), allocatable :: unstable
    type(flavor_t) :: flv

    write (u, "(A)")  "* Test output: decays_3"
    write (u, "(A)")  "* Purpose: Connect a decay configuration &
      &with a process"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize environment and integrate process"
    write (u, "(A)")

```

```

call os_data%init ()

prefix = "decays_3"
call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
    scattering=.false., decay=.true., decay_rest_frame=.false.)

procname2 = prefix // "_d"
process => process_stack%get_process_ptr (procname2)
model => process%get_model_ptr ()
call process%write (.false., u)

write (u, "(A)")
write (u, "(A)")  "* Set up branching and decay"
write (u, "(A)")

call flv%init (25, model)

allocate (unstable)
call unstable%init (flv)
call unstable%init_decays ([procname2], model)

write (u, "(A)")  "* Connect decay with process object"
write (u, "(A)")

call unstable%connect_decay (1, process, model)

call unstable%compute ()
call unstable%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call unstable%final ()
call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_3"

end subroutine decays_3

```

Decay and Process Object

Building upon the previous test, we set up a decay instance and generate a decay event.

```

<Decays: execute tests>+≡
    call test (decays_4, "decays_4", &
        "decay instance", &
        u, results)

<Decays: test declarations>+≡
    public :: decays_4

```

<Decays: tests>+≡

```
subroutine decays_4 (u)
  integer, intent(in) :: u
  type(os_data_t) :: os_data
  class(model_data_t), pointer :: model
  type(process_library_t), target :: lib
  type(string_t) :: prefix, procname2
  class(rng_t), allocatable :: rng
  type(process_stack_t) :: process_stack
  type(process_t), pointer :: process
  type(unstable_config_t), allocatable, target :: unstable
  type(flavor_t) :: flv
  type(unstable_t), allocatable :: instance

  write (u, "(A)")  "* Test output: decays_4"
  write (u, "(A)")  "* Purpose: Create a decay process and evaluate &
    &an instance"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize environment, process, &
    &and decay configuration"
  write (u, "(A)")

  call os_data%init ()

  prefix = "decays_4"
  call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
    scattering=.false., decay=.true., decay_rest_frame = .false.)

  procname2 = prefix // "_d"
  process => process_stack%get_process_ptr (procname2)
  model => process%get_model_ptr ()

  call flv%init (25, model)

  allocate (unstable)
  call unstable%init (flv)
  call unstable%init_decays ([procname2], model)

  call model%set_unstable (25, [procname2])

  call unstable%connect_decay (1, process, model)

  call unstable%compute ()

  allocate (rng_test_t :: rng)

  allocate (instance)
  call instance%init (unstable)
  call instance%import_rng (rng)

  call instance%select_chain ()
  call instance%generate ()
```



```

call instance%write (u)

write (u, *)
call instance%write_process_instances (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call instance%final ()
call process_stack%final ()
call unstable%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_4"

end subroutine decays_4

```

Decay with Parent Process

We define a scattering process $ss \rightarrow ss$ and subsequent decays $s \rightarrow f\bar{f}$.

```

<Decays: execute tests>+≡
    call test (decays_5, "decays_5", &
        "parent process and decay", &
        u, results)

<Decays: test declarations>+≡
    public :: decays_5

<Decays: tests>+≡
    subroutine decays_5 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        class(model_data_t), pointer :: model
        type(process_library_t), target :: lib
        type(string_t) :: prefix, procname1, procname2
        type(process_stack_t) :: process_stack
        type(process_t), pointer :: process
        type(process_instance_t), allocatable, target :: process_instance
        type(decay_root_config_t), target :: decay_root_config
        type(decay_root_t) :: decay_root
        type(decay_chain_t) :: decay_chain

        write (u, "(A)")  "* Test output: decays_5"
        write (u, "(A)")  "* Purpose: Handle a process with subsequent decays"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment and parent process"
        write (u, "(A)")

        call os_data%init ()

        prefix = "decays_5"
        procname1 = prefix // "_p"
        procname2 = prefix // "_d"

```

```

call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
     scattering=.true., decay=.true.)

write (u, "(A)")  "* Initialize decay process"
write (u, "(A)")

process => process_stack%get_process_ptr (procname1)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2])

write (u, "(A)")  "* Initialize decay tree configuration"
write (u, "(A)")

call decay_root_config%connect (process, model, process_stack)
call decay_root_config%compute ()
call decay_root_config%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize decay tree"

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
call process_instance%init_simulation (1)

call decay_root%init (decay_root_config, process_instance)

write (u, "(A)")
write (u, "(A)")  "* Select decay chain"
write (u, "(A)")

call decay_root%set_mci (1)
!!! Not yet implemented; there is only one term anyway:
! call process_instance%select_i_term (decay_root%selected_term)
call decay_root%set_term (1)
call decay_root%select_chain ()

call decay_chain%build (decay_root)

call decay_root%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate event"
write (u, "(A)")

call process_instance%generate_unweighted_event (decay_root%get_mci ())
call process_instance%evaluate_event_data ()

call decay_root%generate ()

call pacify (decay_root)

write (u, "(A)")  "* Process instances"

```

```

write (u, "(A)")

call decay_root%write_process_instances (u)

write (u, "(A)")
write (u, "(A)")  "* Generate decay chain"
write (u, "(A)")

call decay_chain%evaluate ()
call decay_chain%write (u)

write (u, *)
write (u, "(A,ES19.12)")  "chain probability =", &
    decay_chain%get_probability ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call decay_chain%final ()
call decay_root%final ()
call decay_root_config%final ()
call process_instance%final ()
deallocate (process_instance)

call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_5"

end subroutine decays_5

```

Decay as Event Transform

Again, we define a scattering process $ss \rightarrow ss$ and subsequent decays $s \rightarrow f\bar{f}$.

```

⟨Decays: execute tests⟩+≡
    call test (decays_6, "decays_6", &
        "evt_decay object", &
        u, results)

⟨Decays: test declarations⟩+≡
    public :: decays_6

⟨Decays: tests⟩+≡
    subroutine decays_6 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        class(model_data_t), pointer :: model
        type(process_library_t), target :: lib
        type(string_t) :: prefix, procname1, procname2
        type(process_stack_t) :: process_stack
        type(process_t), pointer :: process
        type(process_instance_t), allocatable, target :: process_instance
        type(evt_decay_t), target :: evt_decay
        integer :: factorization_mode

```

```

logical :: keep_correlations

write (u, "(A)")  "* Test output: decays_6"
write (u, "(A)")  "* Purpose: Handle a process with subsequent decays"
write (u, "(A)")

write (u, "(A)")  "* Initialize environment and parent process"
write (u, "(A)")

call os_data%init ()

prefix = "decays_6"
procname1 = prefix // "_p"
procname2 = prefix // "_d"
call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
    scattering=.true., decay=.true.)

write (u, "(A)")  "* Initialize decay process"

process => process_stack%get_process_ptr (procname1)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2])

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
call process_instance%init_simulation (1)

write (u, "(A)")
write (u, "(A)")  "* Initialize decay object"

call evt_decay%connect (process_instance, model, process_stack)

write (u, "(A)")
write (u, "(A)")  "* Generate scattering event"

call process_instance%generate_unweighted_event (1)
call process_instance%evaluate_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Select decay chain and generate event"
write (u, "(A)")

call evt_decay%prepare_new_event (1, 1)
call evt_decay%generate_unweighted ()

factorization_mode = FM_IGNORE_HELICITY
keep_correlations = .false.
call evt_decay%make_particle_set (factorization_mode, keep_correlations)

call evt_decay%write (u, verbose = .true.)

write (u, "(A)")

```

```

write (u, "(A)")  "* Cleanup"

call evt_decay%final ()
call process_instance%final ()
deallocate (process_instance)

call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: decays_6"

end subroutine decays_6

```

32.7 Tau decays

```

⟨tau_decays.f90⟩≡
  ⟨File header⟩

  module tau_decays

    ⟨Use kinds⟩
    use io_units
    use format_utils, only: write_separator
    use sm_qcd
    use model_data
    use models
    use event_transforms

    ⟨Standard module head⟩

    ⟨Tau decays: public⟩

    ⟨Tau decays: types⟩

    contains

    ⟨Tau decays: procedures⟩

  end module tau_decays

```

32.7.1 Tau Decays Event Transform

This is the type for the tau decay event transform.

```

⟨Tau decays: public⟩≡
  public :: evt_tau_decays_t

⟨Tau decays: types⟩≡
  type, extends (evt_t) :: evt_tau_decays_t
    type(model_t), pointer :: model_hadrons => null()
    type(qcd_t) :: qcd
  contains

```

```

    <Tau decays: evt tau decays: TBP>
end type evt_tau_decays_t

```

```

<Tau decays: evt tau decays: TBP>≡
    procedure :: write_name => evt_tau_decays_write_name

<Tau decays: procedures>≡
    subroutine evt_tau_decays_write_name (evt, unit)
        class(evt_tau_decays_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Event transform: tau decays"
    end subroutine evt_tau_decays_write_name

```

Output.

```

<Tau decays: evt tau decays: TBP>+≡
    procedure :: write => evt_tau_decays_write

<Tau decays: procedures>+≡
    subroutine evt_tau_decays_write (evt, unit, verbose, more_verbose, testflag)
        class(evt_tau_decays_t), intent(in) :: evt
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: verbose, more_verbose, testflag
        integer :: u
        u = given_output_unit (unit)
        call write_separator (u, 2)
        call evt%write_name (u)
        call write_separator (u)
        call evt%base_write (u, testflag = testflag, show_set = .false.)
        if (evt%particle_set_exists) &
            call evt%particle_set%write &
                (u, summary = .true., compressed = .true., testflag = testflag)
        call write_separator (u)
    end subroutine evt_tau_decays_write

```

Here we take the particle set from the previous event transform and apply the tau decays. What probability should be given back, the product of branching ratios of the corresponding tau decays?

```

<Tau decays: evt tau decays: TBP>+≡
    procedure :: generate_weighted => evt_tau_decays_generate_weighted

<Tau decays: procedures>+≡
    subroutine evt_tau_decays_generate_weighted (evt, probability)
        class(evt_tau_decays_t), intent(inout) :: evt
        real(default), intent(inout) :: probability
        logical :: valid
        evt%particle_set = evt%previous%particle_set
        !!! To be checked or expanded
        probability = 1
        valid = .true.
        evt%particle_set_exists = valid
    end subroutine evt_tau_decays_generate_weighted

```

The factorization parameters are irrelevant.

```

<Tau decays: evt tau decays: TBP>+≡
    procedure :: make_particle_set => evt_tau_decays_make_particle_set

<Tau decays: procedures>+≡
    subroutine evt_tau_decays_make_particle_set &
        (evt, factorization_mode, keep_correlations, r)
        class(evt_tau_decays_t), intent(inout) :: evt
        integer, intent(in) :: factorization_mode
        logical, intent(in) :: keep_correlations
        real(default), dimension(:), intent(in), optional :: r
        logical :: valid
        !!! to be checked and expanded
        valid = .true.
        evt%particle_set_exists = evt%particle_set_exists .and. valid
    end subroutine evt_tau_decays_make_particle_set

<Tau decays: evt tau decays: TBP>+≡
    procedure :: prepare_new_event => evt_tau_decays_prepare_new_event

<Tau decays: procedures>+≡
    subroutine evt_tau_decays_prepare_new_event (evt, i_mci, i_term)
        class(evt_tau_decays_t), intent(inout) :: evt
        integer, intent(in) :: i_mci, i_term
        call evt%reset ()
    end subroutine evt_tau_decays_prepare_new_event

```

32.8 Shower

We might use matrix elements of LO and NLO to increase the accuracy of the shower in the sense of matching as well as merging.

```

<shower.f90>≡
    <File header>

    module shower

    <Use kinds>
    <Use strings>
    <Use debug>
    use io_units
    use format_utils, only: write_separator
    use system_defs, only: LF
    use os_interface
    use diagnostics
    use lorentz
    use pdf
    use subevents, only: PRT_BEAM_REMNANT, PRT_INCOMING, PRT_OUTGOING

    use shower_base
    use matching_base
    use powheg_matching, only: powheg_matching_t

```

```

use sm_qcd
use model_data
use rng_base

use event_transforms
use models
use hep_common
use process, only: process_t
use instances, only: process_instance_t
use process_stacks

<Standard module head>

<Shower: public>

<Shower: parameters>

<Shower: types>

contains

<Shower: procedures>

end module shower

```

32.8.1 Configuration Parameters

POWHEG_TESTING allows to disable the parton shower for validation and testing of the POWHEG procedure.

```

<Shower: parameters>≡
  logical, parameter :: POWHEG_TESTING = .false.

```

32.8.2 Event Transform

The event transforms can do more than mere showering. Especially, it may reweight showered events to fixed-order matrix elements. The `model_hadrons` is supposed to be the SM variant that contains all hadrons that can be generated in the shower.

```

<Shower: public>≡
  public :: evt_shower_t

<Shower: types>≡
  type, extends (evt_t) :: evt_shower_t
    class(shower_base_t), allocatable :: shower
    class(matching_t), allocatable :: matching
    type(model_t), pointer :: model_hadrons => null ()
    type(qcd_t) :: qcd
    type(pdf_data_t) :: pdf_data
    type(os_data_t) :: os_data
    logical :: is_first_event
  contains
  <Shower: evt shower: TBP>

```



```
end type evt_shower_t
```

```
<Shower: evt shower: TBP>≡
  procedure :: write_name => evt_shower_write_name
```

```
<Shower: procedures>≡
  subroutine evt_shower_write_name (evt, unit)
    class(evt_shower_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: shower"
  end subroutine evt_shower_write_name
```

Output.

```
<Shower: evt shower: TBP>+≡
  procedure :: write => evt_shower_write
```

```
<Shower: procedures>+≡
  subroutine evt_shower_write (evt, unit, verbose, more_verbose, testflag)
    class(evt_shower_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
    integer :: u
    u = given_output_unit (unit)
    call write_separator (u, 2)
    call evt%write_name (u)
    call write_separator (u)
    call evt%base_write (u, testflag = testflag, show_set = .false.)
    if (evt%particle_set_exists) call evt%particle_set%write &
      (u, summary = .true., compressed = .true., testflag = testflag)
    call write_separator (u)
    call evt%shower%settings%write (u)
  end subroutine evt_shower_write
```

```
<Shower: evt shower: TBP>+≡
  procedure :: connect => evt_shower_connect
```

```
<Shower: procedures>+≡
  subroutine evt_shower_connect &
    (evt, process_instance, model, process_stack)
    class(evt_shower_t), intent(inout), target :: evt
    type(process_instance_t), intent(in), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    call evt%base_connect (process_instance, model, process_stack)
    call evt%make_rng (evt%process)
    if (allocated (evt%matching)) then
      call evt%matching%connect (process_instance, model, evt%shower)
    end if
  end subroutine evt_shower_connect
```

Initialize the event transformation. This will be executed once during dispatching. The `model_hadrons` is supposed to be the SM variant that contains all hadrons that may be generated in the shower.

```

<Shower: evt shower: TBP>+≡
  procedure :: init => evt_shower_init

<Shower: procedures>+≡
  subroutine evt_shower_init (evt, model_hadrons, os_data)
    class(evt_shower_t), intent(out) :: evt
    type(model_t), intent(in), target :: model_hadrons
    type(os_data_t), intent(in) :: os_data
    evt%os_data = os_data
    evt%model_hadrons => model_hadrons
    evt%is_first_event = .true.
  end subroutine evt_shower_init

```

Create RNG instances, spawned by the process object.

```

<Shower: evt shower: TBP>+≡
  procedure :: make_rng => evt_shower_make_rng

<Shower: procedures>+≡
  subroutine evt_shower_make_rng (evt, process)
    class(evt_shower_t), intent(inout) :: evt
    type(process_t), intent(inout) :: process
    class(rng_t), allocatable :: rng
    call process%make_rng (rng)
    call evt%shower%import_rng (rng)
    if (allocated (evt%matching)) then
      call process%make_rng (rng)
      call evt%matching%import_rng (rng)
    end if
  end subroutine evt_shower_make_rng

```

Things we want to do for a new event before the whole event transformation chain is evaluated.

```

<Shower: evt shower: TBP>+≡
  procedure :: prepare_new_event => evt_shower_prepare_new_event

<Shower: procedures>+≡
  subroutine evt_shower_prepare_new_event (evt, i_mci, i_term)
    class(evt_shower_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    real(default) :: fac_scale, alpha_s
    fac_scale = evt%process_instance%get_fac_scale (i_term)
    alpha_s = evt%process_instance%get_alpha_s (i_term)
    call evt%reset ()
    call evt%shower%prepare_new_event (fac_scale, alpha_s)
  end subroutine evt_shower_prepare_new_event

```

```

<Shower: evt shower: TBP>+≡
  procedure :: first_event => evt_shower_first_event

```

{Shower: procedures}+≡

```

subroutine evt_shower_first_event (evt)
  class(evt_shower_t), intent(inout) :: evt
  double precision :: pdftest
  if (debug_on) call msg_debug (D_TRANSFORMS, "evt_shower_first_event")
  associate (settings => evt%shower%settings)
    settings%hadron_collision = .false.
    !!! !!! !!! Workaround for PGF90 v16.1
    !!! if (all (evt%particle_set%prt(1:2)%flv%get_pdg_abs () <= 39)) then
    if (evt%particle_set%prt(1)%flv%get_pdg_abs () <= 39 .and. &
        evt%particle_set%prt(2)%flv%get_pdg_abs () <= 39) then
      settings%hadron_collision = .false.
    !!! else if (all (evt%particle_set%prt(1:2)%flv%get_pdg_abs () >= 100)) then
    else if (evt%particle_set%prt(1)%flv%get_pdg_abs () >= 100 .and. &
        evt%particle_set%prt(2)%flv%get_pdg_abs () >= 100) then
      settings%hadron_collision = .true.
    else
      call msg_fatal ("evt_shower didn't recognize beams setup")
    end if
    if (debug_on) call msg_debug (D_TRANSFORMS,"hadron_collision", settings%hadron_collision)
    if (allocated (evt%matching)) then
      evt%matching%is_hadron_collision = settings%hadron_collision
      call evt%matching%first_event ()
    end if
    if (.not. settings%hadron_collision .and. settings%isr_active) then
      call msg_fatal ("?ps_isr_active is only intended for hadron-collisions")
    end if
    if (evt%pdf_data%type == STRF_LHAPDF5) then
      if (settings%isr_active .and. settings%hadron_collision) then
        call GetQ2max (0, pdftest)
        if (pdftest < epsilon (pdftest)) then
          call msg_bug ("ISR QCD shower enabled, but LHAPDF not " // &
              "initialized," // LF // "      aborting simulation")
          return
        end if
      end if
    else if (evt%pdf_data%type == STRF_PDF_BUILTIN .and. &
        settings%method == PS_PYTHIA6) then
      call msg_fatal ("Builtin PDFs cannot be used for PYTHIA showers," &
          // LF // "      aborting simulation")
      return
    end if
  end associate
  evt%is_first_event = .false.
end subroutine evt_shower_first_event

```

Here we take the particle set from the previous event transform (assuming that there is always one) and apply the shower algorithm. The result is stored in the event transform of the current object. We always return a probability of unity as we don't have the analytic weight of the combination of shower, MLM matching and hadronization. A subdivision into multiple event transformations is under construction. Invalid or vetoed events have to be discarded by the caller which is why we mark the particle set as invalid. This procedure directly

takes the (MLM) matching into account.

<Shower: evt shower: TBP>+≡

```
procedure :: generate_weighted => evt_shower_generate_weighted
```

<Shower: procedures>+≡

```
subroutine evt_shower_generate_weighted (evt, probability)
  class(evt_shower_t), intent(inout) :: evt
  real(default), intent(inout) :: probability
  logical :: valid, vetoed
  if (debug_on) call msg_debug (D_TRANSFORMS, "evt_shower_generate_weighted")
  if (signal_is_pending ()) return
  evt%particle_set = evt%previous%particle_set
  valid = .true.; vetoed = .false.
  if (evt%is_first_event) call evt%first_event ()
  call evt%shower%import_particle_set (evt%particle_set)
  if (allocated (evt%matching)) then
    call evt%matching%before_shower (evt%particle_set, vetoed)
    if (msg_level(D_TRANSFORMS) >= DEBUG) then
      if (debug_on) call msg_debug (D_TRANSFORMS, "Matching before generate emissions")
      call evt%matching%write ()
    end if
  end if
  if (.not. (vetoed .or. POWHEG_TESTING)) then
    if (evt%shower%settings%method == PS_PYTHIA6 .or. &
      evt%shower%settings%hadronization_active) then
      call assure_heprup (evt%particle_set)
    end if
    call evt%shower%generate_emissions (valid)
  end if
  probability = 1
  evt%particle_set_exists = valid .and. .not. vetoed
end subroutine evt_shower_generate_weighted
```

Here, we fill the particle set with the partons from the shower. The factorization parameters are irrelevant. We make a sanity check that the initial energy lands either in the outgoing particles or add to the beam remnant.

<Shower: evt shower: TBP>+≡

```
procedure :: make_particle_set => evt_shower_make_particle_set
```

<Shower: procedures>+≡

```
subroutine evt_shower_make_particle_set &
  (evt, factorization_mode, keep_correlations, r)
  class(evt_shower_t), intent(inout) :: evt
  integer, intent(in) :: factorization_mode
  logical, intent(in) :: keep_correlations
  real(default), dimension(:), intent(in), optional :: r
  type(vector4_t) :: sum_vec_in, sum_vec_out, sum_vec_beamrem, &
    sum_vec_beamrem_before
  logical :: vetoed, sane
  if (evt%particle_set_exists) then
    vetoed = .false.
    sum_vec_beamrem_before = sum (evt%particle_set%prt%p, &
      mask=evt%particle_set%prt%get_status () == PRT_BEAM_REMNANT)
    call evt%shower%make_particle_set (evt%particle_set, &
```

```

        evt%model, evt%model_hadrons)
    if (allocated (evt%matching)) then
        call evt%matching%after_shower (evt%particle_set, vetoed)
    end if
    if (debug_active (D_TRANSFORMS)) then
        call msg_debug (D_TRANSFORMS, &
            "Shower: obtained particle set after shower + matching")
        call evt%particle_set%write (summary = .true., compressed = .true.)
    end if
    sum_vec_in = sum (evt%particle_set%prt%p, &
        mask=evt%particle_set%prt%get_status () == PRT_INCOMING)
    sum_vec_out = sum (evt%particle_set%prt%p, &
        mask=evt%particle_set%prt%get_status () == PRT_OUTGOING)
    sum_vec_beamrem = sum (evt%particle_set%prt%p, &
        mask=evt%particle_set%prt%get_status () == PRT_BEAM_REMNANT)
    sum_vec_beamrem = sum_vec_beamrem - sum_vec_beamrem_before
    sane = abs(sum_vec_out%p(0) - sum_vec_in%p(0)) < &
        sum_vec_in%p(0) / 10 .or. &
        abs((sum_vec_out%p(0) + sum_vec_beamrem%p(0)) - sum_vec_in%p(0)) < &
        sum_vec_in%p(0) / 10
    sane = .true.
    evt%particle_set_exists = .not. vetoed .and. sane
end if
end subroutine evt_shower_make_particle_set

```

<Shower: evt shower: TBP>+≡

```

    procedure :: contains_powheg_matching => evt_shower_contains_powheg_matching

```

<Shower: procedures>+≡

```

    function evt_shower_contains_powheg_matching (evt) result (val)
        logical :: val
        class(evt_shower_t), intent(in) :: evt
        val = .false.
        if (allocated (evt%matching)) &
            val = evt%matching%get_method () == "POWHEG"
    end function evt_shower_contains_powheg_matching

```

<Shower: evt shower: TBP>+≡

```

    procedure :: disable_powheg_matching => evt_shower_disable_powheg_matching

```

<Shower: procedures>+≡

```

    subroutine evt_shower_disable_powheg_matching (evt)
        class(evt_shower_t), intent(inout) :: evt
        select type (matching => evt%matching)
            type is (powheg_matching_t)
                matching%active = .false.
        class default
            call msg_fatal ("Trying to disable powheg but no powheg matching is allocated!")
        end select
    end subroutine evt_shower_disable_powheg_matching

```

<Shower: evt shower: TBP>+≡

```

    procedure :: enable_powheg_matching => evt_shower_enable_powheg_matching

```

```

<Shower: procedures>+≡
  subroutine evt_shower_enable_powheg_matching (evt)
    class(evt_shower_t), intent(inout) :: evt
    select type (matching => evt%matching)
      type is (powheg_matching_t)
        matching%active = .true.
      class default
        call msg_fatal ("Trying to enable powheg but no powheg matching is allocated!")
      end select
    end subroutine evt_shower_enable_powheg_matching

<Shower: evt shower: TBP>+≡
  procedure :: final => evt_shower_final

<Shower: procedures>+≡
  subroutine evt_shower_final (evt)
    class(evt_shower_t), intent(inout) :: evt
    call evt%base_final ()
    if (allocated (evt%matching)) call evt%matching%final ()
  end subroutine evt_shower_final

```

32.8.3 Unit tests

Test module, followed by the corresponding implementation module.

```

<shower_ut.f90>≡
  <File header>

  module shower_ut
    use unit_tests
    use shower_uti

    <Standard module head>

    <Shower: public test>

    contains

    <Shower: test driver>

  end module shower_ut

<shower_uti.f90>≡
  <File header>

  module shower_uti

    <Use kinds>
    <Use strings>
    use format_utils, only: write_separator
    use os_interface
    use sm_qcd
    use physics_defs, only: BORN
    use model_data

```

```

use models
use state_matrices, only: FM_IGNORE_HELICITY
use process_libraries
use rng_base
use rng_tao
use dispatch_rng, only: dispatch_rng_factory_fallback
use mci_base
use mci_midpoint
use phs_base
use phs_single
use prc_core_def, only: prc_core_def_t
use prc_core
use prc_omega
use variables
use event_transforms
use tauola_interface !NODEP!

use process, only: process_t
use instances, only: process_instance_t

use pdf
use shower_base
use shower_core

use dispatch_rng_ut, only: dispatch_rng_factory_tao

use shower

```

⟨Standard module head⟩

⟨Shower: test declarations⟩

contains

⟨Shower: tests⟩

end module shower_ut

API: driver for the unit tests below.

```

⟨Shower: public test⟩≡
  public :: shower_test

⟨Shower: test driver⟩≡
  subroutine shower_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    ⟨Shower: execute tests⟩
  end subroutine shower_test

```

Testbed

This sequence sets up a two-jet process, ready for generating events.

⟨Shower: tests⟩≡

```

    <setup testbed>
    <setup testbed>≡
    subroutine setup_testbed &
        (prefix, os_data, lib, model_list, process, process_instance)
        type(string_t), intent(in) :: prefix
        type(os_data_t), intent(out) :: os_data
        type(process_library_t), intent(out), target :: lib
        type(model_list_t), intent(out) :: model_list
        type(model_t), pointer :: model
        type(model_t), pointer :: model_tmp
        type(process_t), target, intent(out) :: process
        type(process_instance_t), target, intent(out) :: process_instance
        type(var_list_t), pointer :: model_vars
        type(string_t) :: model_name, libname, procname
        type(process_def_entry_t), pointer :: entry
        type(string_t), dimension(:), allocatable :: prt_in, prt_out
        class(prc_core_t), allocatable :: core_template
        class(phs_config_t), allocatable :: phs_config_template
        real(default) :: sqrts

        model_name = "SM"
        libname = prefix // "_lib"
        procname = prefix // "p"

        call os_data%init ()
        dispatch_rng_factory_fallback => dispatch_rng_factory_tao
        allocate (model_tmp)
        call model_list%read_model (model_name, model_name // ".mdl", &
            os_data, model_tmp)
        model_vars => model_tmp%get_var_list_ptr ()
        call model_vars%set_real (var_str ("me"), 0._default, &
            is_known = .true.)
        model => model_tmp

        call lib%init (libname)

        allocate (prt_in (2), source = [var_str ("e-"), var_str ("e+")])
        allocate (prt_out (2), source = [var_str ("d"), var_str ("dbar")])

        allocate (entry)
        call entry%init (procname, model, n_in = 2, n_components = 1)
        call omega_make_process_component (entry, 1, &
            model_name, prt_in, prt_out, &
            report_progress=.true.)
        call lib%append (entry)

        call lib%configure (os_data)
        call lib%write_makefile (os_data, force = .true., verbose = .false.)
        call lib%clean (os_data, distclean = .false.)
        call lib%write_driver (force = .true.)
        call lib%load (os_data)

        call process%init (procname, lib, os_data, model)

```



```

allocate (prc_omega_t :: core_template)
allocate (phs_single_config_t :: phs_config_template)

call process%setup_cores (dispatch_core_omega_test)

call process%init_components (phs_config_template)

sqrt_s = 1000
call process%setup_beams_sqrt_s (sqrt_s, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_test_midpoint)
call process%setup_terms ()

call process_instance%init (process)
call process_instance%integrate (1, 1, 1000)
call process_instance%final_integration (1)

call process_instance%setup_event_data (i_core = 1)
call process_instance%init_simulation (1)
call process_instance%generate_weighted_event (1)
call process_instance%evaluate_event_data ()

end subroutine setup_testbed

```

A minimal dispatcher version that allocates the core object for testing.

```

<setup testbed>+≡
subroutine dispatch_core_omega_test (core, core_def, model, &
    helicity_selection, qcd, use_color_factors, has_beam_pol)
class(prc_core_t), allocatable, intent(inout) :: core
class(prc_core_def_t), intent(in) :: core_def
class(model_data_t), intent(in), target, optional :: model
type(helicity_selection_t), intent(in), optional :: helicity_selection
type(qcd_t), intent(in), optional :: qcd
logical, intent(in), optional :: use_color_factors
logical, intent(in), optional :: has_beam_pol
allocate (prc_omega_t :: core)
select type (core)
type is (prc_omega_t)
    call core%set_parameters (model)
end select
end subroutine dispatch_core_omega_test

```

MCI record prepared for midpoint integrator.

```

<setup testbed>+≡
subroutine dispatch_mci_test_midpoint (mci, var_list, process_id, is_nlo)
use variables, only: var_list_t
class(mci_t), allocatable, intent(out) :: mci
type(var_list_t), intent(in) :: var_list
type(string_t), intent(in) :: process_id
logical, intent(in), optional :: is_nlo
allocate (mci_midpoint_t :: mci)
end subroutine dispatch_mci_test_midpoint

```

Trivial Test

We generate a two-jet event and shower it using default settings, i.e. in disabled mode.

```
<Shower: execute tests>≡
    call test (shower_1, "shower_1", &
               "disabled shower", &
               u, results)

<Shower: test declarations>≡
    public :: shower_1

<Shower: tests>+≡
    subroutine shower_1 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(process_library_t), target :: lib
        type(model_list_t) :: model_list
        class(model_data_t), pointer :: model
        type(model_t), pointer :: model_hadrons
        type(process_t), target :: process
        type(process_instance_t), target :: process_instance
        type(pdf_data_t) :: pdf_data
        integer :: factorization_mode
        logical :: keep_correlations
        class(evt_t), allocatable, target :: evt_trivial
        class(evt_t), allocatable, target :: evt_shower
        type(shower_settings_t) :: settings
        type(taudec_settings_t) :: taudec_settings

        write (u, "(A)")  "* Test output: shower_1"
        write (u, "(A)")  "* Purpose: Two-jet event with disabled shower"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"), &
             os_data, model_hadrons)
        call setup_testbed (var_str ("shower_1"), &
                             os_data, lib, model_list, process, process_instance)

        write (u, "(A)")  "* Set up trivial transform"
        write (u, "(A)")

        allocate (evt_trivial_t :: evt_trivial)
        model => process%get_model_ptr ()
        call evt_trivial%connect (process_instance, model)
        call evt_trivial%prepare_new_event (1, 1)
        call evt_trivial%generate_unweighted ()

        factorization_mode = FM_IGNORE_HELICITY
```

```

keep_correlations = .false.
call evt_trivial%make_particle_set (factorization_mode, keep_correlations)

select type (evt_trivial)
type is (evt_trivial_t)
  call evt_trivial%write (u)
  call write_separator (u, 2)
end select

write (u, "(A)")
write (u, "(A)")  "* Set up shower event transform"
write (u, "(A)")

allocate (evt_shower_t :: evt_shower)
select type (evt_shower)
type is (evt_shower_t)
  call evt_shower%init (model_hadrons, os_data)
  allocate (shower_t :: evt_shower%shower)
  call evt_shower%shower%init (settings, taudec_settings, pdf_data, os_data)
  call evt_shower%connect (process_instance, model)
end select

evt_trivial%next => evt_shower
evt_shower%previous => evt_trivial

call evt_shower%prepare_new_event (1, 1)
call evt_shower%generate_unweighted ()
call evt_shower%make_particle_set (factorization_mode, keep_correlations)

select type (evt_shower)
type is (evt_shower_t)
  call evt_shower%write (u)
  call write_separator (u, 2)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_shower%final ()
call evt_trivial%final ()
call process_instance%final ()
call process%final ()
call lib%final ()
call model_hadrons%final ()
deallocate (model_hadrons)
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: shower_1"

end subroutine shower_1

```

FSR Shower

We generate a two-jet event and shower it with the Whizard FSR shower.

```
<Shower: execute tests>+≡
    call test (shower_2, "shower_2", &
               "final-state shower", &
               u, results)

<Shower: test declarations>+≡
    public :: shower_2

<Shower: tests>+≡
    subroutine shower_2 (u)
        integer, intent(in) :: u
        type(os_data_t) :: os_data
        type(process_library_t), target :: lib
        type(model_list_t) :: model_list
        type(model_t), pointer :: model_hadrons
        class(model_data_t), pointer :: model
        type(process_t), target :: process
        type(process_instance_t), target :: process_instance
        integer :: factorization_mode
        logical :: keep_correlations
        type(pdf_data_t) :: pdf_data
        class(evt_t), allocatable, target :: evt_trivial
        class(evt_t), allocatable, target :: evt_shower
        type(shower_settings_t) :: settings
        type(taudec_settings_t) :: taudec_settings

        write (u, "(A)")  "* Test output: shower_2"
        write (u, "(A)")  "*   Purpose: Two-jet event with FSR shower"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize environment"
        write (u, "(A)")

        call syntax_model_file_init ()
        call os_data%init ()
        call model_list%read_model &
            (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"), &
             os_data, model_hadrons)
        call setup_testbed (var_str ("shower_2"), &
                            os_data, lib, model_list, process, process_instance)
        model => process%get_model_ptr ()

        write (u, "(A)")  "* Set up trivial transform"
        write (u, "(A)")

        allocate (evt_trivial_t :: evt_trivial)
        call evt_trivial%connect (process_instance, model)
        call evt_trivial%prepare_new_event (1, 1)
        call evt_trivial%generate_unweighted ()

        factorization_mode = FM_IGNORE_HELICITY
        keep_correlations = .false.
```

```

call evt_trivial%make_particle_set (factorization_mode, keep_correlations)

select type (evt_trivial)
type is (evt_trivial_t)
    call evt_trivial%write (u)
    call write_separator (u, 2)
end select

write (u, "(A)")
write (u, "(A)")  "* Set up shower event transform"
write (u, "(A)")

settings%fsr_active = .true.

allocate (evt_shower_t :: evt_shower)
select type (evt_shower)
type is (evt_shower_t)
    call evt_shower%init (model_hadrons, os_data)
    allocate (shower_t :: evt_shower%shower)
    call evt_shower%shower%init (settings, taudec_settings, pdf_data, os_data)
    call evt_shower%connect (process_instance, model)
end select

evt_trivial%next => evt_shower
evt_shower%previous => evt_trivial

call evt_shower%prepare_new_event (1, 1)
call evt_shower%generate_unweighted ()
call evt_shower%make_particle_set (factorization_mode, keep_correlations)

select type (evt_shower)
type is (evt_shower_t)
    call evt_shower%write (u, testflag = .true.)
    call write_separator (u, 2)
end select

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call evt_shower%final ()
call evt_trivial%final ()
call process_instance%final ()
call process%final ()
call lib%final ()
call model_hadrons%final ()
deallocate (model_hadrons)
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: shower_2"

end subroutine shower_2

```

32.9 Fixed Order NLO Events

This section deals with the generation of weighted event samples which take into account next-to-leading order corrections. An approach generating unweighted events is not possible here, because negative weights might occur due to subtraction. Note that the events produced this way are not physical in the sense that they will not keep NLO-accuracy when interfaced to a parton shower. They are rather useful for theoretical consistency checks and a fast estimate of NLO effects.

We generate NLO events in the following way: First, the integration is carried out using the complete divergence-subtracted NLO matrix element. In the subsequent simulation, N -particle kinematics are generated using $\mathcal{B} + \mathcal{V} + \mathcal{C}$ as weight. After that, the program loops over all singular regions and for each of them generates an event with $N + 1$ -particle kinematics. The weight for those events corresponds to the real matrix element \mathcal{R}^α evaluated at the α -region's emitter's phase space point, multiplied with S_α . This procedure is implemented using the `evt_nlo` transform.

```

<evt_nlo.f90>≡
  <File header>

  module evt_nlo

    <Use kinds>
    <Use strings>
    <Use debug>
    use io_units, only: given_output_unit
    use constants
    use lorentz
    use phs_points, only: phs_point_t
    use phs_points, only: assignment(=), operator(*), size
    use diagnostics
    use numeric_utils, only: nearly_equal
    use format_utils, only: write_separator
    use physics_defs, only: BORN, NLO_REAL
    use sm_qcd
    use model_data
    use interactions, only: interaction_t
    use particles
    use instances, only: process_instance_t
    use pcm, only: pcm_nlo_t, pcm_nlo_workspace_t
    use process_stacks
    use event_transforms
    use prc_core, only: prc_core_t
    use prc_external, only: prc_external_t
    use quantum_numbers, only: quantum_numbers_t

    use phs_fks, only: phs_fks_t, phs_fks_generator_t
    use phs_fks, only: phs_identifier_t, phs_point_set_t
    use resonances, only: resonance_contributors_t
    use fks_regions, only: region_data_t

    <Standard module head>

```

```

    <Evt Nlo: public>

    <Evt Nlo: public parameters>

    <Evt Nlo: types>

contains

    <Evt Nlo: procedures>

end module evt_nlo

<Evt Nlo: types>≡
    type :: nlo_event_deps_t
        logical :: lab_is_cm = .true.
        type(phs_point_set_t) :: p_born_cms
        type(phs_point_set_t) :: p_born_lab
        type(phs_point_set_t) :: p_real_cms
        type(phs_point_set_t) :: p_real_lab
        type(resonance_contributors_t), dimension(:), allocatable :: contributors
        type(phs_identifier_t), dimension(:), allocatable :: phs_identifiers
        integer, dimension(:), allocatable :: alr_to_i_con
        integer :: n_phs = 0
    end type nlo_event_deps_t

This event transformation is for the generation of fixed-order NLO events. It
takes an event with Born kinematics and creates  $N_\alpha + 1$  modified weighted
events. The first one has Born kinematics and its weight is the sum of Born,
virtual, subtraction and, if present, also DGLAP matrix elements. The other
 $N_\alpha$  events have a weight which is equal to the real matrix element, evaluated
with the phase space corresponding to the emitter of the  $\alpha$ -region.

As the NLO event transforms have different kinematics, they also differ
in their particle_sets. The NLO event_t object carries a single pointer to a
particle_set. To avoid interference between the different NLO particle_sets,
we save the particle_set of the current  $\alpha$ -region in the array particle_set_nlo.
Otherwise it would be unretrievable if the usual particle set of the event object
was used.

<Evt Nlo: public parameters>≡
    integer, parameter, public :: EVT_NLO_UNDEFINED = 0
    integer, parameter, public :: EVT_NLO_SEPARATE_BORNLIKE = 1
    integer, parameter, public :: EVT_NLO_SEPARATE_REAL = 2
    integer, parameter, public :: EVT_NLO_COMBINED = 3

<Evt Nlo: public>≡
    public :: evt_nlo_t

<Evt Nlo: types>+≡
    type, extends (evt_t) :: evt_nlo_t
        type(phs_fks_generator_t) :: phs_fks_generator
        real(default) :: sqme_rad = zero
        integer :: i_evaluation = 0
        type(particle_set_t), dimension(:), allocatable :: particle_set_nlo

```

```

type(qcd_t) :: qcd
type(nlo_event_deps_t) :: event_deps
integer :: mode = EVT_NLO_UNDEFINED
integer, dimension(:), allocatable :: &
    i_evaluation_to_i_phs, i_evaluation_to_emitter, &
    i_evaluation_to_i_term
logical :: keep_failed_events = .false.
integer :: selected_i_flv = 0
contains
<Evt Nlo: evt nlo: TBP>
end type evt_nlo_t

```

```

<Evt Nlo: evt nlo: TBP>≡
procedure :: write_name => evt_nlo_write_name

```

```

<Evt Nlo: procedures>≡
subroutine evt_nlo_write_name (evt, unit)
    class(evt_nlo_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event transform: NLO"
end subroutine evt_nlo_write_name

```

```

<Evt Nlo: evt nlo: TBP>+≡
procedure :: write => evt_nlo_write

```

```

<Evt Nlo: procedures>+≡
subroutine evt_nlo_write (evt, unit, verbose, more_verbose, testflag)
    class(evt_nlo_t), intent(in) :: evt
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose, more_verbose, testflag
    integer :: u, i
    u = given_output_unit (unit)
    call write_separator (u, 2)
    call evt%write_name (u)
    call write_separator (u)
    call evt%base_write (u, testflag = testflag, show_set = .true.)
    write (u, '(A,ES16.9)') "sqme_rad = ", evt%sqme_rad
    write (u, "(3x,A,I0)") "i_evaluation = ", evt%i_evaluation
    call write_separator (u)
    write (u, "(1x,A)") "Radiated particle sets:"
    do i = 1, size (evt%particle_set_nlo)
        call evt%particle_set_nlo(i)%write (u, testflag = testflag)
        call write_separator (u)
    end do
end subroutine evt_nlo_write

```

Connects the event transform to the process. Here also the phase space is set up by making `real_kinematics` point to the corresponding object in the `pcm.instance`.

```

<Evt Nlo: evt nlo: TBP>+≡
procedure :: connect => evt_nlo_connect

```


(Evt Nlo: procedures) +=

```

subroutine evt_nlo_connect (evt, process_instance, model, process_stack)
  class(evt_nlo_t), intent(inout), target :: evt
  type(process_instance_t), intent(in), target :: process_instance
  class(model_data_t), intent(in), target :: model
  type(process_stack_t), intent(in), optional :: process_stack
  if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_connect")
  call evt%base_connect (process_instance, model, process_stack)
  select type (pcm_work => process_instance%pcm_work)
  class is (pcm_nlo_workspace_t)
    select type (pcm => process_instance%pcm)
    type is (pcm_nlo_t)
      call pcm%setup_phs_generator (pcm_work, evt%phs_fks_generator, &
        process_instance%get_sqrts ())
      call evt%set_i_evaluation_mappings (pcm%region_data, &
        pcm_work%real_kinematics%alr_to_i_phs)
    end select
  end select
  call evt%set_mode (process_instance)
  call evt%setup_general_event_kinematics (process_instance)
  if (evt%mode > EVT_NLO_SEPARATE_BORNLIKE) &
    call evt%setup_real_event_kinematics (process_instance)
  if (debug_on) call msg_debug2 (D_TRANSFORMS, "evt_nlo_connect: success")
end subroutine evt_nlo_connect

```

(Evt Nlo: evt_nlo: TBP) +=

```

procedure :: set_i_evaluation_mappings => evt_nlo_set_i_evaluation_mappings

```

(Evt Nlo: procedures) +=

```

subroutine evt_nlo_set_i_evaluation_mappings (evt, reg_data, alr_to_i_phs)
  class(evt_nlo_t), intent(inout) :: evt
  type(region_data_t), intent(in) :: reg_data
  integer, intent(in), dimension(:) :: alr_to_i_phs
  integer :: n_phs, alr
  integer :: i_evaluation, i_phs, emitter
  logical :: checked
  type :: registered_triple_t
    integer, dimension(2) :: phs_em
    type(registered_triple_t), pointer :: next => null ()
  end type registered_triple_t
  type(registered_triple_t), allocatable, target :: check_list
  i_evaluation = 1
  n_phs = reg_data%n_phs
  allocate (evt%i_evaluation_to_i_phs (n_phs), source = 0)
  allocate (evt%i_evaluation_to_emitter (n_phs), source = -1)
  allocate (evt%i_evaluation_to_i_term (0 : n_phs), source = 0)
  do alr = 1, reg_data%n_regions
    i_phs = alr_to_i_phs (alr)
    emitter = reg_data%regions(alr)%emitter
    call search_check_list (checked)
    if (.not. checked) then
      evt%i_evaluation_to_i_phs (i_evaluation) = i_phs
      evt%i_evaluation_to_emitter (i_evaluation) = emitter
      i_evaluation = i_evaluation + 1
    end if
  end do

```

```

        end if
    end do
    call fill_i_evaluation_to_i_term ()
    if (.not. (all (evt%i_evaluation_to_i_phs > 0) &
        .and. all (evt%i_evaluation_to_emitter > -1))) then
        call msg_fatal ("evt_nlo: Inconsistent mappings!")
    else
        if (debug2_active (D_TRANSFORMS)) then
            print *, 'evt_nlo Mappings, i_evaluation -> '
            print *, 'i_phs: ', evt%i_evaluation_to_i_phs
            print *, 'emitter: ', evt%i_evaluation_to_emitter
        end if
    end if
contains
    subroutine fill_i_evaluation_to_i_term ()
        integer :: i_term, i_evaluation, term_emitter
        !!! First find subtraction component
        i_evaluation = 1
        do i_term = 1, evt%process%get_n_terms ()
            if (evt%process_instance%term(i_term)%nlo_type /= NLO_REAL) cycle
            term_emitter = evt%process_instance%kin(i_term)%emitter
            if (term_emitter < 0) then
                evt%i_evaluation_to_i_term (0) = i_term
            else if (evt%i_evaluation_to_emitter(i_evaluation) == term_emitter) then
                evt%i_evaluation_to_i_term (i_evaluation) = i_term
                i_evaluation = i_evaluation + 1
            end if
        end do
    end subroutine fill_i_evaluation_to_i_term

    subroutine search_check_list (found)
        logical, intent(out) :: found
        type(registered_triple_t), pointer :: current_triple => null ()
        if (allocated (check_list)) then
            current_triple => check_list
            do
                if (all (current_triple%phs_em == [i_phs, emitter])) then
                    found = .true.
                    exit
                end if
                if (.not. associated (current_triple%next)) then
                    allocate (current_triple%next)
                    current_triple%next%phs_em = [i_phs, emitter]
                    found = .false.
                    exit
                else
                    current_triple => current_triple%next
                end if
            end do
        else
            allocate (check_list)
            check_list%phs_em = [i_phs, emitter]
            found = .false.
        end if
    end if

```

```

        end subroutine search_check_list
    end subroutine evt_nlo_set_i_evaluation_mappings

    <Evt Nlo: evt nlo: TBP>+=
        procedure :: get_i_phs => evt_nlo_get_i_phs
    <Evt Nlo: procedures>+=
        function evt_nlo_get_i_phs (evt) result (i_phs)
            integer :: i_phs
            class(evt_nlo_t), intent(in) :: evt
            i_phs = evt%i_evaluation_to_i_phs (evt%i_evaluation)
        end function evt_nlo_get_i_phs

    <Evt Nlo: evt nlo: TBP>+=
        procedure :: get_emitter => evt_nlo_get_emitter
    <Evt Nlo: procedures>+=
        function evt_nlo_get_emitter (evt) result (emitter)
            integer :: emitter
            class(evt_nlo_t), intent(in) :: evt
            emitter = evt%i_evaluation_to_emitter (evt%i_evaluation)
        end function evt_nlo_get_emitter

    <Evt Nlo: evt nlo: TBP>+=
        procedure :: get_i_term => evt_nlo_get_i_term
    <Evt Nlo: procedures>+=
        function evt_nlo_get_i_term (evt) result (i_term)
            integer :: i_term
            class(evt_nlo_t), intent(in) :: evt
            if (evt%mode >= EVT_NLO_SEPARATE_REAL) then
                i_term = evt%i_evaluation_to_i_term (evt%i_evaluation)
            else
                i_term = evt%process_instance%get_first_active_i_term ()
            end if
        end function evt_nlo_get_i_term

```

The event transform has a variable which counts the number of times it has already been called for one generation point. If this variable, `i_evaluation`, is zero, this means that `evt_nlo_generate_weighted` is called for the first time, so that the generation of an N -particle event is required. In all other cases, emission events are generated.

During a separate integration of the real component, the first event of each event group will become the counterevent. In this case, we return the sum of all subtraction matrix elements.

During a combined integration, the first event will be a combination of all Born-like events. To get the sum of their matrix elements, we subtract the sum of all real emissions from the sum of all matrix elements as the real contribution is the only non-Born contribution.

Note that the argument named `probability`, the use of the routine `generate_weighted` and the procedure we use to generate NLO events via an event transformation is an abuse of the interface which should be refactored.

```

    <Evt Nlo: evt nlo: TBP>+=

```

```

procedure :: generate_weighted => evt_nlo_generate_weighted
<Evt Nlo: procedures>+=
subroutine evt_nlo_generate_weighted (evt, probability)
  class(evt_nlo_t), intent(inout) :: evt
  real(default), intent(inout) :: probability
  real(default) :: sqme
  call print_debug_info ()
  sqme = probability
  if (evt%mode > EVT_NLO_SEPARATE_BORNLIKE) then
    if (evt%i_evaluation == 0) then
      call evt%reset_phs_identifiers ()
      call evt%evaluate_real_kinematics ()
      if (evt%mode == EVT_NLO_SEPARATE_REAL) then
        sqme = evt%compute_subtraction_sqmes ()
      else
        sqme = sqme - evt%compute_all_sqme_rad ()
      end if
    else
      call evt%compute_real ()
      sqme = evt%sqme_rad
    end if
  end if
  probability = sqme
  if (debug_on) call msg_debug (D_TRANSFORMS, "probability (after)", probability)
contains
  function status_code_to_string (mode) result (smode)
    type(string_t) :: smode
    integer, intent(in) :: mode
    select case (mode)
    case (EVT_NLO_UNDEFINED)
      smode = var_str ("Undefined")
    case (EVT_NLO_SEPARATE_BORNLIKE)
      smode = var_str ("Born-like")
    case (EVT_NLO_SEPARATE_REAL)
      smode = var_str ("Real")
    case (EVT_NLO_COMBINED)
      smode = var_str ("Combined")
    end select
  end function status_code_to_string

  subroutine print_debug_info ()
    if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_generate_weighted")
    if (debug_on) call msg_debug (D_TRANSFORMS, char ("mode: " // status_code_to_string (evt%mode)))
    if (debug_on) call msg_debug (D_TRANSFORMS, "probability (before)", probability)
    if (debug_on) call msg_debug (D_TRANSFORMS, "evt%i_evaluation", evt%i_evaluation)
    if (debug2_active (D_TRANSFORMS)) then
      if (evt%mode > EVT_NLO_SEPARATE_BORNLIKE) then
        if (evt%i_evaluation == 0) then
          print *, 'Evaluate subtraction component'
        else
          print *, 'Evaluate radiation component'
        end if
      end if
    end if
  end subroutine print_debug_info
end

```

```

    end subroutine print_debug_info
end subroutine evt_nlo_generate_weighted

```

```

(Evt Nlo: evt_nlo: TBP)+≡
  procedure :: reset_phs_identifiers => evt_nlo_reset_phs_identifiers

(Evt Nlo: procedures)+≡
  subroutine evt_nlo_reset_phs_identifiers (evt)
    class(evt_nlo_t), intent(inout) :: evt
    evt%event_deps%phs_identifiers%evaluated = .false.
  end subroutine evt_nlo_reset_phs_identifiers

```

The routine `make_factorized_particle_set` will setup the subevent momenta from the `connected%matrix`. Its initial state momenta correspond to the Born process without IS splitting and thus need to be updated with the real momenta from the `int_hard` to get correct momenta in the events with real radiation.

Ideally the `int_hard` and the `connected` would be setup with correct `source_links` to real momenta so that we would not need to replace momenta of the `connected` here.

The parameter `n_in` from the `int_matrix` is still 0 as it has been shifted to `n_vir`. We thus take `n_in` from the `particle_set`.

```

(Evt Nlo: evt_nlo: TBP)+≡
  procedure :: connected_set_real_IS_momenta => evt_nlo_connected_set_real_IS_momenta

(Evt Nlo: procedures)+≡
  subroutine evt_nlo_connected_set_real_IS_momenta (evt)
    class(evt_nlo_t), intent(inout) :: evt
    type(vector4_t) :: p_hard, p_beam, p_remn
    type(interaction_t), pointer :: int_matrix
    integer :: i, i_term, n_in, i_in_beam, i_in_hard, i_in_remn
    i_term = evt%get_i_term ()
    int_matrix => evt%process_instance%get_matrix_int_ptr (i_term)
    n_in = evt%particle_set%get_n_in ()
    do i = 1, n_in
      i_in_beam = i
      i_in_hard = n_in + i
      i_in_remn = 2 * n_in + i
      p_hard = evt%process_instance%term(i_term)%int_hard%get_momentum (i)
      p_beam = int_matrix%get_momentum (i_in_beam)
      p_remn = p_beam - p_hard
      call int_matrix%set_momentum (p_hard , i_in_hard)
      call int_matrix%set_momentum (p_remn , i_in_remn)
    end do
  end subroutine evt_nlo_connected_set_real_IS_momenta

```

```

(Evt Nlo: evt_nlo: TBP)+≡
  procedure :: make_particle_set => evt_nlo_make_particle_set

(Evt Nlo: procedures)+≡
  subroutine evt_nlo_make_particle_set &
    (evt, factorization_mode, keep_correlations, r)
    class(evt_nlo_t), intent(inout) :: evt
    integer, intent(in) :: factorization_mode

```

```

logical, intent(in) :: keep_correlations
real(default), dimension(:), intent(in), optional :: r
if (evt%mode >= EVT_NLO_SEPARATE_BORNLIKE) then
    call make_factorized_particle_set (evt, factorization_mode, &
        keep_correlations, r, evt%get_i_term (), &
        evt%get_selected_quantum_numbers (evt%selected_i_flv))
else
    call make_factorized_particle_set (evt, factorization_mode, &
        keep_correlations, r)
end if
end subroutine evt_nlo_make_particle_set

```

(Evt Nlo: evt nlo: TBP)+≡

```

procedure :: evaluate_real_kinematics => evt_nlo_evaluate_real_kinematics

```

(Evt Nlo: procedures)+≡

```

subroutine evt_nlo_evaluate_real_kinematics (evt)
    class(evt_nlo_t), intent(inout) :: evt
    integer :: alr, i_phs, i_con, emitter
    real(default), dimension(3) :: x_rad
    logical :: use_contributors
    integer :: n_regions
    integer :: i_term
    type(vector4_t), dimension(:), allocatable :: p_real

    select type (pcm_work => evt%process_instance%pcm_work)
    class is (pcm_nlo_workspace_t)
        x_rad = pcm_work%real_kinematics%x_rad
        associate (event_deps => evt%event_deps)
            i_term = evt%get_i_term ()
            event_deps%p_born_lab%phs_point(1) = &
                evt%process_instance%term(i_term)%p_seed
            event_deps%p_born_cms%phs_point(1) &
                = evt%boost_to_cms (event_deps%p_born_lab%phs_point(1))
            call evt%phs_fks_generator%set_sqrts_hat &
                (event_deps%p_born_cms%get_energy (1, 1))
            use_contributors = allocated (event_deps%contributors)
            select type (pcm => evt%process_instance%pcm)
            type is (pcm_nlo_t)
                n_regions = pcm%region_data%n_regions
            end select
            do alr = 1, n_regions
                i_phs = pcm_work%real_kinematics%alr_to_i_phs(alr)
                if (event_deps%phs_identifiers(i_phs)%evaluated) cycle
                emitter = event_deps%phs_identifiers(i_phs)%emitter
                associate (generator => evt%phs_fks_generator)
                    if (emitter <= evt%process%get_n_in ()) then
                        call generator%prepare_generation (x_rad, i_phs, emitter, &
                            event_deps%p_born_cms%phs_point(1)%get (), &
                            event_deps%phs_identifiers)
                        ! TODO wk 19-02-28: intent of p_real (also below)?
                        p_real = event_deps%p_real_lab%phs_point(i_phs)
                        call generator%generate_isr (i_phs, &
                            event_deps%p_born_lab%phs_point(1)%get (), &

```

```

        p_real)
    event_deps%p_real_lab%phs_point(i_phs) = p_real
    event_deps%p_real_cms%phs_point(i_phs) &
        = evt%boost_to_cms (event_deps%p_real_lab%phs_point(i_phs))
else
    if (use_contributors) then
        i_con = event_deps%alr_to_i_con(alr)
        call generator%prepare_generation (x_rad, i_phs, emitter, &
            event_deps%p_born_cms%phs_point(1)%get (), &
            event_deps%phs_identifiers, event_deps%contributors, i_con)
        p_real = event_deps%p_real_cms%phs_point(i_phs)
        call generator%generate_fsr (emitter, i_phs, i_con, &
            event_deps%p_born_cms%phs_point(1)%get (), &
            p_real)
        event_deps%p_real_cms%phs_point(i_phs) = p_real
    else
        call generator%prepare_generation (x_rad, i_phs, emitter, &
            event_deps%p_born_cms%phs_point(1)%get (), &
            event_deps%phs_identifiers)
        p_real = event_deps%p_real_cms%phs_point(i_phs)
        call generator%generate_fsr (emitter, i_phs, &
            event_deps%p_born_cms%phs_point(1)%get (), &
            p_real)
        event_deps%p_real_cms%phs_point(i_phs) = p_real
    end if
    event_deps%p_real_lab%phs_point(i_phs) &
        = evt%boost_to_lab (event_deps%p_real_cms%phs_point(i_phs))
end if
end associate
call pcm_work%set_momenta &
    (event_deps%p_born_lab%phs_point(1)%get (), &
    event_deps%p_real_lab%phs_point(i_phs)%get (), &
    i_phs)
call pcm_work%set_momenta &
    (event_deps%p_born_cms%phs_point(1)%get (), &
    event_deps%p_real_cms%phs_point(i_phs)%get (), &
    i_phs, cms = .true.)
event_deps%phs_identifiers(i_phs)%evaluated = .true.
end do
end associate
end select
end subroutine evt_nlo_evaluate_real_kinematics

```

This routine calls the evaluation of the singular regions only for the subtraction terms.

(Evt Nlo: evt nlo: TBP)+≡

```
procedure :: compute_subtraction_sqmes => evt_nlo_compute_subtraction_sqmes
```

(Evt Nlo: procedures)+≡

```

function evt_nlo_compute_subtraction_sqmes (evt) result (sqme)
    class(evt_nlo_t), intent(inout) :: evt
    real(default) :: sqme
    integer :: i_phs, i_term
    if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_compute_subtraction_sqmes")

```

```

sqme = zero
associate (event_deps => evt%event_deps)
  i_phs = 1; i_term = evt%i_evaluation_to_i_term(0)
  call evt%process_instance%compute_sqme_rad (i_term, i_phs, is_subtraction = .true.)
  sqme = sqme + evt%process_instance%get_sqme (i_term)
end associate
end function evt_nlo_compute_subtraction_sqmes

```

This routine calls the evaluation of the singular regions only for emission matrix elements.

```

<Evt Nlo: evt nlo: TBP>+≡
  procedure :: compute_real => evt_nlo_compute_real

<Evt Nlo: procedures>+≡
  subroutine evt_nlo_compute_real (evt)
    class(evt_nlo_t), intent(inout) :: evt
    integer :: i_phs, i_term
    if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_compute_real")
    i_phs = evt%get_i_phs ()
    i_term = evt%i_evaluation_to_i_term (evt%i_evaluation)
    associate (event_deps => evt%event_deps)
      call evt%process_instance%compute_sqme_rad (i_term, i_phs, &
        is_subtraction = .false.)
      evt%sqme_rad = evt%process_instance%get_sqme (i_term)
    end associate
  end subroutine evt_nlo_compute_real

```

This routine calls the evaluation of the singular regions only for all emission matrix elements. This is needed for the combined mode. It returns the sum of all valid real matrix elements.

```

<Evt Nlo: evt nlo: TBP>+≡
  procedure :: compute_all_sqme_rad => evt_nlo_compute_all_sqme_rad

<Evt Nlo: procedures>+≡
  function evt_nlo_compute_all_sqme_rad (evt) result (sqme)
    class(evt_nlo_t), intent(inout) :: evt
    real(default) :: sqme
    integer :: i_phs, i_term
    if (debug_on) call msg_debug (D_TRANSFORMS, "evt_nlo_compute_all_sqme_rad")
    sqme = zero
    do i_term = 1, size (evt%process_instance%term)
      if (evt%is_valid_event (i_term)) then
        associate (term => evt%process_instance%term(i_term))
          if (term%nlo_type == NLO_REAL .and. .not. term%is_subtraction ()) then
            i_phs = evt%process_instance%kin(i_term)%i_phs
            call evt%process_instance%compute_sqme_rad ( &
              i_term, i_phs, is_subtraction = .false.)
            sqme = sqme + evt%process_instance%get_sqme (i_term)
          end if
        end associate
      end if
    end do
  end function evt_nlo_compute_all_sqme_rad

```


Boosts the given four vector `p_lab` to the Born or real CMS depending on the number of given momenta. Unfortunately, all boosts available via `get_boost_to_cms` are Born-like, so we need to compute the boost to the real CMS here manually. We cannot rely on `i_term` in order to determine whether to apply a Born-like or a real boost as we also need a real boost to compute the weights of the Born-like subevents as implemented in `evt_nlo_generate_weighted`.

```

(Evt Nlo: evt nlo: TBP)+≡
  procedure :: boost_to_cms => evt_nlo_boost_to_cms

(Evt Nlo: procedures)+≡
  function evt_nlo_boost_to_cms (evt, p_lab) result (p_cms)
    type(phs_point_t), intent(in) :: p_lab
    type(vector4_t) :: p0, p1
    class(evt_nlo_t), intent(in) :: evt
    type(phs_point_t) :: p_cms
    type(lorentz_transformation_t) :: lt_lab_to_cms, lt
    real(default) :: sqrts_hat
    integer :: i_boost, n_legs_born
    if (evt%event_deps%lab_is_cm) then
      lt_lab_to_cms = identity
    else
      n_legs_born = size (evt%event_deps%p_born_lab%phs_point(1))
      if (size (p_lab) == n_legs_born) then
        i_boost = evt%get_i_term ()
        lt_lab_to_cms = evt%process_instance%get_boost_to_cms (i_boost)
      else
        sqrts_hat = (p_lab%select (1) + p_lab%select (2))*1
        p0 = p_lab%select (1) + p_lab%select (2)
        lt = boost (p0, sqrts_hat)
        p1 = inverse(lt) * p_lab%select (1)
        lt_lab_to_cms = inverse (lt * rotation_to_2nd (3, space_part (p1)))
      end if
    end if
    p_cms = lt_lab_to_cms * p_lab
  end function evt_nlo_boost_to_cms

```

Boosts the given four vector `p_cms` from the Born CMS to the lab system. It should not be called for ISR as in this case, the Born CMS and the real CMS differ.

```

(Evt Nlo: evt nlo: TBP)+≡
  procedure :: boost_to_lab => evt_nlo_boost_to_lab

(Evt Nlo: procedures)+≡
  function evt_nlo_boost_to_lab (evt, p_cms) result (p_lab)
    type(phs_point_t) :: p_lab
    class(evt_nlo_t), intent(in) :: evt
    type(phs_point_t), intent(in) :: p_cms
    type(lorentz_transformation_t) :: lt_cms_to_lab
    integer :: i_boost
    if (evt%event_deps%lab_is_cm) then
      lt_cms_to_lab = identity
    else
      i_boost = evt%get_i_term ()
      lt_cms_to_lab = evt%process_instance%get_boost_to_lab (i_boost)
    end if
  end function evt_nlo_boost_to_lab

```

```

end if
p_lab = lt_cms_to_lab * p_cms
end function evt_nlo_boost_to_lab

```

(Evt Nlo: evt nlo: TBP)+≡

```

procedure :: setup_general_event_kinematics => evt_nlo_setup_general_event_kinematics

```

(Evt Nlo: procedures)+≡

```

subroutine evt_nlo_setup_general_event_kinematics (evt, process_instance)
  class(evt_nlo_t), intent(inout) :: evt
  type(process_instance_t), intent(in) :: process_instance
  integer :: n_born
  associate (event_deps => evt%event_deps)
    event_deps%lab_is_cm = process_instance%lab_is_cm (1)
    select type (pcm => process_instance%pcm)
      type is (pcm_nlo_t)
        n_born = pcm%region_data%n_legs_born
    end select
    call event_deps%p_born_cms%init (n_born, 1)
    call event_deps%p_born_lab%init (n_born, 1)
  end associate
end subroutine evt_nlo_setup_general_event_kinematics

```

(Evt Nlo: evt nlo: TBP)+≡

```

procedure :: setup_real_event_kinematics => evt_nlo_setup_real_event_kinematics

```

(Evt Nlo: procedures)+≡

```

subroutine evt_nlo_setup_real_event_kinematics (evt, process_instance)
  class(evt_nlo_t), intent(inout) :: evt
  type(process_instance_t), intent(in) :: process_instance
  integer :: n_real, n_phs
  integer :: i_real
  associate (event_deps => evt%event_deps)
    select type (pcm => process_instance%pcm)
      class is (pcm_nlo_t)
        n_real = pcm%region_data%n_legs_real
    end select
    i_real = evt%process%get_first_real_term ()
    select type (phs => process_instance%kin(i_real)%phs)
      type is (phs_fks_t)
        event_deps%phs_identifiers = phs%phs_identifiers
    end select
    n_phs = size (event_deps%phs_identifiers)
    call event_deps%p_real_cms%init (n_real, n_phs)
    call event_deps%p_real_lab%init (n_real, n_phs)
    select type (pcm => process_instance%pcm)
      type is (pcm_nlo_t)
        if (allocated (pcm%region_data%alr_contributors)) then
          allocate (event_deps%contributors (size (pcm%region_data%alr_contributors)))
          event_deps%contributors = pcm%region_data%alr_contributors
        end if
        if (allocated (pcm%region_data%alr_to_i_contributor)) then
          allocate (event_deps%alr_to_i_con &
                    (size (pcm%region_data%alr_to_i_contributor)))

```

```

        event_deps%alr_to_i_con = pcm%region_data%alr_to_i_contributor
    end if
end select
end associate
end subroutine evt_nlo_setup_real_event_kinematics

```

<Evt Nlo: evt nlo: TBP>+≡

```

    procedure :: set_mode => evt_nlo_set_mode

```

<Evt Nlo: procedures>+≡

```

subroutine evt_nlo_set_mode (evt, process_instance)
    class(evt_nlo_t), intent(inout) :: evt
    type(process_instance_t), intent(in) :: process_instance
    integer :: i_real
    select type (pcm => process_instance%pcm)
    type is (pcm_nlo_t)
        if (pcm%settings%combined_integration) then
            evt%mode = EVT_NLO_COMBINED
        else
            i_real = evt%process%get_first_real_component ()
            if (i_real == evt%process%extract_active_component_mci ()) then
                evt%mode = EVT_NLO_SEPARATE_REAL
            else
                evt%mode = EVT_NLO_SEPARATE_BORNLIKE
            end if
        end if
    end select
end subroutine evt_nlo_set_mode

```

<Evt Nlo: evt nlo: TBP>+≡

```

    procedure :: is_valid_event => evt_nlo_is_valid_event

```

<Evt Nlo: procedures>+≡

```

function evt_nlo_is_valid_event (evt, i_term) result (valid)
    logical :: valid
    class(evt_nlo_t), intent(in) :: evt
    integer, intent(in) :: i_term
    valid = evt%process_instance%term(i_term)%passed
end function evt_nlo_is_valid_event

```

Retrieves the actual quantum numbers chosen in `evt_nlo_prepare_new_event`.

<Evt Nlo: evt nlo: TBP>+≡

```

    procedure :: get_selected_quantum_numbers => evt_nlo_get_selected_quantum_numbers

```

<Evt Nlo: procedures>+≡

```

function evt_nlo_get_selected_quantum_numbers (evt, i_flv) result (qn_select)
    class(evt_nlo_t), intent(in) :: evt
    integer, intent(in) :: i_flv
    type(quantum_numbers_t), dimension(:), allocatable :: qn_select
    integer :: i_term, index
    i_term = evt%get_i_term ()
    associate (term => evt%process_instance%term(i_term))
        index = term%connected%matrix%get_qn_index (i_flv, i_sub = 0)
        qn_select = term%connected%matrix%get_quantum_numbers (index)
    end associate
end function evt_nlo_get_selected_quantum_numbers

```

```

end associate
end function evt_nlo_get_selected_quantum_numbers

```

Selects a flavor structure for Born subevents, such that each possible flavor structure is as probable as its portion of the sum of Born matrix elements over all flavors. For non-Born Born-like subevents, no Born matrix elements are available. We always choose `i_flv = 1` in this case. If all terms are active, i.e. in a full NLO calculation, the flavors of Born-like subevents will be distributed according to the Born matrix elements only, to avoid issues with matrix elements of different sign and assure a LO flavor distribution.

Likewise, the real-like event flavors are distributed according to the real matrix elements. Here, we need to make sure to not mix matrix elements from different real terms and instead determine the flavor for each subevent based on just the matrix elements for one of the terms. The implementation below assumes that in the sequence of NLO terms, the Born term is immediately followed by all the real terms which are again followed by the subtraction, the virtual and the DGLAP term.

Both flavor structures can be determined without correlation as the flavors will only become important for events to be matched to a parton shower and in this case we will only generate either a single Born-like or a single real-like event which are not part of an event group.

In case all subevents failed the cuts, all `sqmes` were set to 0 so we cannot determine the flavor in this way. In this case, we always choose the first flavor structure given by the matrix-element generator with `i_flv = 1`.

Ideally, having to choose a particle set here would not be necessary as it is also chosen in `particle_set_init_interaction` which in the current approach is disabled by supplying `qn_select` explicitly based on the flavors chosen here.

```

(Evt Nlo: evt_nlo: TBP)+≡
  procedure :: prepare_new_event => evt_nlo_prepare_new_event

(Evt Nlo: procedures)+≡
  subroutine evt_nlo_prepare_new_event (evt, i_mci, i_term)
    class(evt_nlo_t), intent(inout) :: evt
    integer, intent(in) :: i_mci, i_term
    real(default) :: s, x
    real(default) :: sqme_total
    real(default), dimension(:), allocatable :: sqme_flv
    integer :: i, i_flv, i_core, emitter, n_in
    logical, save :: warn_once = .true.
    class(prc_core_t), pointer :: core => null ()
    call evt%reset ()
    call evt%rng%generate (x)
    do i = 1, size (evt%process_instance%term)
      associate (term => evt%process_instance%term(i))
        if (evt%i_evaluation == 0) then
          if (term%nlo_type == BORN) then
            allocate (sqme_flv (term%config%data%n_flv))
            exit
          end if
        else
          if (term%nlo_type == NLO_REAL .and. .not. term%is_subtraction()) then
            allocate (sqme_flv (term%config%data%n_flv))

```

```

        exit
    end if
end if
end associate
end do
sqme_total = zero
sqme_flv = zero
i_core = evt%process%get_i_core (i_term)
core => evt%process%get_core_ptr (i_core)
do i = 1, size (evt%process_instance%term)
    associate (term => evt%process_instance%term(i))
        if (i == evt%i_evaluation + 1 .and. (term%nlo_type == BORN .or. &
            (term%nlo_type == NLO_REAL .and. .not. term%is_subtraction())) ) then
            sqme_total = sqme_total + real (sum ( term%connected%matrix%get_matrix_element ()))
            !!! TODO (VR 2020-02-19) figure out why this select type is needed for prc_omega_t
            !!! For NLO and prc_omega_t the connected trace seems to be set up incorrectly!
            !!! (PS 2020-11-05) This leads to real events of processes with structure functions
            !!! having a wrong flavor distribution if computed with O'Mega.
            !!! The flavor distributions are identical with and also without the special case
            !!! for O'Mega and wrong in both cases.
            !!! However, this case it is not critical as long as O'Mega does not provide matrix e
            !!! exclusive in coupling orders and is thus only rarely used for NLO applications an
            select type (core)
            class is (prc_external_t)
                do i_flv = 1, size (sqme_flv)
                    sqme_flv(i_flv) = sqme_flv(i_flv) &
                        + real (term%connected%matrix%get_matrix_element ( &
                            term%connected%matrix%get_qn_index (i_flv, i_sub = 0)))
                end do
            class default
                sqme_flv = sqme_flv &
                    + real (term%connected%matrix%get_matrix_element ())
                emitter = evt%process_instance%kin(i)%emitter
                n_in = evt%process_instance%kin(i)%n_in
                if (warn_once .and. term%nlo_type == NLO_REAL .and. emitter <= n_in) then
                    warn_once = .false.
                    call msg_warning("evt_nlo_prepare_new_event: fNLO flavor&
                        & distributions with O'Mega are wrong.")
                end if
            end select
        end if
    end associate
end do
if (debug2_active (D_TRANSFORMS)) then
    if (.not. nearly_equal(sqme_total, sum (sqme_flv))) then
        call msg_warning ("evt_nlo_prepare_new_event: &
            &sum over flavored sqmes does not match total sqme.")
    end if
end if
!!! Need absolute values to take into account negative weights
x = x * abs (sqme_total)
s = abs (sqme_flv (1))
evt%selected_i_flv = 1
if (s < x) then

```

```

do i_flv = 2, size (sqme_flv)
  s = s + abs (sqme_flv (i_flv))
  if (s > x) then
    evt%selected_i_flv = i_flv
    exit
  end if
end do
end if
if (debug2_active (D_TRANSFORMS)) then
  call msg_print_color ("Selected i_flv: ", COL_GREEN)
  print *, evt%selected_i_flv
end if
end subroutine evt_nlo_prepare_new_event

```

32.10 Complete Events

This module combines hard processes with decay chains, shower, and hadronization (not implemented yet) to complete events. It also manages the input and output of event records in various formats.

```

<events.f90>≡
  <File header>

  module events

    <Use kinds>
    <Use strings>
    <Use debug>

    use constants, only: one
    use io_units
    use format_utils, only: pac_fmt, write_separator
    use format_defs, only: FMT_12, FMT_19
    use numeric_utils
    use diagnostics
    use variables
    use expr_base
    use model_data
    use state_matrices, only: FM_IGNORE_HELICITY, &
      FM_SELECT_HELICITY, FM_FACTOR_HELICITY, FM_CORRELATED_HELICITY
    use particles
    use subvt_expr
    use rng_base
    use process, only: process_t
    use instances, only: process_instance_t
    use pcm, only: pcm_nlo_workspace_t
    use process_stacks
    use event_base
    use event_transforms
    use decays
    use evt_nlo

    <Standard module head>

```

```

    <Events: public>

    <Events: types>

    <Events: interfaces>

contains

    <Events: procedures>

end module events

```

32.10.1 Event configuration

The parameters govern the transformation of an event to a particle set.

The **safety_factor** reduces the acceptance probability for unweighting. If greater than one, excess events become less likely, but the reweighting efficiency also drops.

The **sigma** and **n** values, if nontrivial, allow for reweighting the events according to the requested **norm_mode**.

Various **parse_node_t** objects are taken from the SINDARIN input. They encode expressions that apply to the current event. The workspaces for evaluating those expressions are set up in the **event_expr_t** objects. Note that these are really pointers, so the actual nodes are not stored inside the event object.

```

<Events: types>≡
    type :: event_config_t
        logical :: unweighted = .false.
        integer :: norm_mode = NORM_UNDEFINED
        integer :: factorization_mode = FM_IGNORE_HELICITY
        logical :: keep_correlations = .false.
        logical :: colorize_subevt = .false.
        real(default) :: sigma = 1
        integer :: n = 1
        real(default) :: safety_factor = 1
        class(expr_factory_t), allocatable :: ef_selection
        class(expr_factory_t), allocatable :: ef_reweight
        class(expr_factory_t), allocatable :: ef_analysis
    contains
        <Events: event config: TBP>
    end type event_config_t

```

Output.

```

<Events: event config: TBP>≡
    procedure :: write => event_config_write

<Events: procedures>≡
    subroutine event_config_write (object, unit, show_expressions)
        class(event_config_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: show_expressions
        integer :: u
        u = given_output_unit (unit)
    end subroutine event_config_write

```

```

write (u, "(3x,A,L1)") "Unweighted          = ", object%unweighted
write (u, "(3x,A,A)") "Normalization        = ", &
    char (event_normalization_string (object%norm_mode))
write (u, "(3x,A)", advance="no") "Helicity handling = "
select case (object%factorization_mode)
case (FM_IGNORE_HELICITY)
    write (u, "(A)") "drop"
case (FM_SELECT_HELICITY)
    write (u, "(A)") "select"
case (FM_FACTOR_HELICITY)
    write (u, "(A)") "factorize"
end select
write (u, "(3x,A,L1)") "Keep correlations = ", object%keep_correlations
if (object%colorize_subevt) then
    write (u, "(3x,A,L1)") "Colorize subevent = ", object%colorize_subevt
end if
if (.not. nearly_equal (object%safety_factor, one)) then
    write (u, "(3x,A," // FMT_12 // ")") &
        "Safety factor          = ", object%safety_factor
end if
if (present (show_expressions)) then
    if (show_expressions) then
        if (allocated (object%ef_selection)) then
            call write_separator (u)
            write (u, "(3x,A)") "Event selection expression:"
            call object%ef_selection%write (u)
        end if
        if (allocated (object%ef_reweight)) then
            call write_separator (u)
            write (u, "(3x,A)") "Event reweighting expression:"
            call object%ef_reweight%write (u)
        end if
        if (allocated (object%ef_analysis)) then
            call write_separator (u)
            write (u, "(3x,A)") "Analysis expression:"
            call object%ef_analysis%write (u)
        end if
    end if
end if
end subroutine event_config_write

```

32.10.2 The event type

This is the concrete implementation of the `generic_event_t` core that is defined above in the `event_base` module. The core manages the main (dressed) particle set pointer and the current values for weights and sqme. The implementation adds configuration data, expressions, process references, and event transforms.

Each event refers to a single elementary process. This process may be dressed by a shower, a decay chain etc. We maintain pointers to a process instance.

A list of event transforms (class `evt_t`) transform the connected interactions of the process instance into the final particle set. In this list, the first transform is always the trivial one, which just factorizes the process instance. Subsequent

transforms may apply decays, etc. The `particle_set` pointer identifies the particle set that we want to be analyzed and returned by the event, usually the last one.

Squared matrix element and weight values: when reading events from file, the `ref` value is the number in the file, while the `prc` value is the number that we calculate from the momenta in the file, possibly with different parameters. When generating events the first time, or if we do not recalculate, the numbers should coincide. Furthermore, the array of `alt` values is copied from an array of alternative event records. These values should represent calculated values.

The `sqme` and `weight` values mirror corresponding values in the `expr` sub-object. The idea is that when generating or reading events, the event record is filled first, then the `expr` object acquires copies. These copies are used for writing events and as targets for pointer variables in the analysis expression.

All data that involve user-provided expressions (selection, reweighting, analysis) are handled by the `expr` subobject. In particular, evaluating the event-selection expression sets the `passed` flag. Furthermore, the `expr` subobject collects data that can be used in the analysis and should be written to file, including copies of `sqme` and `weight`.

```

<Events: public>≡
  public :: event_t

<Events: types>+≡
  type, extends (generic_event_t) :: event_t
    type(event_config_t) :: config
    type(process_t), pointer :: process => null ()
    type(process_instance_t), pointer :: instance => null ()
    class(rng_t), allocatable :: rng
    integer :: selected_i_mci = 0
    integer :: selected_i_term = 0
    integer :: selected_channel = 0
    logical :: is_complete = .false.
    class(evt_t), pointer :: transform_first => null ()
    class(evt_t), pointer :: transform_last => null ()
    type(event_expr_t) :: expr
    logical :: selection_evaluated = .false.
    logical :: passed = .false.
    real(default), allocatable :: alpha_qcd_forced
    real(default), allocatable :: scale_forced
    real(default) :: reweight = 1
    logical :: analysis_flag = .false.
    integer :: i_event = 0
  contains
    <Events: event: TBP>
  end type event_t

<Events: event: TBP>≡
  procedure :: clone => event_clone

<Events: procedures>+≡
  subroutine event_clone (event, event_new)
    class(event_t), intent(in), target :: event
    class(event_t), intent(out), target :: event_new
    type(string_t) :: id

```

```

integer :: num_id
event_new%config = event%config
event_new%process => event%process
event_new%instance => event%instance
if (allocated (event%rng)) &
    allocate(event_new%rng, source=event%rng)
event_new%selected_i_mci = event%selected_i_mci
event_new%selected_i_term = event%selected_i_term
event_new%selected_channel = event%selected_channel
event_new%is_complete = event%is_complete
event_new%transform_first => event%transform_first
event_new%transform_last => event%transform_last
event_new%selection_evaluated = event%selection_evaluated
event_new%passed = event%passed
if (allocated (event%alpha_qcd_forced)) &
    allocate(event_new%alpha_qcd_forced, source=event%alpha_qcd_forced)
if (allocated (event%scale_forced)) &
    allocate(event_new%scale_forced, source=event%scale_forced)
event_new%reweight = event%reweight
event_new%analysis_flag = event%analysis_flag
event_new%i_event = event%i_event
id = event_new%process%get_id ()
if (id /= "") call event_new%expr%set_process_id (id)
num_id = event_new%process%get_num_id ()
if (num_id /= 0) call event_new%expr%set_process_num_id (num_id)
call event_new%expr%setup_vars (event_new%process%get_sqrts ())
call event_new%expr%link_var_list (event_new%process%get_var_list_ptr ())
end subroutine event_clone

```

Finalizer: the list of event transforms is deleted iteratively.

```

<Events: event: TBP>+≡
procedure :: final => event_final

<Events: procedures>+≡
subroutine event_final (object)
class(event_t), intent(inout) :: object
class(evt_t), pointer :: evt
if (allocated (object%rng)) call object%rng%final ()
call object%expr%final ()
do while (associated (object%transform_first))
    evt => object%transform_first
    object%transform_first => evt%next
    call evt%final ()
    deallocate (evt)
end do
end subroutine event_final

```

Output.

The event index is written in the header, it should coincide with the `event_index` variable that can be used in selection and analysis.

Particle set: this is a pointer to one of the event transforms, so it should suffice to print the latter.

```

<Events: event: TBP>+≡

```

```

procedure :: write => event_write

<Events: procedures>+≡
subroutine event_write (object, unit, show_process, show_transforms, &
    show_decay, verbose, testflag)
    class(event_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: show_process, show_transforms, show_decay
    logical, intent(in), optional :: verbose
    logical, intent(in), optional :: testflag
    logical :: prc, trans, dec, verb
    class(evt_t), pointer :: evt
    character(len=7) :: fmt
    integer :: u, i
    call pac_fmt (fmt, FMT_19, FMT_12, testflag)
    u = given_output_unit (unit)
    prc = .true.; if (present (show_process)) prc = show_process
    trans = .true.; if (present (show_transforms)) trans = show_transforms
    dec = .true.; if (present (show_decay)) dec = show_decay
    verb = .false.; if (present (verbose)) verb = verbose
    call write_separator (u, 2)
    write (u, "(1x,A)", advance="no") "Event"
    if (object%has_index ()) then
        write (u, "(1x,'#',I0)", advance="no") object%get_index ()
    end if
    if (object%is_complete) then
        write (u, *)
    else
        write (u, "(1x,A)") "[incomplete]"
    end if
    call write_separator (u)
    call object%config%write (u)
    if (object%sqme_ref_is_known () .or. object%weight_ref_is_known ()) then
        call write_separator (u)
    end if
    if (object%sqme_ref_is_known ()) then
        write (u, "(3x,A," // fmt // ")") &
            "Squared matrix el. (ref) = ", object%get_sqme_ref ()
        if (object%sqme_alt_is_known ()) then
            do i = 1, object%get_n_alt ()
                write (u, "(5x,A," // fmt // ",1x,I0)") &
                    "alternate sqme = ", object%get_sqme_alt(i), i
            end do
        end if
    end if
    if (object%sqme_prc_is_known ()) &
        write (u, "(3x,A," // fmt // ")") &
            "Squared matrix el. (prc) = ", object%get_sqme_prc ()

    if (object%weight_ref_is_known ()) then
        write (u, "(3x,A," // fmt // ")") &
            "Event weight (ref) = ", object%get_weight_ref ()
        if (object%weight_alt_is_known ()) then
            do i = 1, object%get_n_alt ()
                write (u, "(5x,A," // fmt // ",1x,I0)") &

```

```

        "alternate weight      = ", object%get_weight_alt(i), i
    end do
end if
end if
if (object%weight_prc_is_known ()) &
    write (u, "(3x,A," // fmt // ")") &
        "Event weight (prc)      = ", object%get_weight_prc ()

if (object%selected_i_mci /= 0) then
    call write_separator (u)
    write (u, "(3x,A,I0)") "Selected MCI group = ", object%selected_i_mci
    write (u, "(3x,A,I0)") "Selected term      = ", object%selected_i_term
    write (u, "(3x,A,I0)") "Selected channel   = ", object%selected_channel
end if
if (object%selection_evaluated) then
    call write_separator (u)
    write (u, "(3x,A,L1)") "Passed selection   = ", object%passed
    if (object%passed) then
        write (u, "(3x,A," // fmt // ")") &
            "Reweighting factor = ", object%reweight
        write (u, "(3x,A,L1)") &
            "Analysis flag      = ", object%analysis_flag
    end if
end if
if (associated (object%instance)) then
    if (prc) then
        if (verb) then
            call object%instance%write (u, testflag)
        else
            call object%instance%write_header (u)
        end if
    end if
    if (trans) then
        evt => object%transform_first
        do while (associated (evt))
            select type (evt)
            type is (evt_decay_t)
                call evt%write (u, verbose = dec, more_verbose = verb, &
                    testflag = testflag)
            class default
                call evt%write (u, verbose = verb, testflag = testflag)
            end select
            call write_separator (u, 2)
            evt => evt%next
        end do
    else
        call write_separator (u, 2)
    end if
    if (object%expr%subevt_filled) then
        call object%expr%write (u, pacified = testflag)
        call write_separator (u, 2)
    end if
else
    call write_separator (u, 2)

```

```

        write (u, "(1x,A)") "Process instance: [undefined]"
        call write_separator (u, 2)
    end if
end subroutine event_write

```

32.10.3 Initialization

Initialize: set configuration parameters, using a variable list. We do not call this `init`, because this method name will be used by a type extension.

The default normalization is `NORM_SIGMA`, since the default generation mode is weighted.

For unweighted events, we may want to apply a safety factor to event rejection. (By default, this factor is unity and can be ignored.)

We also allocate the trivial event transform, which is always the first one.

```

<Events: event: TBP>+≡
    procedure :: basic_init => event_init

<Events: procedures>+≡
    subroutine event_init (event, var_list, n_alt)
        class(event_t), intent(out) :: event
        type(var_list_t), intent(in), optional :: var_list
        integer, intent(in), optional :: n_alt
        type(string_t) :: norm_string, mode_string
        logical :: polarized_events
        if (present (n_alt)) then
            call event%base_init (n_alt)
            call event%expr%init (n_alt)
        else
            call event%base_init (0)
        end if
        if (present (var_list)) then
            event%config%unweighted = var_list%get_lval (&
                var_str ("?unweighted"))
            norm_string = var_list%get_sval (&
                var_str ("sample_normalization"))
            event%config%norm_mode = &
                event_normalization_mode (norm_string, event%config%unweighted)
            polarized_events = &
                var_list%get_lval (var_str ("?polarized_events"))
            if (polarized_events) then
                mode_string = &
                    var_list%get_sval (var_str ("polarization_mode"))
                select case (char (mode_string))
                case ("ignore")
                    event%config%factorization_mode = FM_IGNORE_HELICITY
                case ("helicity")
                    event%config%factorization_mode = FM_SELECT_HELICITY
                case ("factorized")
                    event%config%factorization_mode = FM_FACTOR_HELICITY
                case ("correlated")
                    event%config%factorization_mode = FM_CORRELATED_HELICITY
                case default

```

```

        call msg_fatal ("Polarization mode " &
            // char (mode_string) // " is undefined")
    end select
else
    event%config%factorization_mode = FM_IGNORE_HELICITY
end if
event%config%colorize_subevt = &
    var_list%get_lval (var_str ("?colorize_subevt"))
if (event%config%unweighted) then
    event%config%safety_factor = var_list%get_rval (&
        var_str ("safety_factor"))
end if
else
    event%config%norm_mode = NORM_SIGMA
end if
allocate (evt_trivial_t :: event%transform_first)
event%transform_last => event%transform_first
end subroutine event_init

```

Set the `sigma` and `n` values in the configuration record that determine non-standard event normalizations. If these numbers are not set explicitly, the default value for both is unity, and event renormalization has no effect.

```

<Events: event: TBP>+≡
    procedure :: set_sigma => event_set_sigma
    procedure :: set_n => event_set_n

<Events: procedures>+≡
    elemental subroutine event_set_sigma (event, sigma)
        class(event_t), intent(inout) :: event
        real(default), intent(in) :: sigma
        event%config%sigma = sigma
    end subroutine event_set_sigma

    elemental subroutine event_set_n (event, n)
        class(event_t), intent(inout) :: event
        integer, intent(in) :: n
        event%config%n = n
    end subroutine event_set_n

```

Append an event transform (decays, etc.). The transform is not yet connected to a process. The transform is then considered to belong to the event object, and will be finalized together with it. The original pointer is removed.

We can assume that the trivial transform is already present in the event object, at least.

```

<Events: event: TBP>+≡
    procedure :: import_transform => event_import_transform

<Events: procedures>+≡
    subroutine event_import_transform (event, evt)
        class(event_t), intent(inout) :: event
        class(evt_t), intent(inout), pointer :: evt
        event%transform_last%next => evt
        evt%previous => event%transform_last
    end subroutine event_import_transform

```

```

    event%transform_last => evt
    evt => null ()
end subroutine event_import_transform

```

We link the event to an existing process instance. This includes the variable list, which is linked to the process variable list. Note that this is not necessarily identical to the variable list used for event initialization.

The variable list will contain pointers to `event` subobjects, therefore the `target` attribute.

Once we have a process connected, we can use it to obtain an event generator instance.

The model and process stack may be needed by event transforms. The current model setting may be different from the model in the process (regarding unstable particles, etc.). The process stack can be used for assigning extra processes that we need for the event transforms.

```

<Events: event: TBP>+≡
  procedure :: connect => event_connect

<Events: procedures>+≡
  subroutine event_connect (event, process_instance, model, process_stack)
    class(event_t), intent(inout), target :: event
    type(process_instance_t), intent(in), target :: process_instance
    class(model_data_t), intent(in), target :: model
    type(process_stack_t), intent(in), optional :: process_stack
    type(string_t) :: id
    integer :: num_id
    class(evt_t), pointer :: evt
    event%process => process_instance%process
    event%instance => process_instance
    id = event%process%get_id ()
    if (id /= "") call event%expr%set_process_id (id)
    num_id = event%process%get_num_id ()
    if (num_id /= 0) call event%expr%set_process_num_id (num_id)
    call event%expr%setup_vars (event%process%get_sqrts ())
    call event%expr%link_var_list (event%process%get_var_list_ptr ())
    call event%process%make_rng (event%rng)
    evt => event%transform_first
    do while (associated (evt))
      call evt%connect (process_instance, model, process_stack)
      evt => evt%next
    end do
  end subroutine event_connect

```

Set the parse nodes for the associated expressions, individually. The parse-node pointers may be null.

```

<Events: event: TBP>+≡
  procedure :: set_selection => event_set_selection
  procedure :: set_reweight => event_set_reweight
  procedure :: set_analysis => event_set_analysis

<Events: procedures>+≡
  subroutine event_set_selection (event, ef_selection)
    class(event_t), intent(inout) :: event

```

```

        class(expr_factory_t), intent(in) :: ef_selection
        allocate (event%config%ef_selection, source = ef_selection)
    end subroutine event_set_selection

    subroutine event_set_reweight (event, ef_reweight)
        class(event_t), intent(inout) :: event
        class(expr_factory_t), intent(in) :: ef_reweight
        allocate (event%config%ef_reweight, source = ef_reweight)
    end subroutine event_set_reweight

    subroutine event_set_analysis (event, ef_analysis)
        class(event_t), intent(inout) :: event
        class(expr_factory_t), intent(in) :: ef_analysis
        allocate (event%config%ef_analysis, source = ef_analysis)
    end subroutine event_set_analysis

```

Create evaluation trees from the parse trees. The `target` attribute is required because the expressions contain pointers to event subobjects.

```

<Events: event: TBP>+≡
    procedure :: setup_expressions => event_setup_expressions

<Events: procedures>+≡
    subroutine event_setup_expressions (event)
        class(event_t), intent(inout), target :: event
        call event%expr%setup_selection (event%config%ef_selection)
        call event%expr%setup_analysis (event%config%ef_analysis)
        call event%expr%setup_reweight (event%config%ef_reweight)
        call event%expr%colorize (event%config%colorize_subevt)
    end subroutine event_setup_expressions

```

32.10.4 Evaluation

To fill the `particle_set`, i.e., the event record proper, we have to apply all event transforms in order. The last transform should fill its associated particle set, factorizing the state matrix according to the current settings. There are several parameters in the event configuration that control this.

We always fill the particle set for the first transform (the hard process) and the last transform, if different from the first (the fully dressed process).

Each event transform is an event generator of its own. We choose to generate an *unweighted* event for each of them, even if the master event is assumed to be weighted. Thus, the overall event weight is the one of the hard process only. (There may be more options in future extensions.)

We can generate the two random numbers that the factorization needs. For testing purpose, we allow for providing them explicitly, as an option.

```

<Events: event: TBP>+≡
    procedure :: evaluate_transforms => event_evaluate_transforms

<Events: procedures>+≡
    subroutine event_evaluate_transforms (event, r)
        class(event_t), intent(inout) :: event
        real(default), dimension(:), intent(in), optional :: r

```



```

class(evt_t), pointer :: evt
real(default) :: weight_over_sqme
integer :: i_term, emitter, n_in
logical :: failed_but_keep
failed_but_keep = .false.
if (debug_on) call msg_debug (D_TRANSFORMS, "event_evaluate_transforms")
call event%discard_particle_set ()
call event%check ()
if (event%instance%is_complete_event ()) then
  i_term = event%instance%select_i_term ()
  event%selected_i_term = i_term
  evt => event%transform_first
  do while (associated (evt))
    call evt%prepare_new_event &
      (event%selected_i_mci, event%selected_i_term)
    evt => evt%next
  end do
  if (debug_on) call msg_debug &
    (D_TRANSFORMS, "Before event transformations")
  if (debug_on) call msg_debug &
    (D_TRANSFORMS, "event%weight_prc", event%weight_prc)
  if (debug_on) call msg_debug &
    (D_TRANSFORMS, "event%sqme_prc", event%sqme_prc)
  evt => event%transform_first
  do while (associated (evt))
    call print_transform_name_if_debug ()
    if (evt%only_weighted_events) then
      select type (evt)
      type is (evt_nlo_t)
        i_term = evt%get_i_term ()
        failed_but_keep = .not. evt%is_valid_event (i_term) &
          .and. evt%keep_failed_events
        if (.not. any(evt%process_instance%term%passed .and. evt%process_instance%term%act
          .and. .not. evt%keep_failed_events) return
      end select
      if (abs (event%weight_prc) > 0._default) then
        weight_over_sqme = event%weight_prc / event%sqme_prc
        call evt%generate_weighted (event%sqme_prc)
        event%weight_prc = weight_over_sqme * event%sqme_prc
        select type (evt)
        type is (evt_nlo_t)
          if (.not. evt%is_valid_event (i_term)) event%weight_prc = 0
        end select
      else
        if (.not. failed_but_keep) exit
      end if
    else
      call evt%generate_unweighted ()
    end if
    if (signal_is_pending ()) return
    select type (evt)
    type is (evt_nlo_t)
      if (evt%i_evaluation > 0) then
        emitter = evt%process_instance%kin(i_term)%emitter

```

```

        n_in = evt%process_instance%kin(i_term)%n_in
        if (emitter <= n_in) then
            call evt%connected_set_real_IS_momenta ()
        end if
    end if
end select
call evt%make_particle_set (event%config%factorization_mode, &
    event%config%keep_correlations)
if (signal_is_pending ()) return
if (.not. evt%particle_set_exists) exit
evt => evt%next
end do
evt => event%transform_last
if ((associated (evt) .and. evt%particle_set_exists) .or. failed_but_keep) then
    if (event%is_nlo ()) then
        select type (evt)
        type is (evt_nlo_t)
            evt%particle_set_nlo (event%i_event + 1) = evt%particle_set
            evt%i_evaluation = evt%i_evaluation + 1
            call event%link_particle_set &
                (evt%particle_set_nlo(event%i_event + 1))
        end select
    else
        call event%link_particle_set (evt%particle_set)
    end if
end if
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "After event transformations")
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "event%weight_prc", event%weight_prc)
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "event%sqme_prc", event%sqme_prc)
if (debug_on) call msg_debug &
    (D_TRANSFORMS, "evt%particle_set_exists", evt%particle_set_exists)
end if
contains
subroutine print_transform_name_if_debug ()
    if (debug_active (D_TRANSFORMS)) then
        print *, 'Current event transform: '
        call evt%write_name ()
    end if
end subroutine print_transform_name_if_debug
end subroutine event_evaluate_transforms

```

Set / increment the event index for the current event. There is no condition for this to happen. The event index is actually stored in the subevent expression, because this allows us to access it in subevent expressions as a variable.

(Events: event: TBP)+≡

```

    procedure :: set_index => event_set_index
    procedure :: increment_index => event_increment_index

```

(Events: procedures)+≡

```

    subroutine event_set_index (event, index)
        class(event_t), intent(inout) :: event

```

```

integer, intent(in) :: index
call event%expr%set_event_index (index)
end subroutine event_set_index

subroutine event_increment_index (event, offset)
class(event_t), intent(inout) :: event
integer, intent(in), optional :: offset
call event%expr%increment_event_index (offset)
end subroutine event_increment_index

```

Evaluate the event-related expressions, given a valid `particle_set`. If `update_sqme` is set, we use the process instance for the `sqme_prc` value. The `sqme_ref` value is always taken from the event record.

```

⟨Events: event: TBP⟩+≡
  procedure :: evaluate_expressions => event_evaluate_expressions

⟨Events: procedures⟩+≡
  subroutine event_evaluate_expressions (event)
class(event_t), intent(inout) :: event
if (event%has_valid_particle_set ()) then
  call event%expr%fill_subevt (event%get_particle_set_ptr ())
end if
if (event%weight_ref_is_known ()) then
  call event%expr%set (weight_ref = event%get_weight_ref ())
end if
if (event%weight_prc_is_known ()) then
  call event%expr%set (weight_prc = event%get_weight_prc ())
end if
if (event%excess_prc_is_known ()) then
  call event%expr%set (excess_prc = event%get_excess_prc ())
end if
if (event%sqme_ref_is_known ()) then
  call event%expr%set (sqme_ref = event%get_sqme_ref ())
end if
if (event%sqme_prc_is_known ()) then
  call event%expr%set (sqme_prc = event%get_sqme_prc ())
end if
if (event%has_valid_particle_set ()) then
  call event%expr%evaluate &
    (event%passed, event%reweight, event%analysis_flag)
  event%selection_evaluated = .true.
end if
end subroutine event_evaluate_expressions

```

Report the result of the selection evaluation.

```

⟨Events: event: TBP⟩+≡
  procedure :: passed_selection => event_passed_selection

⟨Events: procedures⟩+≡
  function event_passed_selection (event) result (flag)
class(event_t), intent(in) :: event
logical :: flag
flag = event%passed
end function event_passed_selection

```

Set alternate sqme and weight arrays. This should be merged with the previous routine, if the expressions are allowed to refer to these values.

```

<Events: event: TBP>+≡
    procedure :: store_alt_values => event_store_alt_values

<Events: procedures>+≡
    subroutine event_store_alt_values (event)
        class(event_t), intent(inout) :: event
        if (event%weight_alt_is_known ()) then
            call event%expr%set (weight_alt = event%get_weight_alt ())
        end if
        if (event%sqme_alt_is_known ()) then
            call event%expr%set (sqme_alt = event%get_sqme_alt ())
        end if
    end subroutine event_store_alt_values

<Events: event: TBP>+≡
    procedure :: is_nlo => event_is_nlo

<Events: procedures>+≡
    function event_is_nlo (event) result (is_nlo)
        logical :: is_nlo
        class(event_t), intent(in) :: event
        if (associated (event%instance)) then
            select type (pcm_work => event%instance%pcm_work)
            type is (pcm_nlo_workspace_t)
                is_nlo = pcm_work%is_fixed_order_nlo_events ()
            class default
                is_nlo = .false.
            end select
        else
            is_nlo = .false.
        end if
    end function event_is_nlo

```

32.10.5 Reset to empty state

Applying this, current event contents are marked as incomplete but are not deleted. In particular, the initialization is kept. The event index is also kept, this can be reset separately.

```

<Events: event: TBP>+≡
    procedure :: reset_contents => event_reset_contents
    procedure :: reset_index => event_reset_index

<Events: procedures>+≡
    subroutine event_reset_contents (event)
        class(event_t), intent(inout) :: event
        class(evt_t), pointer :: evt
        call event%base_reset_contents ()
        event%selected_i_mci = 0
        event%selected_i_term = 0
    end subroutine event_reset_contents

```

```

event%selected_channel = 0
event%is_complete = .false.
call event%expr%reset_contents ()
event%selection_evaluated = .false.
event%passed = .false.
event%analysis_flag = .false.
if (associated (event%instance)) then
  call event%instance%reset (reset_mci = .true.)
end if
if (allocated (event%alpha_qcd_forced)) deallocate (event%alpha_qcd_forced)
if (allocated (event%scale_forced)) deallocate (event%scale_forced)
evt => event%transform_first
do while (associated (evt))
  call evt%reset ()
  evt => evt%next
end do
end subroutine event_reset_contents

subroutine event_reset_index (event)
  class(event_t), intent(inout) :: event
  call event%expr%reset_event_index ()
end subroutine event_reset_index

```

32.10.6 Squared Matrix Element and Weight

Transfer the result of the process instance calculation to the event record header.

```

<Events: event: TBP>+≡
  procedure :: import_instance_results => event_import_instance_results

<Events: procedures>+≡
  subroutine event_import_instance_results (event)
    class(event_t), intent(inout) :: event
    if (associated (event%instance)) then
      if (event%instance%has_evaluated_trace ()) then
        call event%set ( &
          sqme_prc = event%instance%get_sqme (), &
          weight_prc = event%instance%get_weight (), &
          excess_prc = event%instance%get_excess (), &
          n_dropped = event%instance%get_n_dropped () &
        )
      end if
    end if
  end subroutine event_import_instance_results

```

Duplicate the instance result / the reference result in the event record.

```

<Events: event: TBP>+≡
  procedure :: accept_sqme_ref => event_accept_sqme_ref
  procedure :: accept_sqme_prc => event_accept_sqme_prc
  procedure :: accept_weight_ref => event_accept_weight_ref
  procedure :: accept_weight_prc => event_accept_weight_prc

```

<Events: procedures>+≡

```

subroutine event_accept_sqme_ref (event)
  class(event_t), intent(inout) :: event
  if (event%sqme_ref_is_known ()) then
    call event%set (sqme_prc = event%get_sqme_ref ())
  end if
end subroutine event_accept_sqme_ref

subroutine event_accept_sqme_prc (event)
  class(event_t), intent(inout) :: event
  if (event%sqme_prc_is_known ()) then
    call event%set (sqme_ref = event%get_sqme_prc ())
  end if
end subroutine event_accept_sqme_prc

subroutine event_accept_weight_ref (event)
  class(event_t), intent(inout) :: event
  if (event%weight_ref_is_known ()) then
    call event%set (weight_prc = event%get_weight_ref ())
  end if
end subroutine event_accept_weight_ref

subroutine event_accept_weight_prc (event)
  class(event_t), intent(inout) :: event
  if (event%weight_prc_is_known ()) then
    call event%set (weight_ref = event%get_weight_prc ())
  end if
end subroutine event_accept_weight_prc

```

Update the weight normalization, just after generation. Unweighted and weighted events are generated with a different default normalization. The intended normalization is stored in the configuration record.

<Events: event: TBP>+≡

```

procedure :: update_normalization => event_update_normalization

```

<Events: procedures>+≡

```

subroutine event_update_normalization (event, mode_ref)
  class(event_t), intent(inout) :: event
  integer, intent(in), optional :: mode_ref
  integer :: mode_old
  real(default) :: weight, excess
  if (present (mode_ref)) then
    mode_old = mode_ref
  else if (event%config%unweighted) then
    mode_old = NORM_UNIT
  else
    mode_old = NORM_SIGMA
  end if
  weight = event%get_weight_prc ()
  call event_normalization_update (weight, &
    event%config%sigma, event%config%n, &
    mode_new = event%config%norm_mode, &
    mode_old = mode_old)
  call event%set_weight_prc (weight)

```

```

    excess = event%get_excess_prc ()
    call event_normalization_update (excess, &
        event%config%sigma, event%config%n, &
        mode_new = event%config%norm_mode, &
        mode_old = mode_old)
    call event%set_excess_prc (excess)
end subroutine event_update_normalization

```

The event is complete if it has a particle set plus valid entries for the sqme and weight values.

```

<Events: event: TBP>+≡
    procedure :: check => event_check

<Events: procedures>+≡
    subroutine event_check (event)
        class(event_t), intent(inout) :: event
        event%is_complete = event%has_valid_particle_set () &
            .and. event%sqme_ref_is_known () &
            .and. event%sqme_prc_is_known () &
            .and. event%weight_ref_is_known () &
            .and. event%weight_prc_is_known ()
        if (event%get_n_alt () /= 0) then
            event%is_complete = event%is_complete &
                .and. event%sqme_alt_is_known () &
                .and. event%weight_alt_is_known ()
        end if
    end subroutine event_check

```

32.10.7 Generation

Assuming that we have a valid process associated to the event, we generate an event. We complete the event data, then factorize the spin density matrix and transfer it to the particle set.

When done, we retrieve squared matrix element and weight. In case of explicit generation, the reference values coincide with the process values, so we **accept** the latter.

The explicit random number argument `r` should be generated by a random-number generator. It is taken for the factorization algorithm, bypassing the event-specific random-number generator. This is useful for deterministic testing.

```

<Events: event: TBP>+≡
    procedure :: generate => event_generate

<Events: procedures>+≡
    subroutine event_generate (event, i_mci, r, i_nlo)
        class(event_t), intent(inout) :: event
        integer, intent(in) :: i_mci
        real(default), dimension(:), intent(in), optional :: r
        integer, intent(in), optional :: i_nlo
        logical :: generate_new
        generate_new = .true.
        if (present (i_nlo)) generate_new = (i_nlo == 1)
        if (generate_new) call event%reset_contents ()
    end subroutine event_generate

```

```

event%selected_i_mci = i_mci
if (event%config%unweighted) then
  call event%instance%generate_unweighted_event (i_mci)
  if (signal_is_pending ()) return
  call event%instance%evaluate_event_data ()
  call event%instance%normalize_weight ()
else
  if (generate_new) &
    call event%instance%generate_weighted_event (i_mci)
  if (signal_is_pending ()) return
  call event%instance%evaluate_event_data ()
end if
event%selected_channel = event%instance%get_channel ()
call event%import_instance_results ()
call event%accept_sqme_prc ()
call event%update_normalization ()
call event%accept_weight_prc ()
call event%evaluate_transforms (r)
if (signal_is_pending ()) return
call event%check ()
end subroutine event_generate

```

Get a copy of the particle set belonging to the hard process.

```

<Events: event: TBP>+≡
  procedure :: get_hard_particle_set => event_get_hard_particle_set

<Events: procedures>+≡
  subroutine event_get_hard_particle_set (event, pset)
    class(event_t), intent(in) :: event
    type(particle_set_t), intent(out) :: pset
    class(evt_t), pointer :: evt
    evt => event%transform_first
    pset = evt%particle_set
  end subroutine event_get_hard_particle_set

```

32.10.8 Recovering an event

Select MC group, term, and integration channel.

```

<Events: event: TBP>+≡
  procedure :: select => event_select

<Events: procedures>+≡
  subroutine event_select (event, i_mci, i_term, channel)
    class(event_t), intent(inout) :: event
    integer, intent(in) :: i_mci, i_term, channel
    if (associated (event%instance)) then
      event%selected_i_mci = i_mci
      event%selected_i_term = i_term
      event%selected_channel = channel
    else
      event%selected_i_mci = 0
      event%selected_i_term = 0
      event%selected_channel = 0
    end if
  end subroutine event_select

```



```

        end if
    end subroutine event_select

```

Copy a particle set into the event record.

We deliberately use the first (the trivial) transform for this, i.e., the hard process. The event reader may either read in the transformed event separately, or apply all event transforms to the hard particle set to (re)generate a fully dressed event.

Since this makes all subsequent event transforms invalid, we call `reset` on them.

```

<Events: event: TBP>+≡
    procedure :: set_hard_particle_set => event_set_hard_particle_set

<Events: procedures>+≡
    subroutine event_set_hard_particle_set (event, particle_set)
        class(event_t), intent(inout) :: event
        type(particle_set_t), intent(in) :: particle_set
        class(evt_t), pointer :: evt
        evt => event%transform_first
        call evt%set_particle_set (particle_set, &
            event%selected_i_mci, event%selected_i_term)
        call event%link_particle_set (evt%particle_set)
        evt => evt%next
        do while (associated (evt))
            call evt%reset ()
            evt => evt%next
        end do
    end subroutine event_set_hard_particle_set

```

Set the α_s value that should be used in a recalculation. This should be called only if we explicitly want to override the QCD setting of the process core.

```

<Events: event: TBP>+≡
    procedure :: set_alpha_qcd_forced => event_set_alpha_qcd_forced

<Events: procedures>+≡
    subroutine event_set_alpha_qcd_forced (event, alpha_qcd)
        class(event_t), intent(inout) :: event
        real(default), intent(in) :: alpha_qcd
        if (allocated (event%alpha_qcd_forced)) then
            event%alpha_qcd_forced = alpha_qcd
        else
            allocate (event%alpha_qcd_forced, source = alpha_qcd)
        end if
    end subroutine event_set_alpha_qcd_forced

```

Analogously, for the common scale. This forces also renormalization and factorization scale.

```

<Events: event: TBP>+≡
    procedure :: set_scale_forced => event_set_scale_forced

<Events: procedures>+≡
    subroutine event_set_scale_forced (event, scale)
        class(event_t), intent(inout) :: event

```

```

real(default), intent(in) :: scale
if (allocated (event%scale_forced)) then
    event%scale_forced = scale
else
    allocate (event%scale_forced, source = scale)
end if
end subroutine event_set_scale_forced

```

Here we try to recover an event from the `particle_set` subobject and recalculate the structure functions and matrix elements. We have the appropriate `process` object and an initialized `process_instance` at hand, so beam and configuration data are known. From the `particle_set`, we get the momenta.

The quantum-number information may be incomplete, e.g., helicity information may be partial or absent. We recover the event just from the momentum configuration.

We do not transfer the matrix element from the process instance to the event record, as we do when generating an event. The event record may contain the matrix element as read from file, and the current calculation may use different parameters. We thus can compare old and new values.

The event `weight` may also be known already. If yes, we pass it to the `evaluate_event_data` procedure. It should already be normalized. If we have a `weight_factor` value, we obtain the event weight by multiplying the computed `sqme` by this factor. Otherwise, we make use of the MCI setup (which should be valid then) to compute the event weight, and we should normalize the result just as when generating events.

Evaluating event expressions must also be done separately.

If `recover_phs` is set (and false), do not attempt any phase-space calculation, including MCI evaluation. Useful if we need only matrix elements.

```

<Events: event: TBP>+≡
    procedure :: recalculate => event_recalculate

<Events: procedures>+≡
    subroutine event_recalculate (event, update_sqme, weight_factor, &
        recover_beams, recover_phs, check_match, success)
        class(event_t), intent(inout) :: event
        logical, intent(in) :: update_sqme
        real(default), intent(in), optional :: weight_factor
        logical, intent(in), optional :: recover_beams
        logical, intent(in), optional :: recover_phs
        logical, intent(in), optional :: check_match
        logical, intent(out), optional :: success
        type(particle_set_t), pointer :: particle_set
        integer :: i_mci, i_term, channel
        logical :: rec_phs_mci
        rec_phs_mci = .true.; if (present (recover_phs)) rec_phs_mci = recover_phs
        if (present (success)) success = .false.
        if (event%has_valid_particle_set ()) then
            particle_set => event%get_particle_set_ptr ()
            i_mci = event%selected_i_mci
            i_term = event%selected_i_term
            channel = event%selected_channel
            if (i_mci == 0 .or. i_term == 0 .or. channel == 0) then

```

```

        call msg_bug ("Event: recalculate: undefined selection parameters")
    end if
    call event%instance%choose_mci (i_mci)
    call event%instance%set_trace &
        (particle_set, i_term, recover_beams, check_match, success)
    if (present (success)) then
        if (.not. success) return
    end if
    if (allocated (event%alpha_qcd_forced)) then
        call event%instance%set_alpha_qcd_forced &
            (i_term, event%alpha_qcd_forced)
    end if
    call event%instance%recover (channel, i_term, &
        update_sqme, rec_phs_mci, event%scale_forced)
    if (signal_is_pending ()) return
    if (update_sqme .and. present (weight_factor)) then
        call event%instance%evaluate_event_data &
            (weight = event%instance%get_sqme () * weight_factor)
    else if (event%weight_ref_is_known ()) then
        call event%instance%evaluate_event_data &
            (weight = event%get_weight_ref ())
    else if (rec_phs_mci) then
        call event%instance%recover_event ()
        if (signal_is_pending ()) return
        call event%instance%evaluate_event_data ()
        if (event%config%unweighted) then
            call event%instance%normalize_weight ()
        end if
    end if
    if (signal_is_pending ()) return
    if (update_sqme) then
        call event%import_instance_results ()
    else
        call event%accept_sqme_ref ()
        call event%accept_weight_ref ()
    end if
else
    call msg_bug ("Event: can't recalculate, particle set is undefined")
end if
end subroutine event_recalculate

```

32.10.9 Access content

Pointer to the associated process object (the associated model).

(Events: event: TBP)+≡

```

procedure :: get_process_ptr => event_get_process_ptr
procedure :: get_process_instance_ptr => event_get_process_instance_ptr
procedure :: get_model_ptr => event_get_model_ptr

```

(Events: procedures)+≡

```

function event_get_process_ptr (event) result (ptr)
    class(event_t), intent(in) :: event
    type(process_t), pointer :: ptr

```

```

    ptr => event%process
end function event_get_process_ptr

function event_get_process_instance_ptr (event) result (ptr)
    class(event_t), intent(in) :: event
    type(process_instance_t), pointer :: ptr
    ptr => event%instance
end function event_get_process_instance_ptr

function event_get_model_ptr (event) result (model)
    class(event_t), intent(in) :: event
    class(model_data_t), pointer :: model
    if (associated (event%process)) then
        model => event%process%get_model_ptr ()
    else
        model => null ()
    end if
end function event_get_model_ptr

```

Return the current values of indices: the MCI group of components, the term index (different terms corresponding, potentially, to different effective kinematics), and the MC integration channel. The `i_mci` call is delegated to the current process instance.

```

<Events: event: TBP>+≡
    procedure :: get_i_mci => event_get_i_mci
    procedure :: get_i_term => event_get_i_term
    procedure :: get_channel => event_get_channel

<Events: procedures>+≡
    function event_get_i_mci (event) result (i_mci)
        class(event_t), intent(in) :: event
        integer :: i_mci
        i_mci = event%selected_i_mci
    end function event_get_i_mci

    function event_get_i_term (event) result (i_term)
        class(event_t), intent(in) :: event
        integer :: i_term
        i_term = event%selected_i_term
    end function event_get_i_term

    function event_get_channel (event) result (channel)
        class(event_t), intent(in) :: event
        integer :: channel
        channel = event%selected_channel
    end function event_get_channel

```

This flag tells us whether the event consists just of a hard process (i.e., holds at most the first, trivial transform), or is a dressed events with additional transforms.

```

<Events: event: TBP>+≡
    procedure :: has_transform => event_has_transform

```

```

<Events: procedures>+≡
function event_has_transform (event) result (flag)
  class(event_t), intent(in) :: event
  logical :: flag
  if (associated (event%transform_first)) then
    flag = associated (event%transform_first%next)
  else
    flag = .false.
  end if
end function event_has_transform

```

Return the currently selected normalization mode, or alternate normalization mode.

```

<Events: event: TBP>+≡
  procedure :: get_norm_mode => event_get_norm_mode

<Events: procedures>+≡
  elemental function event_get_norm_mode (event) result (norm_mode)
    class(event_t), intent(in) :: event
    integer :: norm_mode
    norm_mode = event%config%norm_mode
  end function event_get_norm_mode

```

Return the kinematical weight, defined as the ratio of event weight and squared matrix element.

```

<Events: event: TBP>+≡
  procedure :: get_kinematical_weight => event_get_kinematical_weight

<Events: procedures>+≡
function event_get_kinematical_weight (event) result (f)
  class(event_t), intent(in) :: event
  real(default) :: f
  if (event%sqme_ref_is_known () .and. event%weight_ref_is_known () &
    .and. abs (event%get_sqme_ref ()) > 0) then
    f = event%get_weight_ref () / event%get_sqme_ref ()
  else
    f = 0
  end if
end function event_get_kinematical_weight

```

Return data used by external event formats.

```

<Events: event: TBP>+≡
  procedure :: has_index => event_has_index
  procedure :: get_index => event_get_index
  procedure :: get_fac_scale => event_get_fac_scale
  procedure :: get_alpha_s => event_get_alpha_s
  procedure :: get_sqrts => event_get_sqrts
  procedure :: get_polarization => event_get_polarization
  procedure :: get_beam_file => event_get_beam_file
  procedure :: get_process_name => event_get_process_name

```

```

<Events: procedures>+≡
function event_has_index (event) result (flag)
  class(event_t), intent(in) :: event
  logical :: flag
  flag = event%expr%has_event_index ()
end function event_has_index

function event_get_index (event) result (index)
  class(event_t), intent(in) :: event
  integer :: index
  index = event%expr%get_event_index ()
end function event_get_index

function event_get_fac_scale (event) result (fac_scale)
  class(event_t), intent(in) :: event
  real(default) :: fac_scale
  fac_scale = event%instance%get_fac_scale (event%selected_i_term)
end function event_get_fac_scale

function event_get_alpha_s (event) result (alpha_s)
  class(event_t), intent(in) :: event
  real(default) :: alpha_s
  alpha_s = event%instance%get_alpha_s (event%selected_i_term)
end function event_get_alpha_s

function event_get_sqrts (event) result (sqrts)
  class(event_t), intent(in) :: event
  real(default) :: sqrts
  sqrts = event%instance%get_sqrts ()
end function event_get_sqrts

function event_get_polarization (event) result (pol)
  class(event_t), intent(in) :: event
  real(default), dimension(2) :: pol
  pol = event%instance%get_polarization ()
end function event_get_polarization

function event_get_beam_file (event) result (file)
  class(event_t), intent(in) :: event
  type(string_t) :: file
  file = event%instance%get_beam_file ()
end function event_get_beam_file

function event_get_process_name (event) result (name)
  class(event_t), intent(in) :: event
  type(string_t) :: name
  name = event%instance%get_process_name ()
end function event_get_process_name

```

Return the actual number of calls, as stored in the process instance.

```

<Events: event: TBP>+≡
  procedure :: get_actual_calls_total => event_get_actual_calls_total
<Events: procedures>+≡

```

```

elemental function event_get_actual_calls_total (event) result (n)
  class(event_t), intent(in) :: event
  integer :: n
  if (associated (event%instance)) then
    n = event%instance%get_actual_calls_total ()
  else
    n = 0
  end if
end function event_get_actual_calls_total

```

Eliminate numerical noise in the `subevt` expression and in the event transforms (which includes associated process instances).

```

⟨Events: public⟩+≡
  public :: pacify

⟨Events: interfaces⟩≡
  interface pacify
    module procedure pacify_event
  end interface pacify

⟨Events: procedures⟩+≡
  subroutine pacify_event (event)
    class(event_t), intent(inout) :: event
    class(evt_t), pointer :: evt
    call event%pacify_particle_set ()
    if (event%expr%subevt_filled) call pacify (event%expr)
    evt => event%transform_first
    do while (associated (evt))
      select type (evt)
        type is (evt_decay_t); call pacify (evt)
      end select
      evt => evt%next
    end do
  end subroutine pacify_event

```

32.10.10 Unit tests

Test module, followed by the corresponding implementation module.

```

⟨events_ut.f90⟩≡
  ⟨File header⟩

  module events_ut
    use unit_tests
    use events_utl

    ⟨Standard module head⟩

    ⟨Events: public test⟩

    contains

    ⟨Events: test driver⟩

```

```

    end module events_ut

    <events_uti.f90>≡
    <File header>

    module events_uti

    <Use kinds>
    <Use strings>
    use os_interface
    use model_data
    use particles
    use process_libraries
    use process_stacks
    use event_transforms
    use decays
    use decays_ut, only: prepare_testbed

    use process, only: process_t
    use instances, only: process_instance_t

    use events

    <Standard module head>

    <Events: test declarations>

    contains

    <Events: tests>

    end module events_uti

```

API: driver for the unit tests below.

```

    <Events: public test>≡
    public :: events_test

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

```

Empty event record

```

    <Events: execute tests>≡
    call test (events_1, "events_1", &
    "empty event record", &
    u, results)

    <Events: test declarations>≡
    public :: events_1

```



```

<Events: tests>≡
subroutine events_1 (u)
  integer, intent(in) :: u
  type(event_t), target :: event

  write (u, "(A)")  "* Test output: events_1"
  write (u, "(A)")  "* Purpose: display an empty event object"
  write (u, "(A)")

  call event%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: events_1"

end subroutine events_1

```

Simple event

```

<Events: execute tests>+≡
call test (events_2, "events_2", &
  "generate event", &
  u, results)

<Events: test declarations>+≡
public :: events_2

<Events: tests>+≡
subroutine events_2 (u)
  use processes_ut, only: prepare_test_process, cleanup_test_process
  integer, intent(in) :: u
  type(event_t), allocatable, target :: event
  type(process_t), allocatable, target :: process
  type(process_instance_t), allocatable, target :: process_instance
  type(model_data_t), target :: model

  write (u, "(A)")  "* Test output: events_2"
  write (u, "(A)")  "* Purpose: generate and display an event"
  write (u, "(A)")

  call model%init_test ()

  write (u, "(A)")  "* Generate test process event"

  allocate (process)
  allocate (process_instance)
  call prepare_test_process (process, process_instance, model)
  call process_instance%setup_event_data ()

  write (u, "(A)")
  write (u, "(A)")  "* Initialize event object"

  allocate (event)
  call event%basic_init ()
  call event%connect (process_instance, process%get_model_ptr ())

```

```

write (u, "(A)")
write (u, "(A)")  "* Generate test process event"

call process_instance%generate_weighted_event (1)

write (u, "(A)")
write (u, "(A)")  "* Fill event object"
write (u, "(A)")

call event%generate (1, [0.4_default, 0.4_default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call event%final ()
deallocate (event)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_2"

end subroutine events_2

```

Recovering an event

Generate an event and store the particle set. Then reset the event record, recall the particle set, and recover the event from that.

```

<Events: execute tests>+≡
  call test (events_4, "events_4", &
    "recover event", &
    u, results)

<Events: test declarations>+≡
  public :: events_4

<Events: tests>+≡
  subroutine events_4 (u)
    use processes_ut, only: prepare_test_process, cleanup_test_process
    integer, intent(in) :: u
    type(event_t), allocatable, target :: event
    type(process_t), allocatable, target :: process
    type(process_instance_t), allocatable, target :: process_instance
    type(process_t), allocatable, target :: process2
    type(process_instance_t), allocatable, target :: process2_instance

```

```

type(particle_set_t) :: particle_set
type(model_data_t), target :: model

write (u, "(A)")  "* Test output: events_4"
write (u, "(A)")  "* Purpose: generate and recover an event"
write (u, "(A)")

call model%init_test ()

write (u, "(A)")  "* Generate test process event and save particle set"
write (u, "(A)")

allocate (process)
allocate (process_instance)
call prepare_test_process (process, process_instance, model)
call process_instance%setup_event_data ()

allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())

call event%generate (1, [0.4_default, 0.4_default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)

particle_set = event%get_particle_set_ptr ()
! NB: 'particle_set' contains pointers to the model within 'process'

call event%final ()
deallocate (event)

write (u, "(A)")
write (u, "(A)")  "* Recover event from particle set"
write (u, "(A)")

allocate (process2)
allocate (process2_instance)
call prepare_test_process (process2, process2_instance, model)
call process2_instance%setup_event_data ()

allocate (event)
call event%basic_init ()
call event%connect (process2_instance, process2%get_model_ptr ())

call event%select (1, 1, 1)
call event%set_hard_particle_set (particle_set)
call event%recalculate (update_sqme = .true.)
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Transfer sqme and evaluate expressions"
write (u, "(A)")

```

```

call event%accept_sqme_prc ()
call event%accept_weight_prc ()
call event%check ()
call event%set_index (1)
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Reset contents"
write (u, "(A)")

call event%reset_contents ()
call event%reset_index ()
event%transform_first%particle_set_exists = .false.
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call particle_set%final ()

call event%final ()
deallocate (event)

call cleanup_test_process (process2, process2_instance)
deallocate (process2_instance)
deallocate (process2)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_4"

end subroutine events_4

```

Partially Recovering an event

Generate an event and store the particle set. Then reset the event record, recall the particle set, and recover the event as far as possible without recomputing the squared matrix element.

```

(Events: execute tests)+≡
  call test (events_5, "events_5", &
    "partially recover event", &
    u, results)

(Events: test declarations)+≡
  public :: events_5

```

```

<Events: tests>+≡
subroutine events_5 (u)
  use processes_ut, only: prepare_test_process, cleanup_test_process
  integer, intent(in) :: u
  type(event_t), allocatable, target :: event
  type(process_t), allocatable, target :: process
  type(process_instance_t), allocatable, target :: process_instance
  type(process2_t), allocatable, target :: process2
  type(process_instance2_t), allocatable, target :: process2_instance
  type(particle_set_t) :: particle_set
  real(default) :: sqme, weight
  type(model_data_t), target :: model

  write (u, "(A)")  "* Test output: events_5"
  write (u, "(A)")  "* Purpose: generate and recover an event"
  write (u, "(A)")

  call model%init_test ()

  write (u, "(A)")  "* Generate test process event and save particle set"
  write (u, "(A)")

  allocate (process)
  allocate (process_instance)
  call prepare_test_process (process, process_instance, model)
  call process_instance%setup_event_data ()

  allocate (event)
  call event%basic_init ()
  call event%connect (process_instance, process%get_model_ptr ())

  call event%generate (1, [0.4_default, 0.4_default])
  call event%increment_index ()
  call event%evaluate_expressions ()
  call event%write (u)

  particle_set = event%get_particle_set_ptr ()
  sqme = event%get_sqme_ref ()
  weight = event%get_weight_ref ()

  call event%final ()
  deallocate (event)

  write (u, "(A)")
  write (u, "(A)")  "* Recover event from particle set"
  write (u, "(A)")

  allocate (process2)
  allocate (process2_instance)
  call prepare_test_process (process2, process2_instance, model)
  call process2_instance%setup_event_data ()

  allocate (event)
  call event%basic_init ()

```

```

call event%connect (process2_instance, process2%get_model_ptr ())

call event%select (1, 1, 1)
call event%set_hard_particle_set (particle_set)
call event%recalculate (update_sqme = .false.)
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Manually set sqme and evaluate expressions"
write (u, "(A)")

call event%set (sqme_ref = sqme, weight_ref = weight)
call event%accept_sqme_ref ()
call event%accept_weight_ref ()
call event%set_index (1)
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call particle_set%final ()

call event%final ()
deallocate (event)

call cleanup_test_process (process2, process2_instance)
deallocate (process2_instance)
deallocate (process2)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_5"

end subroutine events_5

```

Decays

Generate an event with subsequent decays.

```

<Events: execute tests>+≡
  call test (events_6, "events_6", &
    "decays", &
    u, results)

<Events: test declarations>+≡
  public :: events_6

<Events: tests>+≡
  subroutine events_6 (u)

```

```

integer, intent(in) :: u
type(os_data_t) :: os_data
class(model_data_t), pointer :: model
type(string_t) :: prefix, procname1, procname2
type(process_library_t), target :: lib
type(process_stack_t) :: process_stack
class(evt_t), pointer :: evt_decay
type(event_t), allocatable, target :: event
type(process_t), pointer :: process
type(process_instance_t), allocatable, target :: process_instance

write (u, "(A)")  "* Test output: events_6"
write (u, "(A)")  "* Purpose: generate an event with subsequent decays"
write (u, "(A)")

write (u, "(A)")  "* Generate test process and decay"
write (u, "(A)")

call os_data%init ()

prefix = "events_6"
procname1 = prefix // "_p"
procname2 = prefix // "_d"
call prepare_testbed &
      (lib, process_stack, prefix, os_data, &
       scattering=.true., decay=.true.)

write (u, "(A)")  "* Initialize decay process"

process => process_stack%get_process_ptr (procname1)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2])

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
call process_instance%init_simulation (1)

write (u, "(A)")
write (u, "(A)")  "* Initialize event transform: decay"

allocate (evt_decay_t :: evt_decay)
call evt_decay%connect (process_instance, model, process_stack)

write (u, "(A)")
write (u, "(A)")  "* Initialize event object"
write (u, "(A)")

allocate (event)
call event%basic_init ()
call event%connect (process_instance, model)
call event%import_transform (evt_decay)

call event%write (u, show_decay = .true.)

```

```

write (u, "(A)")
write (u, "(A)")  "* Generate event"
write (u, "(A)")

call event%generate (1, [0.4_default, 0.4_default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call event%final ()
deallocate (event)

call process_instance%final ()
deallocate (process_instance)

call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_6"

end subroutine events_6

```

Decays

Generate a decay event with varying options.

```

<Events: execute tests>+≡
  call test (events_7, "events_7", &
    "decay options", &
    u, results)

<Events: test declarations>+≡
  public :: events_7

<Events: tests>+≡
  subroutine events_7 (u)
    integer, intent(in) :: u
    type(os_data_t) :: os_data
    class(model_data_t), pointer :: model
    type(string_t) :: prefix, procname2
    type(process_library_t), target :: lib
    type(process_stack_t) :: process_stack
    type(process_t), pointer :: process
    type(process_instance_t), allocatable, target :: process_instance

    write (u, "(A)")  "* Test output: events_7"
    write (u, "(A)")  "* Purpose: check decay options"
    write (u, "(A)")

    write (u, "(A)")  "* Prepare test process"
    write (u, "(A)")

```



```

call os_data%init ()

prefix = "events_7"
procname2 = prefix // "_d"
call prepare_testbed &
    (lib, process_stack, prefix, os_data, &
    scattering=.false., decay=.true.)

write (u, "(A)")  "* Generate decay event, default options"
write (u, "(A)")

process => process_stack%get_process_ptr (procname2)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2])

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data (model)
call process_instance%init_simulation (1)

call process_instance%generate_weighted_event (1)
call process_instance%write (u)

call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Generate decay event, helicity-diagonal decay"
write (u, "(A)")

process => process_stack%get_process_ptr (procname2)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2], diagonal = .true.)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data (model)
call process_instance%init_simulation (1)

call process_instance%generate_weighted_event (1)
call process_instance%write (u)

call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Generate decay event, isotropic decay, &
    &polarized final state"
write (u, "(A)")

process => process_stack%get_process_ptr (procname2)
model => process%get_model_ptr ()
call model%set_unstable (25, [procname2], isotropic = .true.)

```

```

call model%set_polarized (6)
call model%set_polarized (-6)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data (model)
call process_instance%init_simulation (1)

call process_instance%generate_weighted_event (1)
call process_instance%write (u)

call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_stack%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_7"

end subroutine events_7

```

32.11 Raw Event I/O

The raw format is for internal use only. All data are stored unformatted, so they can be efficiently be re-read on the same machine, but not necessarily on another machine.

This module explicitly depends on the `events` module which provides the concrete implementation of `event_base`. The other I/O formats access only the methods that are defined in `event_base`.

```

<eio_raw.f90>≡
  <File header>

  module eio_raw

    <Use kinds>
    <Use strings>
    use io_units
    use diagnostics
    use model_data
    use particles
    use event_base
    use event_handles, only: event_handle_t
    use eio_data
    use eio_base
    use events

    <Standard module head>

```

⟨EIO raw: public⟩

⟨EIO raw: parameters⟩

⟨EIO raw: types⟩

contains

⟨EIO raw: procedures⟩

end module eio_raw

32.11.1 File Format Version

This is the current default file version.

```
⟨EIO raw: parameters⟩≡  
  integer, parameter :: CURRENT_FILE_VERSION = 2
```

The user may change this number; this should force some compatibility mode for reading and writing. In any case, the file version stored in a event file that we read has to match the expected file version.

History of version numbers:

1. Format for WHIZARD 2.2.0 to 2.2.3. No version number stored in the raw file.
2. Format from 2.2.4 on. File contains version number. The file contains the transformed particle set (if applicable) after the hard-process particle set.

32.11.2 Type

Note the file version number. The default may be reset during initialization, which should enforce some compatibility mode.

```
⟨EIO raw: public⟩≡  
  public :: eio_raw_t  
  
⟨EIO raw: types⟩≡  
  type, extends (eio_t) :: eio_raw_t  
    logical :: reading = .false.  
    logical :: writing = .false.  
    integer :: unit = 0  
    integer :: norm_mode = NORM_UNDEFINED  
    real(default) :: sigma = 1  
    integer :: n = 1  
    integer :: n_alt = 0  
    logical :: check = .false.  
    logical :: use_alphas_from_file = .false.  
    logical :: use_scale_from_file = .false.  
    logical :: fixed_order_nlo = .false.  
    integer :: file_version = CURRENT_FILE_VERSION  
  contains  
    ⟨EIO raw: eio raw: TBP⟩  
  end type eio_raw_t
```

Output. This is not the actual event format, but a readable account of the current object status.

```

(EIO raw: eio raw: TBP)≡
  procedure :: write => eio_raw_write

(EIO raw: procedures)≡
  subroutine eio_raw_write (object, unit)
    class(eio_raw_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Raw event stream:"
    write (u, "(3x,A,L1)") "Check MD5 sum      = ", object%check
    if (object%n_alt > 0) then
      write (u, "(3x,A,I0)") "Alternate weights = ", object%n_alt
    end if
    write (u, "(3x,A,L1)") "Alpha_s from file = ", &
      object%use_alphas_from_file
    write (u, "(3x,A,L1)") "Scale from file   = ", &
      object%use_scale_from_file
    write (u, "(3x,A,L1)") "Events for fNLO   = ", &
      object%fixed_order_nlo
    if (object%reading) then
      write (u, "(3x,A,A)") "Reading from file = ", char (object%filename)
    else if (object%writing) then
      write (u, "(3x,A,A)") "Writing to file   = ", char (object%filename)
    else
      write (u, "(3x,A)") "[closed]"
    end if
  end subroutine eio_raw_write

```

Finalizer: close any open file.

```

(EIO raw: eio raw: TBP)+≡
  procedure :: final => eio_raw_final

(EIO raw: procedures)+≡
  subroutine eio_raw_final (object)
    class(eio_raw_t), intent(inout) :: object
    if (object%reading .or. object%writing) then
      write (msg_buffer, "(A,A,A)") "Events: closing raw file '", &
        char (object%filename), "'"
      call msg_message ()
      close (object%unit)
      object%reading = .false.
      object%writing = .false.
    end if
  end subroutine eio_raw_final

```

Set the `check` flag which determines whether we compare checksums on input.

```

(EIO raw: eio raw: TBP)+≡
  procedure :: set_parameters => eio_raw_set_parameters

```

(EIO raw: procedures)+≡

```

subroutine eio_raw_set_parameters (eio, check, use_alphas_from_file, &
    use_scale_from_file, fixed_order_nlo, version_string, extension)
    class(eio_raw_t), intent(inout) :: eio
    logical, intent(in), optional :: check, use_alphas_from_file, &
        use_scale_from_file, fixed_order_nlo
    type(string_t), intent(in), optional :: version_string
    type(string_t), intent(in), optional :: extension
    if (present (check)) eio%check = check
    if (present (use_alphas_from_file)) eio%use_alphas_from_file = &
        use_alphas_from_file
    if (present (use_scale_from_file)) eio%use_scale_from_file = &
        use_scale_from_file
    if (present (fixed_order_nlo)) eio%fixed_order_nlo = &
        fixed_order_nlo
    if (present (version_string)) then
        select case (char (version_string))
        case ("", "2.2.4")
            eio%file_version = CURRENT_FILE_VERSION
        case ("2.2")
            eio%file_version = 1
        case default
            call msg_fatal ("Raw event I/O: unsupported version '" &
                // char (version_string) // "'")
            eio%file_version = 0
        end select
    end if
    if (present (extension)) then
        eio%extension = extension
    else
        eio%extension = "evx"
    end if
end subroutine eio_raw_set_parameters

```

Initialize event writing.

(EIO raw: eio raw: TBP)+≡

```

procedure :: init_out => eio_raw_init_out

```

(EIO raw: procedures)+≡

```

subroutine eio_raw_init_out (eio, sample, data, success, extension)
    class(eio_raw_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(event_sample_data_t), intent(in), optional :: data
    logical, intent(out), optional :: success
    type(string_t), intent(in), optional :: extension
    character(32) :: md5sum_prc, md5sum_cfg
    character(32), dimension(:), allocatable :: md5sum_alt
    integer :: i
    if (present (extension)) then
        eio%extension = extension
    else
        eio%extension = "evx"
    end if
    eio%filename = sample // "." // eio%extension

```

```

eio%unit = free_unit ()
write (msg_buffer, "(A,A,A)") "Events: writing to raw file '", &
    char (eio%filename), "'"
call msg_message ()
eio%writing = .true.
if (present (data)) then
    md5sum_prc = data%md5sum_prc
    md5sum_cfg = data%md5sum_cfg
    eio%norm_mode = data%norm_mode
    eio%sigma = data%total_cross_section
    eio%n = data%n_evt
    eio%n_alt = data%n_alt
    if (eio%n_alt > 0) then
        !!! !!! !!! Workaround for gfortran 5.0 ICE
        allocate (md5sum_alt (data%n_alt))
        md5sum_alt = data%md5sum_alt
        !!! allocate (md5sum_alt (data%n_alt), source = data%md5sum_alt)
    end if
else
    md5sum_prc = ""
    md5sum_cfg = ""
end if
open (eio%unit, file = char (eio%filename), form = "unformatted", &
    action = "write", status = "replace")
select case (eio%file_version)
case (2:); write (eio%unit) eio%file_version
end select
write (eio%unit) md5sum_prc
write (eio%unit) md5sum_cfg
write (eio%unit) eio%norm_mode
write (eio%unit) eio%n_alt
if (allocated (md5sum_alt)) then
    do i = 1, eio%n_alt
        write (eio%unit) md5sum_alt(i)
    end do
end if
if (present (success)) success = .true.
end subroutine eio_raw_init_out

```

Initialize event reading.

(EIO raw: eio raw: TBP)+≡

```

procedure :: init_in => eio_raw_init_in

```

(EIO raw: procedures)+≡

```

subroutine eio_raw_init_in (eio, sample, data, success, extension)
    class(eio_raw_t), intent(inout) :: eio
    type(string_t), intent(in) :: sample
    type(event_sample_data_t), intent(inout), optional :: data
    logical, intent(out), optional :: success
    type(string_t), intent(in), optional :: extension
    character(32) :: md5sum_prc, md5sum_cfg
    character(32), dimension(:), allocatable :: md5sum_alt
    integer :: i, file_version
    if (present (success)) success = .true.

```

```

if (present (extension)) then
    eio%extension = extension
else
    eio%extension = "evx"
end if
eio%filename = sample // "." // eio%extension
eio%unit = free_unit ()
if (present (data)) then
    eio%sigma = data%total_cross_section
    eio%n = data%n_evt
end if
write (msg_buffer, "(A,A,A)") "Events: reading from raw file '", &
    char (eio%filename), "'"
call msg_message ()
eio%reading = .true.
open (eio%unit, file = char (eio%filename), form = "unformatted", &
    action = "read", status = "old")
select case (eio%file_version)
case (2:); read (eio%unit) file_version
case default; file_version = 1
end select
if (file_version /= eio%file_version) then
    call msg_error ("Reading event file: raw-file version mismatch.")
    if (present (success)) success = .false.
    return
else if (file_version /= CURRENT_FILE_VERSION) then
    call msg_warning ("Reading event file: compatibility mode.")
end if
read (eio%unit) md5sum_prc
read (eio%unit) md5sum_cfg
read (eio%unit) eio%norm_mode
read (eio%unit) eio%n_alt
if (present (data)) then
    if (eio%n_alt /= data%n_alt) then
        if (present (success)) success = .false.
        return
    end if
end if
allocate (md5sum_alt (eio%n_alt))
do i = 1, eio%n_alt
    read (eio%unit) md5sum_alt(i)
end do
if (present (success)) then
    if (present (data)) then
        if (eio%check) then
            if (data%md5sum_prc /= "") then
                success = success .and. md5sum_prc == data%md5sum_prc
            end if
            if (data%md5sum_cfg /= "") then
                success = success .and. md5sum_cfg == data%md5sum_cfg
            end if
            do i = 1, eio%n_alt
                if (data%md5sum_alt(i) /= "") then
                    success = success .and. md5sum_alt(i) == data%md5sum_alt(i)
                end if
            end do
        end if
    end if
end if

```

```

        end if
    end do
    else
        call msg_warning ("Reading event file: MD5 sum check disabled")
    end if
end if
end if
end if
end subroutine eio_raw_init_in

```

Switch from input to output: reopen the file for reading.

```

<EIO raw: eio raw: TBP>+≡
    procedure :: switch_inout => eio_raw_switch_inout

<EIO raw: procedures>+≡
    subroutine eio_raw_switch_inout (eio, success)
        class(eio_raw_t), intent(inout) :: eio
        logical, intent(out), optional :: success
        write (msg_buffer, "(A,A,A)") "Events: appending to raw file '", &
            char (eio%filename), "'"
        call msg_message ()
        close (eio%unit, status = "keep")
        eio%reading = .false.
        open (eio%unit, file = char (eio%filename), form = "unformatted", &
            action = "write", position = "append", status = "old")
        eio%writing = .true.
        if (present (success)) success = .true.
    end subroutine eio_raw_switch_inout

```

Output an event. Write first the event indices, then weight and squared matrix element, then the particle set.

We always write the particle set of the hard process. (Note: this should be reconsidered.) We do make a physical copy.

On output, we write the `prc` values for weight and `sqme`, since these are the values just computed. On input, we store the values as `ref` values. The caller can then decide whether to recompute values and thus obtain distinct `prc` values, or just accept them.

The `passed` flag is not written. This allow us to apply different selection criteria upon rereading.

```

<EIO raw: eio raw: TBP>+≡
    procedure :: output => eio_raw_output

<EIO raw: procedures>+≡
    subroutine eio_raw_output &
        (eio, event, i_prc, reading, passed, pacify, event_handle)
        class(eio_raw_t), intent(inout) :: eio
        class(generic_event_t), intent(in), target :: event
        logical, intent(in), optional :: reading, passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        integer, intent(in) :: i_prc
        type(particle_set_t), pointer :: pset
        integer :: i
        if (eio%writing) then
            if (event%has_valid_particle_set ()) then

```



```

select type (event)
type is (event_t)
  write (eio%unit) i_prc
  write (eio%unit) event%get_index ()
  write (eio%unit) event%get_i_mci ()
  write (eio%unit) event%get_i_term ()
  write (eio%unit) event%get_channel ()
  write (eio%unit) event%expr%weight_prc
  write (eio%unit) event%expr%excess_prc
  write (eio%unit) event%get_n_dropped ()
  write (eio%unit) event%expr%sqme_prc
  do i = 1, eio%n_alt
    write (eio%unit) event%expr%weight_alt(i)
    write (eio%unit) event%expr%sqme_alt(i)
  end do
  allocate (pset)
  call event%get_hard_particle_set (pset)
  call pset%write_raw (eio%unit)
  call pset%final ()
  deallocate (pset)
  select case (eio%file_version)
  case (2:)
    if (event%has_transform ()) then
      write (eio%unit) .true.
      pset => event%get_particle_set_ptr ()
      call pset%write_raw (eio%unit)
    else
      write (eio%unit) .false.
    end if
  end select
class default
  call msg_bug ("Event: write raw: defined only for full event_t")
end select
else
  call msg_bug ("Event: write raw: particle set is undefined")
end if
else
  call eio%write ()
  call msg_fatal ("Raw event file is not open for writing")
end if
end subroutine eio_raw_output

```

Input an event.

Note: the particle set is physically copied. If there is a performance issue, we might choose to pointer-assign it instead, with a different version of `event%set_hard_particle_set`.

```

<EIO raw: eio raw: TBP>+≡
  procedure :: input_i_prc => eio_raw_input_i_prc
  procedure :: input_event => eio_raw_input_event

<EIO raw: procedures>+≡
  subroutine eio_raw_input_i_prc (eio, i_prc, iostat)
    class(eio_raw_t), intent(inout) :: eio
    integer, intent(out) :: i_prc

```

```

integer, intent(out) :: iostat
if (eio%reading) then
    read (eio%unit, iostat = iostat) i_prc
else
    call eio%write ()
    call msg_fatal ("Raw event file is not open for reading")
end if
end subroutine eio_raw_input_i_prc

subroutine eio_raw_input_event (eio, event, iostat, event_handle)
class(eio_raw_t), intent(inout) :: eio
class(generic_event_t), intent(inout), target :: event
integer, intent(out) :: iostat
class(event_handle_t), intent(inout), optional :: event_handle
integer :: event_index, i_mci, i_term, channel, i
real(default) :: weight, excess, sqme
integer :: n_dropped
real(default), dimension(:), allocatable :: weight_alt, sqme_alt
logical :: has_transform
type(particle_set_t), pointer :: pset
class(model_data_t), pointer :: model
if (eio%reading) then
    select type (event)
    type is (event_t)
        read (eio%unit, iostat = iostat) event_index
        if (iostat /= 0) return
        read (eio%unit, iostat = iostat) i_mci
        if (iostat /= 0) return
        read (eio%unit, iostat = iostat) i_term
        if (iostat /= 0) return
        read (eio%unit, iostat = iostat) channel
        if (iostat /= 0) return
        read (eio%unit, iostat = iostat) weight
        if (iostat /= 0) return
        read (eio%unit, iostat = iostat) excess
        if (iostat /= 0) return
        read (eio%unit, iostat = iostat) n_dropped
        if (iostat /= 0) return
        read (eio%unit, iostat = iostat) sqme
        if (iostat /= 0) return
        call event%reset_contents ()
        call event%set_index (event_index)
        call event%select (i_mci, i_term, channel)
        if (eio%norm_mode /= NORM_UNDEFINED) then
            call event_normalization_update (weight, &
                eio%sigma, eio%n, event%get_norm_mode (), eio%norm_mode)
            call event_normalization_update (excess, &
                eio%sigma, eio%n, event%get_norm_mode (), eio%norm_mode)
        end if
        call event%set (sqme_ref = sqme, weight_ref = weight, &
            excess_prc = excess, &
            n_dropped = n_dropped)
        if (eio%n_alt /= 0) then
            allocate (sqme_alt (eio%n_alt), weight_alt (eio%n_alt))

```

```

do i = 1, eio%n_alt
  read (eio%unit, iostat = iostat) weight_alt(i)
  if (iostat /= 0) return
  read (eio%unit, iostat = iostat) sqme_alt(i)
  if (iostat /= 0) return
end do
call event%set (sqme_alt = sqme_alt, weight_alt = weight_alt)
end if
model => null ()
if (associated (event%process)) then
  model => event%process%get_model_ptr ()
end if
allocate (pset)
call pset%read_raw (eio%unit, iostat)
if (iostat /= 0) return
if (associated (model)) call pset%set_model (model)
call event%set_hard_particle_set (pset)
if (eio%use_alphas_from_file .or. eio%use_scale_from_file) then
  call event%recalculate (update_sqme = .true.)
  if (eio%fixed_order_nlo) then
    if (event%weight_prc /= event%weight_ref .and. &
        event%weight_prc == 0) then
      event%weight_prc = event%weight_ref
    end if
  end if
end if
call pset%final ()
deallocate (pset)
select case (eio%file_version)
case (2:)
  read (eio%unit, iostat = iostat) has_transform
  if (iostat /= 0) return
  if (has_transform) then
    allocate (pset)
    call pset%read_raw (eio%unit, iostat)
    if (iostat /= 0) return
    if (associated (model)) &
      call pset%set_model (model)
    call event%link_particle_set (pset)
  end if
end select
class default
  call msg_bug ("Event: read raw: defined only for full event_t")
end select
else
  call eio%write ()
  call msg_fatal ("Raw event file is not open for reading")
end if
end subroutine eio_raw_input_event

```

(EIO raw: eio raw: TBP)+≡
 procedure :: skip => eio_raw_skip
(EIO raw: procedures)+≡

```

subroutine eio_raw_skip (eio, iostat)
  class(eio_raw_t), intent(inout) :: eio
  integer, intent(out) :: iostat
  if (eio%reading) then
    read (eio%unit, iostat = iostat)
  else
    call eio%write ()
    call msg_fatal ("Raw event file is not open for reading")
  end if
end subroutine eio_raw_skip

```

32.11.3 Unit tests

Test module, followed by the corresponding implementation module.

<eio_raw_ut.f90>≡

<File header>

```

module eio_raw_ut
  use unit_tests
  use eio_raw_uti

```

<Standard module head>

<EIO raw: public test>

contains

<EIO raw: test driver>

```

end module eio_raw_ut

```

<eio_raw_uti.f90>≡

<File header>

```

module eio_raw_uti

```

<Use kinds>

<Use strings>

```

  use model_data
  use variables
  use events
  use eio_data
  use eio_base

```

```

  use eio_raw

```

```

  use process, only: process_t

```

```

  use instances, only: process_instance_t

```

<Standard module head>

<EIO raw: test declarations>

contains

<EIO raw: tests>

end module eio_raw_util

API: driver for the unit tests below.

<EIO raw: public test>≡

public :: eio_raw_test

<EIO raw: test driver>≡

subroutine eio_raw_test (u, results)

integer, intent(in) :: u

type(test_results_t), intent(inout) :: results

<EIO raw: execute tests>

end subroutine eio_raw_test

Test I/O methods

We test the implementation of all I/O methods.

<EIO raw: execute tests>≡

call test (eio_raw_1, "eio_raw_1", &
"read and write event contents", &
u, results)

<EIO raw: test declarations>≡

public :: eio_raw_1

<EIO raw: tests>≡

subroutine eio_raw_1 (u)

use processes_util, only: prepare_test_process, cleanup_test_process

integer, intent(in) :: u

type(model_data_t), target :: model

type(event_t), allocatable, target :: event

type(process_t), allocatable, target :: process

type(process_instance_t), allocatable, target :: process_instance

class(eio_t), allocatable :: eio

integer :: i_prc, iostat

type(string_t) :: sample

write (u, "(A)") "* Test output: eio_raw_1"

write (u, "(A)") "* Purpose: generate and read/write an event"

write (u, "(A)")

write (u, "(A)") "* Initialize test process"

call model%init_test ()

allocate (process)

allocate (process_instance)

call prepare_test_process (process, process_instance, model, &

run_id = var_str ("run_test"))

call process_instance%setup_event_data ()

```

allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_raw_1"

allocate (eio_raw_t :: eio)

call eio%init_out (sample)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)
write (u, "(A)")

call eio%output (event, i_prc = 42)
call eio%write (u)
call eio%final ()

call event%final ()
deallocate (event)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event"
write (u, "(A)")

call eio%init_in (sample)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())

call eio%input_i_prc (i_prc, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (i_prc):", iostat
call eio%input_event (event, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (event):", iostat
call eio%write (u)

write (u, "(A)")
write (u, "(1x,A,I0)") "i_prc = ", i_prc
write (u, "(A)")
call event%write (u)
write (u, "(A)")
write (u, "(A)")  "* Generate and append another event"
write (u, "(A)")

```

```

call eio%switch_inout ()
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%write (u)
write (u, "(A)")

call eio%output (event, i_prc = 5)
call eio%write (u)
call eio%final ()

call event%final ()
deallocate (event)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Re-read both events"
write (u, "(A)")

call eio%init_in (sample)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())

call eio%input_i_prc (i_prc, iostat)
if (iostat /= 0) write (u, "(A,I0)")  "I/O error (i_prc/1):", iostat
call eio%input_event (event, iostat)
if (iostat /= 0) write (u, "(A,I0)")  "I/O error (event/1):", iostat
call eio%input_i_prc (i_prc, iostat)
if (iostat /= 0) write (u, "(A,I0)")  "I/O error (i_prc/2):", iostat
call eio%input_event (event, iostat)
if (iostat /= 0) write (u, "(A,I0)")  "I/O error (event/2):", iostat
call eio%write (u)

write (u, "(A)")
write (u, "(1x,A,I0)")  "i_prc = ", i_prc
write (u, "(A)")
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
deallocate (eio)

call event%final ()
deallocate (event)

```

```

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_raw_1"

end subroutine eio_raw_1

```

Test I/O methods

We test the implementation of all I/O methods.

```

<EIO raw: execute tests>+≡
call test (eio_raw_2, "eio_raw_2", &
    "handle multiple weights", &
    u, results)

<EIO raw: test declarations>+≡
public :: eio_raw_2

<EIO raw: tests>+≡
subroutine eio_raw_2 (u)
    use processes_ut, only: prepare_test_process, cleanup_test_process
    integer, intent(in) :: u
    type(model_data_t), target :: model
    type(var_list_t) :: var_list
    type(event_t), allocatable, target :: event
    type(process_t), allocatable, target :: process
    type(process_instance_t), allocatable, target :: process_instance
    type(event_sample_data_t) :: data
    class(eio_t), allocatable :: eio
    integer :: i_prc, iostat
    type(string_t) :: sample

    write (u, "(A)")  "* Test output: eio_raw_2"
    write (u, "(A)")  "* Purpose: generate and read/write an event"
    write (u, "(A)")  "*           with multiple weights"
    write (u, "(A)")

    call model%init_test ()

    write (u, "(A)")  "* Initialize test process"

    allocate (process)
    allocate (process_instance)
    call prepare_test_process (process, process_instance, model, &
        run_id = var_str ("run_test"))
    call process_instance%setup_event_data ()

    call data%init (n_proc = 1, n_alt = 2)

    call var_list_append_log (var_list, var_str ("?unweighted"), .false., &

```



```

        intrinsic = .true.)
call var_list_append_string (var_list, var_str ("sample_normalization"), &
    var_str ("auto"), intrinsic = .true.)
call var_list_append_real (var_list, var_str ("safety_factor"), &
    1._default, intrinsic = .true.)

allocate (event)
call event%basic_init (var_list, n_alt = 2)
call event%connect (process_instance, process%get_model_ptr ())

write (u, "(A)")
write (u, "(A)")  "* Generate and write an event"
write (u, "(A)")

sample = "eio_raw_2"

allocate (eio_raw_t :: eio)

call eio%init_out (sample, data)
call event%generate (1, [0._default, 0._default])
call event%increment_index ()
call event%evaluate_expressions ()
call event%set (sqme_alt = [2._default, 3._default])
call event%set (weight_alt = &
    [2 * event%get_weight_ref (), 3 * event%get_weight_ref ()])
call event%store_alt_values ()
call event%check ()

call event%write (u)
write (u, "(A)")

call eio%output (event, i_prc = 42)
call eio%write (u)
call eio%final ()

call event%final ()
deallocate (event)
call process_instance%final ()
deallocate (process_instance)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event"
write (u, "(A)")

call eio%init_in (sample, data)

allocate (process_instance)
call process_instance%init (process)
call process_instance%setup_event_data ()
allocate (event)
call event%basic_init (var_list, n_alt = 2)
call event%connect (process_instance, process%get_model_ptr ())

call eio%input_i_prc (i_prc, iostat)

```

```

if (iostat /= 0) write (u, "(A,I0)") "I/O error (i_prc):", iostat
call eio%input_event (event, iostat)
if (iostat /= 0) write (u, "(A,I0)") "I/O error (event):", iostat
call eio%write (u)

write (u, "(A)")
write (u, "(1x,A,I0)") "i_prc = ", i_prc
write (u, "(A)")
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
deallocate (eio)

call event%final ()
deallocate (event)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call model%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: eio_raw_2"

end subroutine eio_raw_2

```

32.12 Dispatch

An event transform is responsible for dressing a partonic event. Since event transforms are not mutually exclusive but are concatenated, we provide individual dispatchers for each of them.

```

(dispatch_transforms.f90)≡
  <File header>

  module dispatch_transforms

    <Use kinds>
    <Use strings>
    use process
    use variables
    use system_defs, only: LF
    use system_dependencies, only: LHAPDF6_AVAILABLE
    use sf_lhapdf, only: lhapdf_initialize
    use diagnostics
    use models
    use os_interface
    use beam_structures

```

```

use resonances, only: resonance_history_set_t
use instances, only: process_instance_t, process_instance_hook_t

use event_base, only: event_callback_t, event_callback_nop_t
use hepmc_interface, only: HEPMC3_MODE_HEPMC2, HEPMC3_MODE_HEPMC3
use hepmc_interface, only: HEPMC3_MODE_ROOT, HEPMC3_MODE_ROOTTREE
use hepmc_interface, only: HEPMC3_MODE_HEPEVT
use eio_base
use eio_raw
use eio_checkpoints
use eio_callback
use eio_lhef
use eio_hepmc
use eio_lcio
use eio_stdhep
use eio_ascii
use eio_weights
use eio_dump

use event_transforms
use resonance_insertion
use isr_epa_handler
use decays
use shower_base
use shower_core
use shower
use shower_pythia6
use shower_pythia8
use hadrons
use mlm_matching
use powheg_matching
use ckkw_matching
use tauola_interface !NODEP!
use evt_nlo

<Standard module head>

<Dispatch transforms: public>

contains

<Dispatch transforms: procedures>

end module dispatch_transforms

<Dispatch transforms: public>≡
  public :: dispatch_evt_nlo

<Dispatch transforms: procedures>≡
  subroutine dispatch_evt_nlo (evt, keep_failed_events)
    class(evt_t), intent(out), pointer :: evt
    logical, intent(in) :: keep_failed_events
    call msg_message ("Simulate: activating fixed-order NLO events")
    allocate (evt_nlo_t :: evt)
    evt%only_weighted_events = .true.

```

```

select type (evt)
type is (evt_nlo_t)
    evt%i_evaluation = 0
    evt%keep_failed_events = keep_failed_events
end select
end subroutine dispatch_evt_nlo

```

<Dispatch transforms: public>+≡

```
public :: dispatch_evt_resonance
```

<Dispatch transforms: procedures>+≡

```

subroutine dispatch_evt_resonance (evt, var_list, res_history_set, libname)
class(evt_t), intent(out), pointer :: evt
type(var_list_t), intent(in) :: var_list
type(resonance_history_set_t), dimension(:), intent(in) :: res_history_set
type(string_t), intent(in) :: libname
logical :: resonance_history
resonance_history = var_list%get_lval (var_str ("?resonance_history"))
if (resonance_history) then
    allocate (evt_resonance_t :: evt)
    call msg_message ("Simulate: activating resonance insertion")
    select type (evt)
    type is (evt_resonance_t)
        call evt%set_resonance_data (res_history_set)
        call evt%set_library (libname)
    end select
else
    evt => null ()
end if
end subroutine dispatch_evt_resonance

```

Initialize the ISR/EPA handler, depending on active settings.

The activation is independent for both handlers, since only one may be needed at a time. However, if both handlers are active, the current implementation requires the handler modes of ISR and EPA to coincide.

<Dispatch transforms: public>+≡

```
public :: dispatch_evt_isr_epa_handler
```

<Dispatch transforms: procedures>+≡

```

subroutine dispatch_evt_isr_epa_handler (evt, var_list)
class(evt_t), intent(out), pointer :: evt
type(var_list_t), intent(in) :: var_list
logical :: isr_recoil
logical :: epa_recoil
logical :: isr_handler_active
logical :: epa_handler_active
type(string_t) :: isr_handler_mode
type(string_t) :: epa_handler_mode
logical :: isr_keep_mass
real(default) :: sqrts
real(default) :: isr_q_max
real(default) :: epa_q_max
real(default) :: isr_mass
real(default) :: epa_mass

```

```

isr_handler_active = var_list%get_lval (var_str ("?isr_handler"))
if (isr_handler_active) then
  call msg_message ("Simulate: activating ISR handler")
  isr_recoil = &
    var_list%get_lval (var_str ("?isr_recoil"))
  isr_handler_mode = &
    var_list%get_sval (var_str ("$isr_handler_mode"))
  isr_keep_mass = &
    var_list%get_lval (var_str ("?isr_handler_keep_mass"))
  if (isr_recoil) then
    call msg_fatal ("Simulate: ISR handler is incompatible &
      &with ?isr_recoil=true")
  end if
end if
epa_handler_active = var_list%get_lval (var_str ("?epa_handler"))
if (epa_handler_active) then
  call msg_message ("Simulate: activating EPA handler")
  epa_recoil = var_list%get_lval (var_str ("?epa_recoil"))
  epa_handler_mode = var_list%get_sval (var_str ("$epa_handler_mode"))
  if (epa_recoil) then
    call msg_fatal ("Simulate: EPA handler is incompatible &
      &with ?epa_recoil=true")
  end if
end if
if (isr_handler_active .and. epa_handler_active) then
  if (isr_handler_mode /= epa_handler_mode) then
    call msg_fatal ("Simulate: ISR/EPA handler: modes must coincide")
  end if
end if
if (isr_handler_active .or. epa_handler_active) then
  allocate (evt_isr_epa_t :: evt)
  select type (evt)
  type is (evt_isr_epa_t)
    if (isr_handler_active) then
      call evt%set_mode_string (isr_handler_mode)
    else
      call evt%set_mode_string (epa_handler_mode)
    end if
    sqrts = var_list%get_rval (var_str ("sqrts"))
    if (isr_handler_active) then
      isr_q_max = var_list%get_rval (var_str ("isr_q_max"))
      isr_mass = var_list%get_rval (var_str ("isr_mass"))
      call evt%set_data_isr (sqrts, isr_q_max, isr_mass, isr_keep_mass)
    end if
    if (epa_handler_active) then
      epa_q_max = var_list%get_rval (var_str ("epa_q_max"))
      epa_mass = var_list%get_rval (var_str ("epa_mass"))
      call evt%set_data_epa (sqrts, epa_q_max, epa_mass)
    end if
    call msg_message ("Simulate: ISR/EPA handler mode: " &
      // char (evt%get_mode_string ()))
  end select
else
  evt => null ()

```

```

        end if
    end subroutine dispatch_evt_isr_epa_handler

    <Dispatch transforms: public>+≡
    public :: dispatch_evt_decay

    <Dispatch transforms: procedures>+≡
    subroutine dispatch_evt_decay (evt, var_list)
        class(evt_t), intent(out), pointer :: evt
        type(var_list_t), intent(in), target :: var_list
        logical :: allow_decays
        allow_decays = var_list%get_lval (var_str ("?allow_decays"))
        if (allow_decays) then
            allocate (evt_decay_t :: evt)
            call msg_message ("Simulate: activating decays")
            select type (evt)
            type is (evt_decay_t)
                call evt%set_var_list (var_list)
            end select
        else
            evt => null ()
        end if
    end subroutine dispatch_evt_decay

    <Dispatch transforms: public>+≡
    public :: dispatch_evt_shower

    <Dispatch transforms: procedures>+≡
    subroutine dispatch_evt_shower (evt, var_list, model, fallback_model, &
        os_data, beam_structure, process)
        class(evt_t), intent(out), pointer :: evt
        type(var_list_t), intent(in) :: var_list
        type(model_t), pointer, intent(in) :: model, fallback_model
        type(os_data_t), intent(in) :: os_data
        type(beam_structure_t), intent(in) :: beam_structure
        type(process_t), intent(in), optional :: process
        type(string_t) :: lhpdf_file, lhpdf_dir, process_name
        integer :: lhpdf_member
        type(shower_settings_t) :: settings
        type(taudec_settings_t) :: taudec_settings
        call msg_message ("Simulate: activating parton shower")
        allocate (evt_shower_t :: evt)
        call settings%init (var_list)
        if (associated (model)) then
            call taudec_settings%init (var_list, model)
        else
            call taudec_settings%init (var_list, fallback_model)
        end if
        if (present (process)) then
            process_name = process%get_id ()
        else
            process_name = 'dispatch_testing'
        end if
        select type (evt)

```

```

type is (evt_shower_t)
  call evt%init (fallback_model, os_data)
  lhpdf_member = &
    var_list%get_ival (var_str ("lhpdf_member"))
  if (LHAPDF6_AVAILABLE) then
    lhpdf_dir = &
      var_list%get_sval (var_str ("lhpdf_dir"))
    lhpdf_file = &
      var_list%get_sval (var_str ("lhpdf_file"))
    call lhpdf_initialize &
      (1, lhpdf_dir, lhpdf_file, lhpdf_member, evt%pdf_data%pdf)
  end if
  if (present (process)) call evt%pdf_data%setup ("Shower", &
    beam_structure, lhpdf_member, process%get_pdf_set ())
  select case (settings%method)
  case (PS_WHIZARD)
    allocate (shower_t :: evt%shower)
  case (PS_PYTHIA6)
    allocate (shower_pythia6_t :: evt%shower)
  case (PS_PYTHIA8)
    allocate (shower_pythia8_t :: evt%shower)
  case default
    call msg_fatal ('Shower: Method ' // &
      char (var_list%get_sval (var_str ("shower_method")))) // &
      'not implemented!')
  end select
  call evt%shower%init (settings, taudec_settings, evt%pdf_data, os_data)
end select
call dispatch_matching (evt, settings, var_list, process_name)
end subroutine dispatch_evt_shower

```

<Dispatch transforms: public>+≡

```
public :: dispatch_evt_shower_hook
```

<Dispatch transforms: procedures>+≡

```

subroutine dispatch_evt_shower_hook (hook, var_list, process_instance)
  class(process_instance_hook_t), pointer, intent(out) :: hook
  type(var_list_t), intent(in) :: var_list
  class(process_instance_t), intent(in), target :: process_instance
  if (var_list%get_lval (var_str ('?powheg_matching'))) then
    call msg_message ("Integration hook: add POWHEG hook")
    allocate (powheg_matching_hook_t :: hook)
    call hook%init (var_list, process_instance)
  else
    hook => null ()
  end if
end subroutine dispatch_evt_shower_hook

```

<Dispatch transforms: public>+≡

```
public :: dispatch_matching
```

<Dispatch transforms: procedures>+≡

```

subroutine dispatch_matching (evt, settings, var_list, process_name)
  class(evt_t), intent(inout) :: evt

```

```

type(var_list_t), intent(in) :: var_list
type(string_t), intent(in) :: process_name
type(shower_settings_t), intent(in) :: settings
select type (evt)
type is (evt_shower_t)
  if (settings%mlm_matching .and. settings%ckkw_matching) then
    call msg_fatal ("Both MLM and CKKW matching activated," // &
      LF // "      aborting simulation")
  end if
  if (settings%powheg_matching) then
    call msg_message ("Simulate: applying POWHEG matching")
    allocate (powheg_matching_t :: evt%matching)
  end if
  if (settings%mlm_matching) then
    call msg_message ("Simulate: applying MLM matching")
    allocate (mlm_matching_t :: evt%matching)
  end if
  if (settings%ckkw_matching) then
    call msg_warning ("Simulate: CKKW(-L) matching not yet supported")
    allocate (ckkw_matching_t :: evt%matching)
  end if
  if (allocated (evt%matching)) &
    call evt%matching%init (var_list, process_name)
end select
end subroutine dispatch_matching

```

<Dispatch transforms: public>+≡

```
public :: dispatch_evt_hadrons
```

<Dispatch transforms: procedures>+≡

```

subroutine dispatch_evt_hadrons (evt, var_list, fallback_model)
  class(evt_t), intent(out), pointer :: evt
  type(var_list_t), intent(in) :: var_list
  type(model_t), pointer, intent(in) :: fallback_model
  type(shower_settings_t) :: shower_settings
  type(hadron_settings_t) :: hadron_settings
  allocate (evt_hadrons_t :: evt)
  call msg_message ("Simulate: activating hadronization")
  call shower_settings%init (var_list)
  call hadron_settings%init (var_list)
  select type (evt)
  type is (evt_hadrons_t)
    call evt%init (fallback_model)
    select case (hadron_settings%method)
    case (HADRONS_WHIZARD)
      allocate (hadrons_hadrons_t :: evt%hadrons)
    case (HADRONS_PYTHIA6)
      allocate (hadrons_pythia6_t :: evt%hadrons)
    case (HADRONS_PYTHIA8)
      allocate (hadrons_pythia8_t :: evt%hadrons)
    case default
      call msg_fatal ('Hadronization: Method ' // &
        char (var_list%get_sval (var_str ("hadronization_method")))) // &
        'not implemented!')
    end select
  end select
end subroutine

```



```

        end select
        call evt%hadrons%init &
            (shower_settings, hadron_settings, fallback_model)
    end select
end subroutine dispatch_evt_hadrons

```

We cannot put this in the `events` subdir due to `eio_raw_t`, which is defined here.

```

<Dispatch transforms: public>+≡
    public :: dispatch_eio

<Dispatch transforms: procedures>+≡
    subroutine dispatch_eio (eio, method, var_list, fallback_model, &
        event_callback)
        class(eio_t), allocatable, intent(inout) :: eio
        type(string_t), intent(in) :: method
        type(var_list_t), intent(in) :: var_list
        type(model_t), target, intent(in) :: fallback_model
        class(event_callback_t), allocatable, intent(in) :: event_callback
        logical :: check, keep_beams, keep_remnants, recover_beams
        logical :: use_alphas_from_file, use_scale_from_file
        logical :: fixed_order_nlo_events
        logical :: write_sqme_prc, write_sqme_ref, write_sqme_alt
        logical :: output_cross_section, ensure_order
        type(string_t) :: lhef_version, lhef_extension, raw_version
        type(string_t) :: extension_default, debug_extension, dump_extension, &
            extension_hepmc, &
            extension_lha, extension_hepevt, extension_ascii_short, &
            extension_ascii_long, extension_athena, extension_mokka, &
            extension_stdhep, extension_stdhep_up, extension_stdhep_ev4, &
            extension_raw, extension_hepevt_verb, extension_lha_verb, &
            extension_lcio
        integer :: checkpoint
        integer :: lcio_run_id, hepmc3_mode
        logical :: show_process, show_transforms, show_decay, verbose, pacified
        logical :: dump_weights, dump_compressed, dump_summary, dump_screen
        logical :: proc_as_run_id
        keep_beams = &
            var_list%get_lval (var_str ("?keep_beams"))
        keep_remnants = &
            var_list%get_lval (var_str ("?keep_remnants"))
        ensure_order = &
            var_list%get_lval (var_str ("?hepevt_ensure_order"))
        recover_beams = &
            var_list%get_lval (var_str ("?recover_beams"))
        use_alphas_from_file = &
            var_list%get_lval (var_str ("?use_alphas_from_file"))
        use_scale_from_file = &
            var_list%get_lval (var_str ("?use_scale_from_file"))
        fixed_order_nlo_events = &
            var_list%get_lval (var_str ("?fixed_order_nlo_events"))
        select case (char (method))
        case ("raw")
            allocate (eio_raw_t :: eio)

```

```

select type (eio)
type is (eio_raw_t)
  check = &
    var_list%get_lval (var_str ("?check_event_file"))
  raw_version = &
    var_list%get_sval (var_str ("$event_file_version"))
  extension_raw = &
    var_list%get_sval (var_str ("$extension_raw"))
  call eio%set_parameters (check, use_alphas_from_file, &
    use_scale_from_file, fixed_order_nlo_events, &
    raw_version, extension_raw)
end select
case ("checkpoint")
  allocate (eio_checkpoints_t :: eio)
  select type (eio)
  type is (eio_checkpoints_t)
    checkpoint = &
      var_list%get_ival (var_str ("checkpoint"))
    pacified = &
      var_list%get_lval (var_str ("?pacify"))
    call eio%set_parameters (checkpoint, blank = pacified)
  end select
case ("callback")
  allocate (eio_callback_t :: eio)
  select type (eio)
  type is (eio_callback_t)
    checkpoint = &
      var_list%get_ival (var_str ("event_callback_interval"))
    if (allocated (event_callback)) then
      call eio%set_parameters (event_callback, checkpoint)
    else
      call eio%set_parameters (event_callback_nop_t (), 0)
    end if
  end select
case ("lhef")
  allocate (eio_lhef_t :: eio)
  select type (eio)
  type is (eio_lhef_t)
    lhef_version = &
      var_list%get_sval (var_str ("$lhef_version"))
    lhef_extension = &
      var_list%get_sval (var_str ("$lhef_extension"))
    write_sqme_prc = &
      var_list%get_lval (var_str ("?lhef_write_sqme_prc"))
    write_sqme_ref = &
      var_list%get_lval (var_str ("?lhef_write_sqme_ref"))
    write_sqme_alt = &
      var_list%get_lval (var_str ("?lhef_write_sqme_alt"))
    call eio%set_parameters ( &
      keep_beams, keep_remnants, recover_beams, &
      use_alphas_from_file, use_scale_from_file, &
      char (lhef_version), lhef_extension, &
      write_sqme_ref, write_sqme_prc, write_sqme_alt)
  end select

```

```

case ("hepmc")
  allocate (eio_hepmc_t :: eio)
  select type (eio)
  type is (eio_hepmc_t)
    output_cross_section = &
      var_list%get_lval (var_str ("?hepmc_output_cross_section"))
    extension_hepmc = &
      var_list%get_sval (var_str ("$extension_hepmc"))
    select case (char (var_list%get_sval (var_str ("$hepmc3_mode"))))
    case ("HepMC2")
      hepmc3_mode = HEPMC3_MODE_HEPMC2
    case ("HepMC3")
      hepmc3_mode = HEPMC3_MODE_HEPMC3
    case ("Root")
      hepmc3_mode = HEPMC3_MODE_ROOT
    case ("RootTree")
      hepmc3_mode = HEPMC3_MODE_ROOTTREE
    case ("HepEVT")
      hepmc3_mode = HEPMC3_MODE_HEPEVT
    case default
      call msg_fatal ("Only supported HepMC3 modes are: 'HepMC2', " // &
        "'HepMC3', 'HepEVT', 'Root', and 'RootTree'".)
    end select
    call eio%set_parameters (recover_beams, &
      use_alphas_from_file, use_scale_from_file, &
      extension = extension_hepmc, &
      output_cross_section = output_cross_section, &
      hepmc3_mode = hepmc3_mode)
  end select
case ("lcio")
  allocate (eio_lcio_t :: eio)
  select type (eio)
  type is (eio_lcio_t)
    extension_lcio = &
      var_list%get_sval (var_str ("$extension_lcio"))
    proc_as_run_id = &
      var_list%get_lval (var_str ("?proc_as_run_id"))
    lcio_run_id = &
      var_list%get_ival (var_str ("lcio_run_id"))
    call eio%set_parameters (recover_beams, &
      use_alphas_from_file, use_scale_from_file, &
      extension_lcio, proc_as_run_id = proc_as_run_id, &
      lcio_run_id = lcio_run_id)
  end select
case ("stdhep")
  allocate (eio_stdhep_hepevt_t :: eio)
  select type (eio)
  type is (eio_stdhep_hepevt_t)
    extension_stdhep = &
      var_list%get_sval (var_str ("$extension_stdhep"))
    call eio%set_parameters &
      (keep_beams, keep_remnants, ensure_order, recover_beams, &
      use_alphas_from_file, use_scale_from_file, extension_stdhep)
  end select

```

```

case ("stdhep_up")
  allocate (eio_stdhep_hepeup_t :: eio)
  select type (eio)
  type is (eio_stdhep_hepeup_t)
    extension_stdhep_up = &
      var_list%get_sval (var_str ("$extension_stdhep_up"))
    call eio%set_parameters (keep_beams, keep_remnants, ensure_order, &
      recover_beams, use_alphas_from_file, &
      use_scale_from_file, extension_stdhep_up)
  end select
case ("stdhep_ev4")
  allocate (eio_stdhep_hepev4_t :: eio)
  select type (eio)
  type is (eio_stdhep_hepev4_t)
    extension_stdhep_ev4 = &
      var_list%get_sval (var_str ("$extension_stdhep_ev4"))
    call eio%set_parameters &
      (keep_beams, keep_remnants, ensure_order, recover_beams, &
      use_alphas_from_file, use_scale_from_file, extension_stdhep_ev4)
  end select
case ("ascii")
  allocate (eio_ascii_ascii_t :: eio)
  select type (eio)
  type is (eio_ascii_ascii_t)
    extension_default = &
      var_list%get_sval (var_str ("$extension_default"))
    call eio%set_parameters &
      (keep_beams, keep_remnants, ensure_order, extension_default)
  end select
case ("athena")
  allocate (eio_ascii_athena_t :: eio)
  select type (eio)
  type is (eio_ascii_athena_t)
    extension_athena = &
      var_list%get_sval (var_str ("$extension_athena"))
    call eio%set_parameters &
      (keep_beams, keep_remnants, ensure_order, extension_athena)
  end select
case ("debug")
  allocate (eio_ascii_debug_t :: eio)
  select type (eio)
  type is (eio_ascii_debug_t)
    debug_extension = &
      var_list%get_sval (var_str ("$debug_extension"))
    show_process = &
      var_list%get_lval (var_str ("?debug_process"))
    show_transforms = &
      var_list%get_lval (var_str ("?debug_transforms"))
    show_decay = &
      var_list%get_lval (var_str ("?debug_decay"))
    verbose = &
      var_list%get_lval (var_str ("?debug_verbose"))
    call eio%set_parameters ( &
      extension = debug_extension, &

```

```

        show_process = show_process, &
        show_transforms = show_transforms, &
        show_decay = show_decay, &
        verbose = verbose)
    end select
case ("dump")
    allocate (eio_dump_t :: eio)
    select type (eio)
    type is (eio_dump_t)
        dump_extension = &
            var_list%get_sval (var_str ("$dump_extension"))
        pacified = &
            var_list%get_lval (var_str ("?pacify"))
        dump_weights = &
            var_list%get_lval (var_str ("?dump_weights"))
        dump_compressed = &
            var_list%get_lval (var_str ("?dump_compressed"))
        dump_summary = &
            var_list%get_lval (var_str ("?dump_summary"))
        dump_screen = &
            var_list%get_lval (var_str ("?dump_screen"))
        call eio%set_parameters ( &
            extension = dump_extension, &
            pacify = pacified, &
            weights = dump_weights, &
            compressed = dump_compressed, &
            summary = dump_summary, &
            screen = dump_screen)
    end select
case ("hepevt")
    allocate (eio_ascii_hepevt_t :: eio)
    select type (eio)
    type is (eio_ascii_hepevt_t)
        extension_hepevt = &
            var_list%get_sval (var_str ("$extension_hepevt"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_hepevt)
    end select
case ("hepevt_verb")
    allocate (eio_ascii_hepevt_verb_t :: eio)
    select type (eio)
    type is (eio_ascii_hepevt_verb_t)
        extension_hepevt_verb = &
            var_list%get_sval (var_str ("$extension_hepevt_verb"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_hepevt_verb)
    end select
case ("lha")
    allocate (eio_ascii_lha_t :: eio)
    select type (eio)
    type is (eio_ascii_lha_t)
        extension_lha = &
            var_list%get_sval (var_str ("$extension_lha"))
        call eio%set_parameters &

```

```

        (keep_beams, keep_remnants, ensure_order, extension_lha)
    end select
case ("lha_verb")
    allocate (eio_ascii_lha_verb_t :: eio)
    select type (eio)
    type is (eio_ascii_lha_verb_t)
        extension_lha_verb = var_list%get_sval ( &
            var_str ("$extension_lha_verb"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_lha_verb)
    end select
case ("long")
    allocate (eio_ascii_long_t :: eio)
    select type (eio)
    type is (eio_ascii_long_t)
        extension_ascii_long = &
            var_list%get_sval (var_str ("$extension_ascii_long"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_ascii_long)
    end select
case ("mokka")
    allocate (eio_ascii_mokka_t :: eio)
    select type (eio)
    type is (eio_ascii_mokka_t)
        extension_mokka = &
            var_list%get_sval (var_str ("$extension_mokka"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_mokka)
    end select
case ("short")
    allocate (eio_ascii_short_t :: eio)
    select type (eio)
    type is (eio_ascii_short_t)
        extension_ascii_short = &
            var_list%get_sval (var_str ("$extension_ascii_short"))
        call eio%set_parameters &
            (keep_beams, keep_remnants, ensure_order, extension_ascii_short)
    end select
case ("weight_stream")
    allocate (eio_weights_t :: eio)
    select type (eio)
    type is (eio_weights_t)
        pacified = &
            var_list%get_lval (var_str ("?pacify"))
        call eio%set_parameters (pacify = pacified)
    end select
case default
    call msg_fatal ("Event I/O method '" // char (method) &
        // "' not implemented")
end select
call eio%set_fallback_model (fallback_model)
end subroutine dispatch_eio

```

32.12.1 Unit tests

Test module, followed by the corresponding implementation module.

<dispatch_transforms_ut.f90>≡
<File header>

```
module dispatch_transforms_ut
  use unit_tests
  use dispatch_transforms_uti
```

<Standard module head>

<Dispatch transforms: public test>

contains

<Dispatch transforms: test driver>

```
end module dispatch_transforms_ut
```

<dispatch_transforms_uti.f90>≡
<File header>

```
module dispatch_transforms_uti

<Use kinds>
<Use strings>
  use format_utils, only: write_separator
  use variables
  use event_base, only: event_callback_t
  use models, only: model_t, model_list_t
  use models, only: syntax_model_file_init, syntax_model_file_final
  use resonances, only: resonance_history_set_t
  use beam_structures, only: beam_structure_t
  use eio_base, only: eio_t
  use os_interface, only: os_data_t
  use event_transforms, only: evt_t
  use dispatch_transforms
```

<Standard module head>

<Dispatch transforms: test declarations>

contains

<Dispatch transforms: tests>

```
end module dispatch_transforms_uti
```

API: driver for the unit tests below.

<Dispatch transforms: public test>≡
public :: dispatch_transforms_test

<Dispatch transforms: test driver>≡
subroutine dispatch_transforms_test (u, results)
 integer, intent(in) :: u

```

    type(test_results_t), intent(inout) :: results
    <Dispatch transforms: execute tests>
end subroutine dispatch_transforms_test

```

Event I/O

```

<Dispatch transforms: execute tests>≡
    call test (dispatch_transforms_1, "dispatch_transforms_1", &
        "event I/O", &
        u, results)

<Dispatch transforms: test declarations>≡
    public :: dispatch_transforms_1

<Dispatch transforms: tests>≡
    subroutine dispatch_transforms_1 (u)
        integer, intent(in) :: u
        type(var_list_t) :: var_list
        type(model_list_t) :: model_list
        type(model_t), pointer :: model
        type(os_data_t) :: os_data
        class(event_callback_t), allocatable :: event_callback
        class(eio_t), allocatable :: eio

        write (u, "(A)")  "* Test output: dispatch_transforms_1"
        write (u, "(A)")  "* Purpose: allocate an event I/O (eio) stream"
        write (u, "(A)")

        call var_list%init_defaults (0)
        call os_data%init ()
        call syntax_model_file_init ()
        call model_list%read_model (var_str ("SM_hadrons"), &
            var_str ("SM_hadrons.mdl"), os_data, model)

        write (u, "(A)")  "* Allocate as raw"
        write (u, "(A)")

        call dispatch_eio (eio, var_str ("raw"), var_list, &
            model, event_callback)

        call eio%write (u)

        call eio%final ()
        deallocate (eio)

        write (u, "(A)")
        write (u, "(A)")  "* Allocate as checkpoints:"
        write (u, "(A)")

        call dispatch_eio (eio, var_str ("checkpoint"), var_list, &
            model, event_callback)

        call eio%write (u)
    end subroutine dispatch_transforms_1

```



```

call eio%final ()
deallocate (eio)

write (u, "(A)")
write (u, "(A)")  "* Allocate as LHEF:"
write (u, "(A)")

call var_list%set_string (var_str ("lhef_extension"), &
    var_str ("lhe_custom"), is_known = .true.)
call dispatch_eio (eio, var_str ("lhef"), var_list, &
    model, event_callback)

call eio%write (u)

call eio%final ()
deallocate (eio)

write (u, "(A)")
write (u, "(A)")  "* Allocate as HepMC:"
write (u, "(A)")

call dispatch_eio (eio, var_str ("hepmc"), var_list, &
    model, event_callback)

call eio%write (u)

call eio%final ()
deallocate (eio)

write (u, "(A)")
write (u, "(A)")  "* Allocate as weight_stream"
write (u, "(A)")

call dispatch_eio (eio, var_str ("weight_stream"), var_list, &
    model, event_callback)

call eio%write (u)

call eio%final ()
deallocate (eio)

write (u, "(A)")
write (u, "(A)")  "* Allocate as debug format"
write (u, "(A)")

call var_list%set_log (var_str ("?debug_verbose"), &
    .false., is_known = .true.)
call dispatch_eio (eio, var_str ("debug"), var_list, &
    model, event_callback)

call eio%write (u)

write (u, "(A)")

```

```

write (u, "(A)")  "* Cleanup"

call eio%final ()
call var_list%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_transforms_1"

end subroutine dispatch_transforms_1

```

Event transforms

This test dispatches evt (event transform) objects.

```

<Dispatch transforms: execute tests>+≡
  call test (dispatch_transforms_2, "dispatch_transforms_2", &
    "event transforms", &
    u, results)

<Dispatch transforms: test declarations>+≡
  public :: dispatch_transforms_2

<Dispatch transforms: tests>+≡
  subroutine dispatch_transforms_2 (u)
    integer, intent(in) :: u
    type(var_list_t), target :: var_list
    type(model_list_t) :: model_list
    type(model_t), pointer :: model
    type(os_data_t) :: os_data
    type(resonance_history_set_t), dimension(1) :: res_history_set
    type(beam_structure_t) :: beam_structure
    class(evt_t), pointer :: evt

    write (u, "(A)")  "* Test output: dispatch_transforms_2"
    write (u, "(A)")  "* Purpose: configure event transform"
    write (u, "(A)")

    call syntax_model_file_init ()
    call var_list%init_defaults (0)
    call os_data%init ()
    call model_list%read_model (var_str ("SM_hadrons"), &
      var_str ("SM_hadrons.mdl"), os_data, model)

    write (u, "(A)")  "* Resonance insertion"
    write (u, "(A)")

    call var_list%set_log (var_str ("?resonance_history"), .true., &
      is_known = .true.)
    call dispatch_evt_resonance (evt, var_list, &
      res_history_set, &
      var_str ("foo_R"))
    call evt%write (u, verbose = .true., more_verbose = .true.)

    call evt%final ()

```

```

deallocate (evt)

write (u, "(A)")
write (u, "(A)")  "* ISR handler"
write (u, "(A)")

call var_list%set_log (var_str ("?isr_handler"), .true., &
    is_known = .true.)
call var_list%set_log (var_str ("?epa_handler"), .false., &
    is_known = .true.)
call var_list%set_string (var_str ("$isr_handler_mode"), &
    var_str ("recoil"), &
    is_known = .true.)
call var_list%set_real (var_str ("sqrts"), 100._default, &
    is_known = .true.)
call var_list%set_real (var_str ("isr_mass"), 511.e-6_default, &
    is_known = .true.)
call dispatch_evt_isr_epa_handler (evt, var_list)
call evt%write (u, verbose = .true., more_verbose = .true.)

call evt%final ()
deallocate (evt)

write (u, "(A)")
write (u, "(A)")  "* EPA handler"
write (u, "(A)")

call var_list%set_log (var_str ("?isr_handler"), .false., &
    is_known = .true.)
call var_list%set_log (var_str ("?epa_handler"), .true., &
    is_known = .true.)
call var_list%set_string (var_str ("$epa_handler_mode"), &
    var_str ("recoil"), &
    is_known = .true.)
call var_list%set_real (var_str ("sqrts"), 100._default, &
    is_known = .true.)
call var_list%set_real (var_str ("epa_mass"), 511.e-6_default, &
    is_known = .true.)
call dispatch_evt_isr_epa_handler (evt, var_list)
call evt%write (u, verbose = .true., more_verbose = .true.)

call evt%final ()
deallocate (evt)

write (u, "(A)")
write (u, "(A)")  "* Partonic decays"
write (u, "(A)")

call dispatch_evt_decay (evt, var_list)
call evt%write (u, verbose = .true., more_verbose = .true.)

call evt%final ()
deallocate (evt)

```

```

write (u, "(A)")
write (u, "(A)")  "* Shower"
write (u, "(A)")

call var_list%set_log (var_str ("?allow_shower"), .true., &
    is_known = .true.)
call var_list%set_string (var_str ("$shower_method"), &
    var_str ("WHIZARD"), is_known = .true.)
call dispatch_evt_shower (evt, var_list, model, &
    model, os_data, beam_structure)
call evt%write (u)
call write_separator (u, 2)

call evt%final ()
deallocate (evt)

call var_list%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_transforms_2"

end subroutine dispatch_transforms_2

```

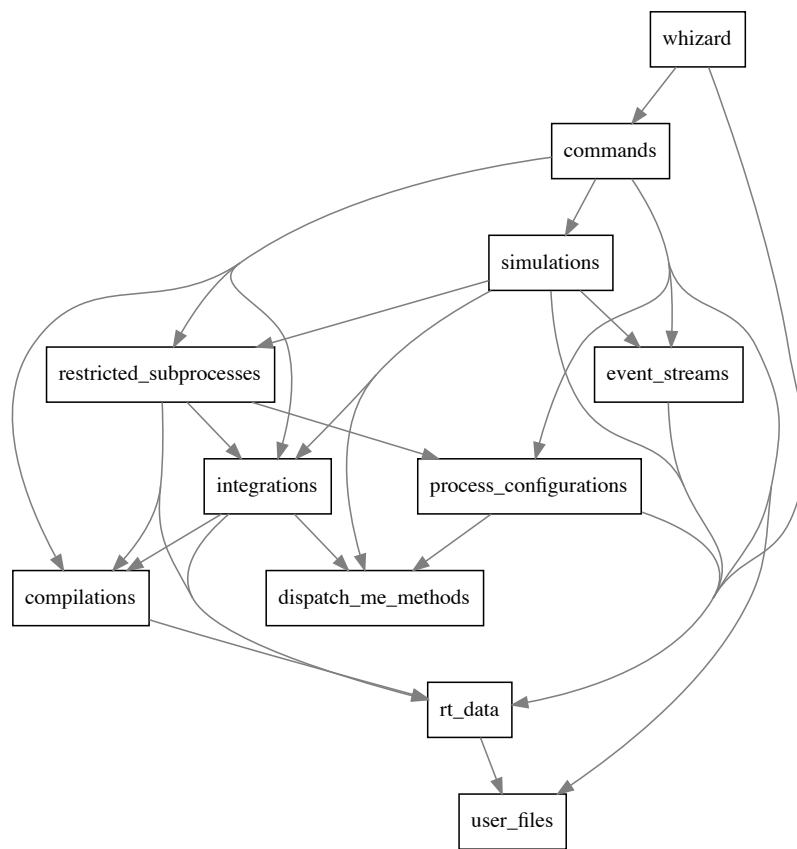


Figure 32.2: Module dependencies in `src/whizard-core`.

Chapter 33

Integration and Simulation

33.1 User-controlled File I/O

The SINDARIN language includes commands that write output to file (input may be added later). We identify files by their name, and manage the unit internally. We need procedures for opening, closing, and printing files.

```
<user_files.f90>≡  
<File header>  
  
module user_files  
  
  <Use strings>  
    use io_units  
    use diagnostics  
    use ifiles  
    use analysis  
  
  <Standard module head>  
  
  <User files: public>  
  
  <User files: types>  
  
  <User files: interfaces>  
  
  contains  
  
  <User files: procedures>  
  
end module user_files
```

33.1.1 The file type

This is a type that describes an open user file and its properties. The entry is part of a doubly-linked list.

```
<User files: types>≡
```

```

type :: file_t
  private
  type(string_t) :: name
  integer :: unit = -1
  logical :: reading = .false.
  logical :: writing = .false.
  type(file_t), pointer :: prev => null ()
  type(file_t), pointer :: next => null ()
end type file_t

```

The initializer opens the file.

```

<User files: procedures>≡
subroutine file_init (file, name, action, status, position)
  type(file_t), intent(out) :: file
  type(string_t), intent(in) :: name
  character(len=*), intent(in) :: action, status, position
  file%unit = free_unit ()
  file%name = name
  open (unit = file%unit, file = char (file%name), &
        action = action, status = status, position = position)
  select case (action)
  case ("read")
    file%reading = .true.
  case ("write")
    file%writing = .true.
  case ("readwrite")
    file%reading = .true.
    file%writing = .true.
  end select
end subroutine file_init

```

The finalizer closes it.

```

<User files: procedures>+≡
subroutine file_final (file)
  type(file_t), intent(inout) :: file
  close (unit = file%unit)
  file%unit = -1
end subroutine file_final

```

Check if a file is open with correct status.

```

<User files: procedures>+≡
function file_is_open (file, action) result (flag)
  logical :: flag
  type(file_t), intent(in) :: file
  character(*), intent(in) :: action
  select case (action)
  case ("read")
    flag = file%reading
  case ("write")
    flag = file%writing
  case ("readwrite")
    flag = file%reading .and. file%writing
  end select
end function file_is_open

```

```

        case default
            call msg_bug ("Checking file '" // char (file%name) &
                // "' : illegal action specifier")
        end select
    end function file_is_open

```

Return the unit number of a file for direct access. It should be checked first whether the file is open.

```

<User files: procedures>+≡
    function file_get_unit (file) result (unit)
        integer :: unit
        type(file_t), intent(in) :: file
        unit = file%unit
    end function file_get_unit

```

Write to the file. Error if in wrong mode. If there is no string, just write an empty record. If there is a string, respect the `advancing` option.

```

<User files: procedures>+≡
    subroutine file_write_string (file, string, advancing)
        type(file_t), intent(in) :: file
        type(string_t), intent(in), optional :: string
        logical, intent(in), optional :: advancing
        if (file%writing) then
            if (present (string)) then
                if (present (advancing)) then
                    if (advancing) then
                        write (file%unit, "(A)") char (string)
                    else
                        write (file%unit, "(A)", advance="no") char (string)
                    end if
                else
                    write (file%unit, "(A)") char (string)
                end if
            else
                write (file%unit, *)
            end if
        else
            call msg_error ("Writing to file: File '" // char (file%name) &
                // "' is not open for writing.")
        end if
    end subroutine file_write_string

```

Write a whole ifile, line by line.

```

<User files: procedures>+≡
    subroutine file_write_ifile (file, ifile)
        type(file_t), intent(in) :: file
        type(ifile_t), intent(in) :: ifile
        type(line_p) :: line
        call line_init (line, ifile)
        do while (line_is_associated (line))
            call file_write_string (file, line_get_string_advance (line))
        end do
    end subroutine

```



```
end subroutine file_write_ifile
```

Write an analysis object (or all objects) to an open file.

<User files: procedures>+≡

```
subroutine file_write_analysis (file, tag)
  type(file_t), intent(in) :: file
  type(string_t), intent(in), optional :: tag
  if (file%writing) then
    if (present (tag)) then
      call analysis_write (tag, unit = file%unit)
    else
      call analysis_write (unit = file%unit)
    end if
  else
    call msg_error ("Writing analysis to file: File ' " // char (file%name) &
      // "' is not open for writing.")
  end if
end subroutine file_write_analysis
```

33.1.2 The file list

We maintain a list of all open files and their attributes. The list must be doubly-linked because we may delete entries.

<User files: public>≡

```
public :: file_list_t
```

<User files: types>+≡

```
type :: file_list_t
  type(file_t), pointer :: first => null ()
  type(file_t), pointer :: last => null ()
end type file_list_t
```

There is no initialization routine, but a finalizer which deletes all:

<User files: public>+≡

```
public :: file_list_final
```

<User files: procedures>+≡

```
subroutine file_list_final (file_list)
  type(file_list_t), intent(inout) :: file_list
  type(file_t), pointer :: current
  do while (associated (file_list%first))
    current => file_list%first
    file_list%first => current%next
    call file_final (current)
    deallocate (current)
  end do
  file_list%last => null ()
end subroutine file_list_final
```

Find an entry in the list. Return null pointer on failure.

```
<User files: procedures>+≡  
function file_list_get_file_ptr (file_list, name) result (current)  
  type(file_t), pointer :: current  
  type(file_list_t), intent(in) :: file_list  
  type(string_t), intent(in) :: name  
  current => file_list%first  
  do while (associated (current))  
    if (current%name == name) return  
    current => current%next  
  end do  
end function file_list_get_file_ptr
```

Check if a file is open, public version:

```
<User files: public>+≡  
public :: file_list_is_open  
  
<User files: procedures>+≡  
function file_list_is_open (file_list, name, action) result (flag)  
  logical :: flag  
  type(file_list_t), intent(in) :: file_list  
  type(string_t), intent(in) :: name  
  character(len=*), intent(in) :: action  
  type(file_t), pointer :: current  
  current => file_list_get_file_ptr (file_list, name)  
  if (associated (current)) then  
    flag = file_is_open (current, action)  
  else  
    flag = .false.  
  end if  
end function file_list_is_open
```

Return the unit number for a file. It should be checked first whether the file is open.

```
<User files: public>+≡  
public :: file_list_get_unit  
  
<User files: procedures>+≡  
function file_list_get_unit (file_list, name) result (unit)  
  integer :: unit  
  type(file_list_t), intent(in) :: file_list  
  type(string_t), intent(in) :: name  
  type(file_t), pointer :: current  
  current => file_list_get_file_ptr (file_list, name)  
  if (associated (current)) then  
    unit = file_get_unit (current)  
  else  
    unit = -1  
  end if  
end function file_list_get_unit
```

Append a new file entry, i.e., open this file. Error if it is already open.

```
<User files: public>+≡  
public :: file_list_open
```

```

<User files: procedures>+≡
subroutine file_list_open (file_list, name, action, status, position)
  type(file_list_t), intent(inout) :: file_list
  type(string_t), intent(in) :: name
  character(len=*), intent(in) :: action, status, position
  type(file_t), pointer :: current
  if (.not. associated (file_list_get_file_ptr (file_list, name))) then
    allocate (current)
    call msg_message ("Opening file '" // char (name) // "' for output")
    call file_init (current, name, action, status, position)
    if (associated (file_list%last)) then
      file_list%last%next => current
      current%prev => file_list%last
    else
      file_list%first => current
    end if
    file_list%last => current
  else
    call msg_error ("Opening file: File '" // char (name) &
      // "' is already open.")
  end if
end subroutine file_list_open

```

Delete a file entry, i.e., close this file. Error if it is not open.

```

<User files: public>+≡
public :: file_list_close

<User files: procedures>+≡
subroutine file_list_close (file_list, name)
  type(file_list_t), intent(inout) :: file_list
  type(string_t), intent(in) :: name
  type(file_t), pointer :: current
  current => file_list_get_file_ptr (file_list, name)
  if (associated (current)) then
    if (associated (current%prev)) then
      current%prev%next => current%next
    else
      file_list%first => current%next
    end if
    if (associated (current%next)) then
      current%next%prev => current%prev
    else
      file_list%last => current%prev
    end if
    call msg_message ("Closing file '" // char (name) // "' for output")
    call file_final (current)
    deallocate (current)
  else
    call msg_error ("Closing file: File '" // char (name) &
      // "' is not open.")
  end if
end subroutine file_list_close

```

Write a string to file. Error if it is not open.

```
<User files: public>+≡
    public :: file_list_write

<User files: interfaces>≡
    interface file_list_write
        module procedure file_list_write_string
        module procedure file_list_write_ifile
    end interface

<User files: procedures>+≡
    subroutine file_list_write_string (file_list, name, string, advancing)
        type(file_list_t), intent(in) :: file_list
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: string
        logical, intent(in), optional :: advancing
        type(file_t), pointer :: current
        current => file_list_get_file_ptr (file_list, name)
        if (associated (current)) then
            call file_write_string (current, string, advancing)
        else
            call msg_error ("Writing to file: File '" // char (name) &
                // "'is not open.")
        end if
    end subroutine file_list_write_string

    subroutine file_list_write_ifile (file_list, name, ifile)
        type(file_list_t), intent(in) :: file_list
        type(string_t), intent(in) :: name
        type(ifile_t), intent(in) :: ifile
        type(file_t), pointer :: current
        current => file_list_get_file_ptr (file_list, name)
        if (associated (current)) then
            call file_write_ifile (current, ifile)
        else
            call msg_error ("Writing to file: File '" // char (name) &
                // "'is not open.")
        end if
    end subroutine file_list_write_ifile
```

Write an analysis object or all objects to data file. Error if it is not open. If the file name is empty, write to standard output.

```
<User files: public>+≡
    public :: file_list_write_analysis

<User files: procedures>+≡
    subroutine file_list_write_analysis (file_list, name, tag)
        type(file_list_t), intent(in) :: file_list
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: tag
        type(file_t), pointer :: current
        if (name == "") then
            if (present (tag)) then
                call analysis_write (tag)
            else

```

```

        call analysis_write
    end if
else
    current => file_list_get_file_ptr (file_list, name)
    if (associated (current)) then
        call file_write_analysis (current, tag)
    else
        call msg_error ("Writing analysis to file: File '" // char (name) &
            // "' is not open.")
    end if
end if
end subroutine file_list_write_analysis

```

33.2 Runtime data

```
<rt_data.f90>≡  
  <File header>  
  
  module rt_data  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use format_utils, only: write_separator  
    use format_defs, only: FMT_19, FMT_12  
    use system_dependencies  
    use diagnostics  
    use os_interface  
    use lexers  
    use parser  
    use models  
    use subevents  
    use pdg_arrays  
    use variables, only: var_list_t  
    use process_libraries  
    use prclib_stacks  
    use prc_core, only: helicity_selection_t  
    use beam_structures  
    use event_base, only: event_callback_t  
    use user_files  
    use process_stacks  
    use iterations  
  
    <Standard module head>  
  
    <RT data: public>  
  
    <RT data: types>  
  
    contains  
  
    <RT data: procedures>  
  
  end module rt_data
```

33.2.1 Strategy for models and variables

The program manages its data via a main `rt_data_t` object. During program flow, various commands create and use local `rt_data_t` objects. Those transient blocks contain either pointers to global object or local copies which are deleted after use.

Each `rt_data_t` object contains a variable list component. This lists holds (local copies of) all kinds of intrinsic or user-defined variables. The variable list is linked to the variable list contained in the local process library. This, in turn, is linked to the variable list of the `rt_data_t` context, and so on.

A variable lookup will thus be recursively delegated to the linked variable lists, until a match is found. When modifying a variable which is not yet local, the program creates a local copy and uses this afterwards. Thus, when the local `rt_data_t` object is deleted, the context value is recovered.

Models are kept in a model list which is separate from the variable list. Otherwise, they are treated in a similar manner: the local list is linked to the context model list. Model lookup is thus recursively delegated. When a model or any part of it is modified, the model is copied to the local `rt_data_t` object, so the context model is not modified. Commands such as `integrate` will create their own copy of the current model (and of the current variable list) at the point where they are executed.

When a model is encountered for the first time, it is read from file. The reading is automatically delegated to the global context. Thus, this master copy survives until the main `rt_data_t` object is deleted, at program completion.

If there is a currently active model, its variable list is linked to the main variable list. Variable lookups will then start from the model variable list. When the current model is switched, the new active model will get this link instead. Consequently, a change to the current model is kept as long as this model has a local copy; it survives local model switches. On the other hand, a parameter change in the current model doesn't affect any other model, even if the parameter name is identical.

33.2.2 Container for parse nodes

The runtime data set contains a bunch of parse nodes (chunks of code that have not been compiled into evaluation trees but saved for later use). We collect them here.

This implementation has the useful effect that an assignment between two objects of this type will establish a pointer-target relationship for all components.

```

<RT data: types>≡
  type :: rt_parse_nodes_t
    type(parse_node_t), pointer :: cuts_lexpr => null ()
    type(parse_node_t), pointer :: scale_expr => null ()
    type(parse_node_t), pointer :: fac_scale_expr => null ()
    type(parse_node_t), pointer :: ren_scale_expr => null ()
    type(parse_node_t), pointer :: weight_expr => null ()
    type(parse_node_t), pointer :: selection_lexpr => null ()
    type(parse_node_t), pointer :: reweight_expr => null ()
    type(parse_node_t), pointer :: analysis_lexpr => null ()
    type(parse_node_p), dimension(:), allocatable :: alt_setup
  contains
    <RT data: rt parse nodes: TBP>
  end type rt_parse_nodes_t

```

Clear individual components. The parse nodes are nullified. No finalization needed since the pointer targets are part of the global parse tree.

```

<RT data: rt parse nodes: TBP>≡
  procedure :: clear => rt_parse_nodes_clear

```

```

<RT data: procedures>≡
subroutine rt_parse_nodes_clear (rt_pn, name)
  class(rt_parse_nodes_t), intent(inout) :: rt_pn
  type(string_t), intent(in) :: name
  select case (char (name))
  case ("cuts")
    rt_pn%cuts_lexpr => null ()
  case ("scale")
    rt_pn%scale_expr => null ()
  case ("factorization_scale")
    rt_pn%fac_scale_expr => null ()
  case ("renormalization_scale")
    rt_pn%ren_scale_expr => null ()
  case ("weight")
    rt_pn%weight_expr => null ()
  case ("selection")
    rt_pn%selection_lexpr => null ()
  case ("reweight")
    rt_pn%reweight_expr => null ()
  case ("analysis")
    rt_pn%analysis_lexpr => null ()
  end select
end subroutine rt_parse_nodes_clear

```

Output for the parse nodes.

```

<RT data: rt parse nodes: TBP>+≡
  procedure :: write => rt_parse_nodes_write

<RT data: procedures>+≡
subroutine rt_parse_nodes_write (object, unit)
  class(rt_parse_nodes_t), intent(in) :: object
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  call wrt ("Cuts", object%cuts_lexpr)
  call write_separator (u)
  call wrt ("Scale", object%scale_expr)
  call write_separator (u)
  call wrt ("Factorization scale", object%fac_scale_expr)
  call write_separator (u)
  call wrt ("Renormalization scale", object%ren_scale_expr)
  call write_separator (u)
  call wrt ("Weight", object%weight_expr)
  call write_separator (u, 2)
  call wrt ("Event selection", object%selection_lexpr)
  call write_separator (u)
  call wrt ("Event reweighting factor", object%reweight_expr)
  call write_separator (u)
  call wrt ("Event analysis", object%analysis_lexpr)
  if (allocated (object%alt_setup)) then
    call write_separator (u, 2)
    write (u, "(1x,A,':')") "Alternative setups"
    do i = 1, size (object%alt_setup)
      call write_separator (u)
    end do
  end if
end subroutine rt_parse_nodes_write

```



```

        call wrt ("Commands", object%alt_setup(i)%ptr)
    end do
end if
contains
subroutine wrt (title, pn)
    character(*), intent(in) :: title
    type(parse_node_t), intent(in), pointer :: pn
    if (associated (pn)) then
        write (u, "(1x,A,':')") title
        call write_separator (u)
        call parse_node_write_rec (pn, u)
    else
        write (u, "(1x,A,':',1x,A)") title, "[undefined]"
    end if
end subroutine wrt
end subroutine rt_parse_nodes_write

```

Screen output for individual components. (This should eventually be more condensed, currently we print the internal representation tree.)

```

<RT data: rt parse nodes: TBP>+≡
    procedure :: show => rt_parse_nodes_show

<RT data: procedures>+≡
subroutine rt_parse_nodes_show (rt_pn, name, unit)
    class(rt_parse_nodes_t), intent(in) :: rt_pn
    type(string_t), intent(in) :: name
    integer, intent(in), optional :: unit
    type(parse_node_t), pointer :: pn
    integer :: u
    u = given_output_unit (unit)
    select case (char (name))
    case ("cuts")
        pn => rt_pn%cuts_lexpr
    case ("scale")
        pn => rt_pn%scale_expr
    case ("factorization_scale")
        pn => rt_pn%fac_scale_expr
    case ("renormalization_scale")
        pn => rt_pn%ren_scale_expr
    case ("weight")
        pn => rt_pn%weight_expr
    case ("selection")
        pn => rt_pn%selection_lexpr
    case ("reweight")
        pn => rt_pn%reweight_expr
    case ("analysis")
        pn => rt_pn%analysis_lexpr
    end select
    if (associated (pn)) then
        write (u, "(A,1x,A,1x,A)") "Expression:", char (name), "(parse tree):"
        call parse_node_write_rec (pn, u)
    else
        write (u, "(A,1x,A,A)") "Expression:", char (name), ": [undefined]"
    end if
end subroutine

```

```
end subroutine rt_parse_nodes_show
```

33.2.3 The data type

This is a big data container which contains everything that is used and modified during the command flow. A local copy of this can be used to temporarily override defaults. The data set is transparent.

```
<RT data: public>≡
  public :: rt_data_t

<RT data: types>+≡
  type :: rt_data_t
    type(lexer_t), pointer :: lexer => null ()
    type(rt_data_t), pointer :: context => null ()
    type(string_t), dimension(:), allocatable :: export
    type(var_list_t) :: var_list
    type(iterations_list_t) :: it_list
    type(os_data_t) :: os_data
    type(model_list_t) :: model_list
    type(model_t), pointer :: model => null ()
    logical :: model_is_copy = .false.
    type(model_t), pointer :: preload_model => null ()
    type(model_t), pointer :: fallback_model => null ()
    type(prclib_stack_t) :: prclib_stack
    type(process_library_t), pointer :: prclib => null ()
    type(beam_structure_t) :: beam_structure
    type(rt_parse_nodes_t) :: pn
    type(process_stack_t) :: process_stack
    type(string_t), dimension(:), allocatable :: sample_fmt
    class(event_callback_t), allocatable :: event_callback
    type(file_list_t), pointer :: out_files => null ()
    logical :: quit = .false.
    integer :: quit_code = 0
    type(string_t) :: logfile
    logical :: nlo_fixed_order = .false.
    logical, dimension(0:5) :: selected_nlo_parts = .false.
    integer, dimension(:), allocatable :: nlo_component
  contains
    <RT data: rt data: TBP>
  end type rt_data_t
```

33.2.4 Output

```
<RT data: rt data: TBP>≡
  procedure :: write => rt_data_write

<RT data: procedures>+≡
  subroutine rt_data_write (object, unit, vars, pacify)
    class(rt_data_t), intent(in) :: object
    integer, intent(in), optional :: unit
    type(string_t), dimension(:), intent(in), optional :: vars
    logical, intent(in), optional :: pacify
```

```

integer :: u, i
u = given_output_unit (unit)
call write_separator (u, 2)
write (u, "(1x,A)") "Runtime data:"
if (object%get_n_export () > 0) then
    call write_separator (u, 2)
    write (u, "(1x,A)") "Exported objects and variables:"
    call write_separator (u)
    call object%write_exports (u)
end if
if (present (vars)) then
    if (size (vars) /= 0) then
        call write_separator (u, 2)
        write (u, "(1x,A)") "Selected variables:"
        call write_separator (u)
        call object%write_vars (u, vars)
    end if
else
    call write_separator (u, 2)
    if (associated (object%model)) then
        call object%model%write_var_list (u, follow_link=.true.)
    else
        call object%var_list%write (u, follow_link=.true.)
    end if
end if
if (object%it_list%get_n_pass () > 0) then
    call write_separator (u, 2)
    write (u, "(1x)", advance="no")
    call object%it_list%write (u)
end if
if (associated (object%model)) then
    call write_separator (u, 2)
    call object%model%write (u)
end if
call object%prclib_stack%write (u)
call object%beam_structure%write (u)
call write_separator (u, 2)
call object%pn%write (u)
if (allocated (object%sample_fmt)) then
    call write_separator (u)
    write (u, "(1x,A)", advance="no") "Event sample formats = "
    do i = 1, size (object%sample_fmt)
        if (i > 1) write (u, "(A,1x)", advance="no") ", "
        write (u, "(A)", advance="no") char (object%sample_fmt(i))
    end do
    write (u, "(A)")
end if
call write_separator (u)
write (u, "(1x,A)", advance="no") "Event callback:"
if (allocated (object%event_callback)) then
    call object%event_callback%write (u)
else
    write (u, "(1x,A)") "[undefined]"
end if

```

```

    call object%process_stack%write (u, pacify)
    write (u, "(1x,A,1x,L1)") "quit      :", object%quit
    write (u, "(1x,A,1x,I0)") "quit_code:", object%quit_code
    call write_separator (u, 2)
    write (u, "(1x,A,1x,A)") "Logfile  :", "" // trim (char (object%logfile)) // ""
    call write_separator (u, 2)
end subroutine rt_data_write

```

Write only selected variables.

```

<RT data: rt data: TBP>+≡
    procedure :: write_vars => rt_data_write_vars

<RT data: procedures>+≡
    subroutine rt_data_write_vars (object, unit, vars)
        class(rt_data_t), intent(in), target :: object
        integer, intent(in), optional :: unit
        type(string_t), dimension(:), intent(in) :: vars
        type(var_list_t), pointer :: var_list
        integer :: u, i
        u = given_output_unit (unit)
        var_list => object%get_var_list_ptr ()
        do i = 1, size (vars)
            associate (var => vars(i))
                if (var_list%contains (var, follow_link=.true.)) then
                    call var_list%write_var (var, unit = u, &
                        follow_link = .true., defined=.true.)
                end if
            end associate
        end do
    end subroutine rt_data_write_vars

```

Write only the model list.

```

<RT data: rt data: TBP>+≡
    procedure :: write_model_list => rt_data_write_model_list

<RT data: procedures>+≡
    subroutine rt_data_write_model_list (object, unit)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        call object%model_list%write (u)
    end subroutine rt_data_write_model_list

```

Write only the library stack.

```

<RT data: rt data: TBP>+≡
    procedure :: write_libraries => rt_data_write_libraries

<RT data: procedures>+≡
    subroutine rt_data_write_libraries (object, unit, libpath)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: libpath
        integer :: u

```

```

    u = given_output_unit (unit)
    call object%prclib_stack%write (u, libpath)
end subroutine rt_data_write_libraries

```

Write only the beam data.

```

<RT data: rt data: TBP>+≡
    procedure :: write_beams => rt_data_write_beams

<RT data: procedures>+≡
    subroutine rt_data_write_beams (object, unit)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        call write_separator (u, 2)
        call object%beam_structure%write (u)
        call write_separator (u, 2)
    end subroutine rt_data_write_beams

```

Write only the process and event expressions.

```

<RT data: rt data: TBP>+≡
    procedure :: write_expr => rt_data_write_expr

<RT data: procedures>+≡
    subroutine rt_data_write_expr (object, unit)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        call write_separator (u, 2)
        call object%pn%write (u)
        call write_separator (u, 2)
    end subroutine rt_data_write_expr

```

Write only the process stack.

```

<RT data: rt data: TBP>+≡
    procedure :: write_process_stack => rt_data_write_process_stack

<RT data: procedures>+≡
    subroutine rt_data_write_process_stack (object, unit)
        class(rt_data_t), intent(in) :: object
        integer, intent(in), optional :: unit
        call object%process_stack%write (unit)
    end subroutine rt_data_write_process_stack

```

```

<RT data: rt data: TBP>+≡
    procedure :: write_var_descriptions => rt_data_write_var_descriptions

<RT data: procedures>+≡
    subroutine rt_data_write_var_descriptions (rt_data, unit, ascii_output)
        class(rt_data_t), intent(in) :: rt_data
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: ascii_output

```

```

integer :: u
logical :: ao
u = given_output_unit (unit)
ao = .false.; if (present (ascii_output)) ao = ascii_output
call rt_data%var_list%write (u, follow_link=.true., &
    descriptions=.true., ascii_output=ao)
end subroutine rt_data_write_var_descriptions

```

```

<RT data: rt data: TBP>+≡
    procedure :: show_description_of_string => rt_data_show_description_of_string

<RT data: procedures>+≡
    subroutine rt_data_show_description_of_string (rt_data, string, &
        unit, ascii_output)
        class(rt_data_t), intent(in) :: rt_data
        type(string_t), intent(in) :: string
        integer, intent(in), optional :: unit
        logical, intent(in), optional :: ascii_output
        integer :: u
        logical :: ao
        u = given_output_unit (unit)
        ao = .false.; if (present (ascii_output)) ao = ascii_output
        call rt_data%var_list%write_var (string, unit=u, follow_link=.true., &
            defined=.false., descriptions=.true., ascii_output=ao)
    end subroutine rt_data_show_description_of_string

```

33.2.5 Clear

The `clear` command can remove the contents of various subobjects. The objects themselves should stay.

```

<RT data: rt data: TBP>+≡
    procedure :: clear_beams => rt_data_clear_beams

<RT data: procedures>+≡
    subroutine rt_data_clear_beams (global)
        class(rt_data_t), intent(inout) :: global
        call global%beam_structure%final_sf ()
        call global%beam_structure%final_pol ()
        call global%beam_structure%final_mom ()
    end subroutine rt_data_clear_beams

```

33.2.6 Initialization

Initialize runtime data. This defines special variables such as `sqrts`, and should be done only for the instance that is actually global. Local copies will inherit the special variables.

We link the global variable list to the process stack variable list, so the latter is always available (and kept global).

```

<RT data: rt data: TBP>+≡
    procedure :: global_init => rt_data_global_init

```

```

<RT data: procedures>+≡
subroutine rt_data_global_init (global, paths, logfile)
  class(rt_data_t), intent(out), target :: global
  type(paths_t), intent(in), optional :: paths
  type(string_t), intent(in), optional :: logfile
  integer :: seed
  call global%os_data%init (paths)
  if (present (logfile)) then
    global%logfile = logfile
  else
    global%logfile = ""
  end if
  allocate (global%out_files)
  call system_clock (seed)
  call global%var_list%init_defaults (seed, paths)
  call global%init_pointer_variables ()
  call global%process_stack%init_var_list (global%var_list)
end subroutine rt_data_global_init

```

33.2.7 Local copies

This is done at compile time when a local copy of runtime data is needed: Link the variable list and initialize all derived parameters. This allows for synchronizing them with local variable changes without affecting global data.

Also re-initialize pointer variables, so they point to local copies of their targets.

```

<RT data: rt data: TBP>+≡
  procedure :: local_init => rt_data_local_init

<RT data: procedures>+≡
subroutine rt_data_local_init (local, global, env)
  class(rt_data_t), intent(inout), target :: local
  type(rt_data_t), intent(in), target :: global
  integer, intent(in), optional :: env
  local%context => global
  call local%process_stack%link (global%process_stack)
  call local%process_stack%init_var_list (local%var_list)
  call local%process_stack%link_var_list (global%var_list)
  call local%var_list%append_string (var_str ("model_name"), &
    var_str (""), intrinsic=.true.)
  call local%init_pointer_variables ()
  local%fallback_model => global%fallback_model
  local%os_data = global%os_data
  local%logfile = global%logfile
  call local%model_list%link (global%model_list)
  local%model => global%model
  if (associated (local%model)) then
    call local%model%link_var_list (local%var_list)
  end if
  if (allocated (global%event_callback)) then
    allocate (local%event_callback, source = global%event_callback)
  end if

```

```
end subroutine rt_data_local_init
```

These variables point to objects which get local copies:

```
<RT data: rt data: TBP>+≡
  procedure :: init_pointer_variables => rt_data_init_pointer_variables

<RT data: procedures>+≡
  subroutine rt_data_init_pointer_variables (local)
    class(rt_data_t), intent(inout), target :: local
    logical, target, save :: known = .true.
    call local%var_list%append_string_ptr (var_str ("f_c"), &
      local%os_data%f_c, known, intrinsic=.true., &
      description=var_str('This string variable gives the ' // &
        '\ttt{Fortran} compiler used within \whizard. It can ' // &
        'only be accessed, not set by the user. (cf. also ' // &
        '\ttt{\$f_cflags}, \ttt{\$f_clibs}'))
    call local%var_list%append_string_ptr (var_str ("f_cflags"), &
      local%os_data%f_cflags, known, intrinsic=.true., &
      description=var_str('This string variable gives the ' // &
        'compiler flags for the \ttt{Fortran} compiler used ' // &
        'within \whizard. It can only be accessed, not set by ' // &
        'the user. (cf. also \ttt{\$f_c}, \ttt{\$f_clibs}'))
    call local%var_list%append_string_ptr (var_str ("f_clibs"), &
      local%os_data%f_clibs, known, intrinsic=.true., &
      description=var_str('This string variable gives the ' // &
        'linked libraries for the \ttt{Fortran} compiler used ' // &
        'within \whizard. It can only be accessed, not set by ' // &
        'the user. (cf. also \ttt{\$f_c}, \ttt{\$f_cflags}'))
  end subroutine rt_data_init_pointer_variables
```

This is done at execution time: Copy data, transfer pointers. `local` has `intent(inout)` because its local variable list has already been prepared by the previous routine.

To be pedantic, the local pointers to model and library should point to the entries in the local copies. (However, as long as these are just shallow copies with identical content, this is actually irrelevant.)

The process library and process stacks behave as global objects. The copies of the process library and process stacks should be shallow copies, so the contents stay identical. Since objects may be pushed on the stack in the local environment, upon restoring the global environment, we should reverse the assignment. Then the added stack elements will end up on the global stack. (This should be reconsidered in a parallel environment.)

```
<RT data: rt data: TBP>+≡
  procedure :: activate => rt_data_activate

<RT data: procedures>+≡
  subroutine rt_data_activate (local)
    class(rt_data_t), intent(inout), target :: local
    class(rt_data_t), pointer :: global
    global => local%context
    if (associated (global)) then
      local%lexer => global%lexer
      call global%copy_globals (local)
```



```

local%os_data = global%os_data
local%logfile = global%logfile
if (associated (global%prclib)) then
  local%prclib => &
    local%prclib_stack%get_library_ptr (global%prclib%get_name ())
end if
call local%import_values ()
call local%process_stack%link (global%process_stack)
local%it_list = global%it_list
local%beam_structure = global%beam_structure
local%pn = global%pn
if (allocated (local%sample_fmt)) deallocate (local%sample_fmt)
if (allocated (global%sample_fmt)) then
  allocate (local%sample_fmt (size (global%sample_fmt)), &
    source = global%sample_fmt)
end if
local%out_files => global%out_files
local%model => global%model
local%model_is_copy = .false.
else if (.not. associated (local%model)) then
  local%model => local%preload_model
  local%model_is_copy = .false.
end if
if (associated (local%model)) then
  call local%model%link_var_list (local%var_list)
  call local%var_list%set_string (var_str (" $model_name"), &
    local%model%get_name (), is_known = .true.)
else
  call local%var_list%set_string (var_str (" $model_name"), &
    var_str (""), is_known = .false.)
end if
end subroutine rt_data_activate

```

Restore the previous state of data, without actually finalizing the local environment. We also clear the local process stack. Some local modifications (model list and process library stack) are communicated to the global context, if there is any.

If the `keep_local` flag is set, we want to retain current settings in the local environment. In particular, we create an instance of the currently selected model (which thus becomes separated from the model library!). The local variables are also kept.

```

<RT data: rt data: TBP>+≡
  procedure :: deactivate => rt_data_deactivate

<RT data: procedures>+≡
  subroutine rt_data_deactivate (local, global, keep_local)
    class(rt_data_t), intent(inout), target :: local
    class(rt_data_t), intent(inout), optional, target :: global
    logical, intent(in), optional :: keep_local
    type(string_t) :: local_model, local_scheme
    logical :: same_model, delete
    delete = .true.; if (present (keep_local)) delete = .not. keep_local
    if (present (global)) then

```

```

if (associated (global%model) .and. associated (local%model)) then
  local_model = local%model%get_name ()
  if (global%model%has_schemes ()) then
    local_scheme = local%model%get_scheme ()
    same_model = &
      global%model%matches (local_model, local_scheme)
  else
    same_model = global%model%matches (local_model)
  end if
else
  same_model = .false.
end if
if (delete) then
  call local%process_stack%clear ()
  call local%unselect_model ()
  call local%unset_values ()
else if (associated (local%model)) then
  call local%ensure_model_copy ()
end if
if (.not. same_model .and. associated (global%model)) then
  if (global%model%has_schemes ()) then
    call msg_message ("Restoring model '" // &
      char (global%model%get_name ()) // "', scheme '" // &
      char (global%model%get_scheme ()) // "'")
  else
    call msg_message ("Restoring model '" // &
      char (global%model%get_name ()) // "'")
  end if
end if
if (associated (global%model)) then
  call global%model%link_var_list (global%var_list)
end if
call global%restore_globals (local)
else
  call local%unselect_model ()
end if
end subroutine rt_data_deactivate

```

This imports the global objects for which local modifications should be kept. Currently, this is only the process library stack.

```

<RT data: rt data: TBP>+≡
  procedure :: copy_globals => rt_data_copy_globals

<RT data: procedures>+≡
  subroutine rt_data_copy_globals (global, local)
    class(rt_data_t), intent(in) :: global
    class(rt_data_t), intent(inout) :: local
    local%prclib_stack = global%prclib_stack
  end subroutine rt_data_copy_globals

```

This restores global objects for which local modifications should be kept. May also modify (remove) the local objects.

```

<RT data: rt data: TBP>+≡

```

```

    procedure :: restore_globals => rt_data_restore_globals
<RT data: procedures>+≡
    subroutine rt_data_restore_globals (global, local)
        class(rt_data_t), intent(inout) :: global
        class(rt_data_t), intent(inout) :: local
        global%prclib_stack = local%prclib_stack
        call local%handle_exports (global)
    end subroutine rt_data_restore_globals

```

33.2.8 Exported objects

Exported objects are transferred to the global state when a local environment is closed. (For the top-level global data set, there is no effect.)

The current implementation handles only the **results** object, which resolves to the local process stack. The stack elements are appended to the global stack without modification, the local stack becomes empty.

Write names of objects to be exported:

```

<RT data: rt data: TBP>+≡
    procedure :: write_exports => rt_data_write_exports
<RT data: procedures>+≡
    subroutine rt_data_write_exports (rt_data, unit)
        class(rt_data_t), intent(in) :: rt_data
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        do i = 1, rt_data%get_n_export ()
            write (u, "(A)") char (rt_data%export(i))
        end do
    end subroutine rt_data_write_exports

```

The number of entries in the export list.

```

<RT data: rt data: TBP>+≡
    procedure :: get_n_export => rt_data_get_n_export
<RT data: procedures>+≡
    function rt_data_get_n_export (rt_data) result (n)
        class(rt_data_t), intent(in) :: rt_data
        integer :: n
        if (allocated (rt_data%export)) then
            n = size (rt_data%export)
        else
            n = 0
        end if
    end function rt_data_get_n_export

```

Return a specific export Append new names to the export list. If a duplicate occurs, do not transfer it.

```

<RT data: rt data: TBP>+≡
    procedure :: append_exports => rt_data_append_exports

```

<RT data: procedures>+≡

```

subroutine rt_data_append_exports (rt_data, export)
  class(rt_data_t), intent(inout) :: rt_data
  type(string_t), dimension(:), intent(in) :: export
  logical, dimension(:), allocatable :: mask
  type(string_t), dimension(:), allocatable :: tmp
  integer :: i, j, n
  if (.not. allocated (rt_data%export)) allocate (rt_data%export (0))
  n = size (rt_data%export)
  allocate (mask (size (export)), source=.false.)
  do i = 1, size (export)
    mask(i) = all (export(i) /= rt_data%export) &
      .and. all (export(i) /= export(:i-1))
  end do
  if (count (mask) > 0) then
    allocate (tmp (n + count (mask)))
    tmp(1:n) = rt_data%export(:)
    j = n
    do i = 1, size (export)
      if (mask(i)) then
        j = j + 1
        tmp(j) = export(i)
      end if
    end do
    call move_alloc (from=tmp, to=rt_data%export)
  end if
end subroutine rt_data_append_exports

```

Transfer export-objects from the local rt data to the global rt data, as far as supported.

<RT data: rt data: TBP>+≡

```

procedure :: handle_exports => rt_data_handle_exports

```

<RT data: procedures>+≡

```

subroutine rt_data_handle_exports (local, global)
  class(rt_data_t), intent(inout), target :: local
  class(rt_data_t), intent(inout), target :: global
  type(string_t) :: export
  integer :: i
  if (local%get_n_export () > 0) then
    do i = 1, local%get_n_export ()
      export = local%export(i)
      select case (char (export))
        case ("results")
          call msg_message ("Exporting integration results &
            &to outer environment")
          call local%transfer_process_stack (global)
        case default
          call msg_bug ("handle exports: '" &
            // char (export) // "' unsupported")
      end select
    end do
  end if
end subroutine rt_data_handle_exports

```

Export the process stack. One-by-one, take the last process from the local stack and push it on the global stack. Also handle the corresponding result variables: append if the process did not exist yet in the global stack, otherwise update.

TODO: result variables do not work that way yet, require initialization in the global variable list.

```

(RT data: rt data: TBP)+≡
  procedure :: transfer_process_stack => rt_data_transfer_process_stack

(RT data: procedures)+≡
  subroutine rt_data_transfer_process_stack (local, global)
    class(rt_data_t), intent(inout), target :: local
    class(rt_data_t), intent(inout), target :: global
    type(process_entry_t), pointer :: process
    type(string_t) :: process_id
    do
      call local%process_stack%pop_last (process)
      if (.not. associated (process)) exit
      process_id = process%get_id ()
      call global%process_stack%push (process)
      call global%process_stack%fill_result_vars (process_id)
      call global%process_stack%update_result_vars &
        (process_id, global%var_list)
    end do
  end subroutine rt_data_transfer_process_stack

```

33.2.9 Finalization

Finalizer for the variable list and the structure-function list. This is done only for the global RT dataset; local copies contain pointers to this and do not need a finalizer.

```

(RT data: rt data: TBP)+≡
  procedure :: final => rt_data_global_final

(RT data: procedures)+≡
  subroutine rt_data_global_final (global)
    class(rt_data_t), intent(inout) :: global
    call global%process_stack%final ()
    call global%prclib_stack%final ()
    call global%model_list%final ()
    call global%var_list%final (follow_link=.false.)
    if (associated (global%out_files)) then
      call file_list_final (global%out_files)
      deallocate (global%out_files)
    end if
  end subroutine rt_data_global_final

```

The local copy needs a finalizer for the variable list, which consists of local copies. This finalizer is called only when the local environment is finally discarded. (Note that the process stack should already have been cleared after execution, which can occur many times for the same local environment.)

```

(RT data: rt data: TBP)+≡

```

```

    procedure :: local_final => rt_data_local_final
<RT data: procedures>+≡
    subroutine rt_data_local_final (local)
        class(rt_data_t), intent(inout) :: local
        call local%process_stack%clear ()
        call local%model_list%final ()
        call local%var_list%final (follow_link=.false.)
    end subroutine rt_data_local_final

```

33.2.10 Model Management

Read a model, so it becomes available for activation. No variables or model copies, this is just initialization.

If this is a local environment, the model will be automatically read into the global context.

```

<RT data: rt data: TBP>+≡
    procedure :: read_model => rt_data_read_model
<RT data: procedures>+≡
    subroutine rt_data_read_model (global, name, model, scheme)
        class(rt_data_t), intent(inout) :: global
        type(string_t), intent(in) :: name
        type(string_t), intent(in), optional :: scheme
        type(model_t), pointer, intent(out) :: model
        type(string_t) :: filename
        filename = name // ".mdl"
        call global%model_list%read_model &
            (name, filename, global%os_data, model, scheme)
    end subroutine rt_data_read_model

```

Read a UFO model. Create it on the fly if necessary.

```

<RT data: rt data: TBP>+≡
    procedure :: read_ufo_model => rt_data_read_ufo_model
<RT data: procedures>+≡
    subroutine rt_data_read_ufo_model (global, name, model, ufo_path)
        class(rt_data_t), intent(inout) :: global
        type(string_t), intent(in) :: name
        type(model_t), pointer, intent(out) :: model
        type(string_t), intent(in), optional :: ufo_path
        type(string_t) :: filename
        filename = name // ".ufo.mdl"
        call global%model_list%read_model &
            (name, filename, global%os_data, model, ufo=.true., ufo_path=ufo_path)
    end subroutine rt_data_read_ufo_model

```

Initialize the fallback model. This model is used whenever the current model does not describe all physical particles (hadrons, mainly). It is not supposed to be modified, and the pointer should remain linked to this model.

```

<RT data: rt data: TBP>+≡
    procedure :: init_fallback_model => rt_data_init_fallback_model

```

```

<RT data: procedures>+≡
subroutine rt_data_init_fallback_model (global, name, filename)
class(rt_data_t), intent(inout) :: global
type(string_t), intent(in) :: name, filename
call global%model_list%read_model &
    (name, filename, global%os_data, global%fallback_model)
end subroutine rt_data_init_fallback_model

```

Activate a model: assign the current-model pointer and set the model name in the variable list. If necessary, read the model from file. Link the global variable list to the model variable list.

```

<RT data: rt data: TBP>+≡
procedure :: select_model => rt_data_select_model

<RT data: procedures>+≡
subroutine rt_data_select_model (global, name, scheme, ufo, ufo_path)
class(rt_data_t), intent(inout), target :: global
type(string_t), intent(in) :: name
type(string_t), intent(in), optional :: scheme
logical, intent(in), optional :: ufo
type(string_t), intent(in), optional :: ufo_path
logical :: same_model, ufo_model
ufo_model = .false.; if (present (ufo)) ufo_model = ufo
if (associated (global%model)) then
    same_model = global%model%matches (name, scheme, ufo)
else
    same_model = .false.
end if
if (.not. same_model) then
    global%model => global%model_list%get_model_ptr (name, scheme, ufo)
    if (.not. associated (global%model)) then
        if (ufo_model) then
            call global%read_ufo_model (name, global%model, ufo_path)
        else
            call global%read_model (name, global%model)
        end if
        global%model_is_copy = .false.
    else if (associated (global%context)) then
        global%model_is_copy = &
            global%model_list%model_exists (name, scheme, ufo, &
                follow_link=.false.)
    else
        global%model_is_copy = .false.
    end if
end if
if (associated (global%model)) then
    call global%model%link_var_list (global%var_list)
    call global%var_list%set_string (var_str (" $model_name"), &
        name, is_known = .true.)
    if (global%model%is_ufo_model ()) then
        call msg_message ("Switching to model '" // char (name) // "' " &
            // "(generated from UFO source)")
    else if (global%model%has_schemes ()) then
        call msg_message ("Switching to model '" // char (name) // "', " &

```

```

        // "scheme ' " // char (global%model%get_scheme ()) // "'")
    else
        call msg_message ("Switching to model ' " // char (name) // "'")
    end if
else
    call global%var_list%set_string (var_str ("$model_name"), &
        var_str (""), is_known = .false.)
end if
end subroutine rt_data_select_model

```

Remove the model link. Do not unset the model name variable, because this may unset the variable in a parent `rt_data` object (via linked var lists).

```

<RT data: rt_data: TBP>+≡
    procedure :: unselect_model => rt_data_unselect_model

<RT data: procedures>+≡
    subroutine rt_data_unselect_model (global)
        class(rt_data_t), intent(inout), target :: global
        if (associated (global%model)) then
            global%model => null ()
            global%model_is_copy = .false.
        end if
    end subroutine rt_data_unselect_model

```

Create a copy of the currently selected model and append it to the local model list. The model pointer is redirected to the copy. (Not applicable for the global model list, those models will be modified in-place.)

```

<RT data: rt_data: TBP>+≡
    procedure :: ensure_model_copy => rt_data_ensure_model_copy

<RT data: procedures>+≡
    subroutine rt_data_ensure_model_copy (global)
        class(rt_data_t), intent(inout), target :: global
        if (associated (global%context)) then
            if (.not. global%model_is_copy) then
                call global%model_list%append_copy (global%model, global%model)
                global%model_is_copy = .true.
                call global%model%link_var_list (global%var_list)
            end if
        end if
    end subroutine rt_data_ensure_model_copy

```

Modify a model variable. The update mechanism will ensure that the model parameter set remains consistent. This has to take place in a local copy of the current model. If there is none yet, create one.

```

<RT data: rt_data: TBP>+≡
    procedure :: model_set_real => rt_data_model_set_real

<RT data: procedures>+≡
    subroutine rt_data_model_set_real (global, name, rval, verbose, pacified)
        class(rt_data_t), intent(inout), target :: global
        type(string_t), intent(in) :: name
        real(default), intent(in) :: rval

```



```

    logical, intent(in), optional :: verbose, pacified
    call global%ensure_model_copy ()
    call global%model%set_real (name, rval, verbose, pacified)
end subroutine rt_data_model_set_real

```

Modify particle properties. This has to take place in a local copy of the current model. If there is none yet, create one.

```

<RT data: rt data: TBP>+≡
    procedure :: modify_particle => rt_data_modify_particle

<RT data: procedures>+≡
    subroutine rt_data_modify_particle &
        (global, pdg, polarized, stable, decay, &
         isotropic_decay, diagonal_decay, decay_helicity)
    class(rt_data_t), intent(inout), target :: global
    integer, intent(in) :: pdg
    logical, intent(in), optional :: polarized, stable
    logical, intent(in), optional :: isotropic_decay, diagonal_decay
    integer, intent(in), optional :: decay_helicity
    type(string_t), dimension(:), intent(in), optional :: decay
    call global%ensure_model_copy ()
    if (present (polarized)) then
        if (polarized) then
            call global%model%set_polarized (pdg)
        else
            call global%model%set_unpolarized (pdg)
        end if
    end if
    if (present (stable)) then
        if (stable) then
            call global%model%set_stable (pdg)
        else if (present (decay)) then
            call global%model%set_unstable &
                (pdg, decay, isotropic_decay, diagonal_decay, decay_helicity)
        else
            call msg_bug ("Setting particle unstable: missing decay processes")
        end if
    end if
end subroutine rt_data_modify_particle

```

33.2.11 Managing Variables

Return a pointer to the currently active variable list. If there is no model, this is the global variable list. If there is one, it is the model variable list, which should be linked to the former.

```

<RT data: rt data: TBP>+≡
    procedure :: get_var_list_ptr => rt_data_get_var_list_ptr

<RT data: procedures>+≡
    function rt_data_get_var_list_ptr (global) result (var_list)
    class(rt_data_t), intent(in), target :: global
    type(var_list_t), pointer :: var_list

```

```

    if (associated (global%model)) then
        var_list => global%model%get_var_list_ptr ()
    else
        var_list => global%var_list
    end if
end function rt_data_get_var_list_ptr

```

Initialize a local variable: append it to the current variable list. No initial value, yet.

```

<RT data: rt data: TBP>+=
  procedure :: append_log => rt_data_append_log
  procedure :: append_int => rt_data_append_int
  procedure :: append_real => rt_data_append_real
  procedure :: append_cmplx => rt_data_append_cmplx
  procedure :: append_subevt => rt_data_append_subevt
  procedure :: append_pdg_array => rt_data_append_pdg_array
  procedure :: append_string => rt_data_append_string

<RT data: procedures>+=
  subroutine rt_data_append_log (local, name, lval, intrinsic, user)
    class(rt_data_t), intent(inout) :: local
    type(string_t), intent(in) :: name
    logical, intent(in), optional :: lval
    logical, intent(in), optional :: intrinsic, user
    call local%var_list%append_log (name, lval, &
        intrinsic = intrinsic, user = user)
  end subroutine rt_data_append_log

  subroutine rt_data_append_int (local, name, ival, intrinsic, user)
    class(rt_data_t), intent(inout) :: local
    type(string_t), intent(in) :: name
    integer, intent(in), optional :: ival
    logical, intent(in), optional :: intrinsic, user
    call local%var_list%append_int (name, ival, &
        intrinsic = intrinsic, user = user)
  end subroutine rt_data_append_int

  subroutine rt_data_append_real (local, name, rval, intrinsic, user)
    class(rt_data_t), intent(inout) :: local
    type(string_t), intent(in) :: name
    real(default), intent(in), optional :: rval
    logical, intent(in), optional :: intrinsic, user
    call local%var_list%append_real (name, rval, &
        intrinsic = intrinsic, user = user)
  end subroutine rt_data_append_real

  subroutine rt_data_append_cmplx (local, name, cval, intrinsic, user)
    class(rt_data_t), intent(inout) :: local
    type(string_t), intent(in) :: name
    complex(default), intent(in), optional :: cval
    logical, intent(in), optional :: intrinsic, user
    call local%var_list%append_cmplx (name, cval, &
        intrinsic = intrinsic, user = user)
  end subroutine rt_data_append_cmplx

```

```

subroutine rt_data_append_subevt (local, name, pval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(subevt_t), intent(in), optional :: pval
  logical, intent(in) :: intrinsic, user
  call local%var_list%append_subevt (name, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_subevt

subroutine rt_data_append_pdg_array (local, name, aval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(pdg_array_t), intent(in), optional :: aval
  logical, intent(in), optional :: intrinsic, user
  call local%var_list%append_pdg_array (name, aval, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_pdg_array

subroutine rt_data_append_string (local, name, sval, intrinsic, user)
  class(rt_data_t), intent(inout) :: local
  type(string_t), intent(in) :: name
  type(string_t), intent(in), optional :: sval
  logical, intent(in), optional :: intrinsic, user
  call local%var_list%append_string (name, sval, &
    intrinsic = intrinsic, user = user)
end subroutine rt_data_append_string

```

Import values for all local variables, given a global context environment where these variables are defined.

```

<RT data: rt data: TBP>+≡
  procedure :: import_values => rt_data_import_values

<RT data: procedures>+≡
  subroutine rt_data_import_values (local)
    class(rt_data_t), intent(inout) :: local
    type(rt_data_t), pointer :: global
    global => local%context
    if (associated (global)) then
      call local%var_list%import (global%var_list)
    end if
  end subroutine rt_data_import_values

```

Unset all variable values.

```

<RT data: rt data: TBP>+≡
  procedure :: unset_values => rt_data_unset_values

<RT data: procedures>+≡
  subroutine rt_data_unset_values (global)
    class(rt_data_t), intent(inout) :: global
    call global%var_list%undefine (follow_link=.false.)
  end subroutine rt_data_unset_values

```

Set a variable. (Not a model variable, these are handled separately.) We can assume that the variable has been initialized.

```

(RT data: rt data: TBP)+≡
  procedure :: set_log => rt_data_set_log
  procedure :: set_int => rt_data_set_int
  procedure :: set_real => rt_data_set_real
  procedure :: set_cmplx => rt_data_set_cmplx
  procedure :: set_subevt => rt_data_set_subevt
  procedure :: set_pdg_array => rt_data_set_pdg_array
  procedure :: set_string => rt_data_set_string

(RT data: procedures)+≡
  subroutine rt_data_set_log &
    (global, name, lval, is_known, force, verbose)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    logical, intent(in) :: lval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose
    call global%var_list%set_log (name, lval, is_known, &
      force=force, verbose=verbose)
  end subroutine rt_data_set_log

  subroutine rt_data_set_int &
    (global, name, ival, is_known, force, verbose)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    integer, intent(in) :: ival
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose
    call global%var_list%set_int (name, ival, is_known, &
      force=force, verbose=verbose)
  end subroutine rt_data_set_int

  subroutine rt_data_set_real &
    (global, name, rval, is_known, force, verbose, pacified)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    real(default), intent(in) :: rval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose, pacified
    call global%var_list%set_real (name, rval, is_known, &
      force=force, verbose=verbose, pacified=pacified)
  end subroutine rt_data_set_real

  subroutine rt_data_set_cmplx &
    (global, name, cval, is_known, force, verbose, pacified)
    class(rt_data_t), intent(inout) :: global
    type(string_t), intent(in) :: name
    complex(default), intent(in) :: cval
    logical, intent(in) :: is_known
    logical, intent(in), optional :: force, verbose, pacified
    call global%var_list%set_cmplx (name, cval, is_known, &
      force=force, verbose=verbose, pacified=pacified)

```

```

end subroutine rt_data_set_cmplx

subroutine rt_data_set_subevt &
  (global, name, pval, is_known, force, verbose)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  type(subevt_t), intent(in) :: pval
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose
  call global%var_list%set_subevt (name, pval, is_known, &
    force=force, verbose=verbose)
end subroutine rt_data_set_subevt

subroutine rt_data_set_pdg_array &
  (global, name, aval, is_known, force, verbose)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  type(pdg_array_t), intent(in) :: aval
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose
  call global%var_list%set_pdg_array (name, aval, is_known, &
    force=force, verbose=verbose)
end subroutine rt_data_set_pdg_array

subroutine rt_data_set_string &
  (global, name, sval, is_known, force, verbose)
  class(rt_data_t), intent(inout) :: global
  type(string_t), intent(in) :: name
  type(string_t), intent(in) :: sval
  logical, intent(in) :: is_known
  logical, intent(in), optional :: force, verbose
  call global%var_list%set_string (name, sval, is_known, &
    force=force, verbose=verbose)
end subroutine rt_data_set_string

```

Return the value of a variable, assuming that the type is correct.

```

<RT data: rt data: TBP>+≡
  procedure :: get_lval => rt_data_get_lval
  procedure :: get_ival => rt_data_get_ival
  procedure :: get_rval => rt_data_get_rval
  procedure :: get_cval => rt_data_get_cval
  procedure :: get_pval => rt_data_get_pval
  procedure :: get_aval => rt_data_get_aval
  procedure :: get_sval => rt_data_get_sval

<RT data: procedures>+≡
  function rt_data_get_lval (global, name) result (lval)
    logical :: lval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    lval = var_list%get_lval (name)
  end function rt_data_get_lval

```

```

function rt_data_get_ival (global, name) result (ival)
    integer :: ival
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    ival = var_list%get_ival (name)
end function rt_data_get_ival

function rt_data_get_rval (global, name) result (rval)
    real(default) :: rval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    rval = var_list%get_rval (name)
end function rt_data_get_rval

function rt_data_get_cval (global, name) result (cval)
    complex(default) :: cval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    cval = var_list%get_cval (name)
end function rt_data_get_cval

function rt_data_get_aval (global, name) result (aval)
    type(pdg_array_t) :: aval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    aval = var_list%get_aval (name)
end function rt_data_get_aval

function rt_data_get_pval (global, name) result (pval)
    type(subvt_t) :: pval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    pval = var_list%get_pval (name)
end function rt_data_get_pval

function rt_data_get_sval (global, name) result (sval)
    type(string_t) :: sval
    class(rt_data_t), intent(in), target :: global
    type(string_t), intent(in) :: name
    type(var_list_t), pointer :: var_list
    var_list => global%get_var_list_ptr ()
    sval = var_list%get_sval (name)
end function rt_data_get_sval

```

Return true if the variable exists in the global list.

```

<RT data: rt data: TBP>+≡
    procedure :: contains => rt_data_contains

<RT data: procedures>+≡
    function rt_data_contains (global, name) result (lval)
        logical :: lval
        class(rt_data_t), intent(in), target :: global
        type(string_t), intent(in) :: name
        type(var_list_t), pointer :: var_list
        var_list => global%get_var_list_ptr ()
        lval = var_list%contains (name)
    end function rt_data_contains

```

Return true if the value of the variable is known.

```

<RT data: rt data: TBP>+≡
    procedure :: is_known => rt_data_is_known

<RT data: procedures>+≡
    function rt_data_is_known (global, name) result (lval)
        logical :: lval
        class(rt_data_t), intent(in), target :: global
        type(string_t), intent(in) :: name
        type(var_list_t), pointer :: var_list
        var_list => global%get_var_list_ptr ()
        lval = var_list%is_known (name)
    end function rt_data_is_known

```

33.2.12 Further Content

Add a library (available via a pointer of type `prclib_entry_t`) to the stack and update the pointer and variable list to the current library. The pointer association of `prclib_entry` will be discarded.

```

<RT data: rt data: TBP>+≡
    procedure :: add_prclib => rt_data_add_prclib

<RT data: procedures>+≡
    subroutine rt_data_add_prclib (global, prclib_entry)
        class(rt_data_t), intent(inout) :: global
        type(prclib_entry_t), intent(inout), pointer :: prclib_entry
        call global%prclib_stack%push (prclib_entry)
        call global%update_prclib (global%prclib_stack%get_first_ptr ())
    end subroutine rt_data_add_prclib

```

Given a pointer to a process library, make this the currently active library.

```

<RT data: rt data: TBP>+≡
    procedure :: update_prclib => rt_data_update_prclib

```

```

<RT data: procedures>+≡
subroutine rt_data_update_prclib (global, lib)
  class(rt_data_t), intent(inout) :: global
  type(process_library_t), intent(in), target :: lib
  global%prclib => lib
  if (global%var_list%contains (&
    var_str ("library_name"), follow_link = .false.)) then
    call global%var_list%set_string (var_str ("library_name"), &
      global%prclib%get_name (), is_known=.true.)
  else
    call global%var_list%append_string ( &
      var_str ("library_name"), global%prclib%get_name (), &
      intrinsic = .true.)
  end if
end subroutine rt_data_update_prclib

```

33.2.13 Miscellaneous

The helicity selection data are distributed among several parameters. Here, we collect them in a single record.

```

<RT data: rt data: TBP>+≡
  procedure :: get_helicity_selection => rt_data_get_helicity_selection

<RT data: procedures>+≡
function rt_data_get_helicity_selection (rt_data) result (helicity_selection)
  class(rt_data_t), intent(in) :: rt_data
  type(helicity_selection_t) :: helicity_selection
  associate (var_list => rt_data%var_list)
    helicity_selection%active = var_list%get_lval (&
      var_str ("helicity_selection_active"))
    if (helicity_selection%active) then
      helicity_selection%threshold = var_list%get_rval (&
        var_str ("helicity_selection_threshold"))
      helicity_selection%cutoff = var_list%get_ival (&
        var_str ("helicity_selection_cutoff"))
    end if
  end associate
end function rt_data_get_helicity_selection

```

Show the beam setup: beam structure and relevant global variables.

```

<RT data: rt data: TBP>+≡
  procedure :: show_beams => rt_data_show_beams

<RT data: procedures>+≡
subroutine rt_data_show_beams (rt_data, unit)
  class(rt_data_t), intent(in) :: rt_data
  integer, intent(in), optional :: unit
  type(string_t) :: s
  integer :: u
  u = given_output_unit (unit)
  associate (beams => rt_data%beam_structure, var_list => rt_data%var_list)
    call beams%write (u)
    if (.not. beams%asymmetric () .and. beams%get_n_beam () == 2) then

```



```

write (u, "(2x,A," // FMT_19 // ",1x,'GeV')") "sqrts =", &
var_list%get_rval (var_str ("sqrts"))
end if
if (beams%contains ("pdf_builtin")) then
s = var_list%get_sval (var_str ("$pdf_builtin_set"))
if (s /= "") then
write (u, "(2x,A,1x,3A)" "PDF set =", "'", char (s), "'")
else
write (u, "(2x,A,1x,A)" "PDF set =", "[undefined]")
end if
end if
if (beams%contains ("lhpdf")) then
s = var_list%get_sval (var_str ("$lhpdf_dir"))
if (s /= "") then
write (u, "(2x,A,1x,3A)" "LHAPDF dir      =", "'", char (s), "'")
end if
s = var_list%get_sval (var_str ("$lhpdf_file"))
if (s /= "") then
write (u, "(2x,A,1x,3A)" "LHAPDF file      =", "'", char (s), "'")
write (u, "(2x,A,1x,I0)" "LHAPDF member =", &
var_list%get_ival (var_str ("lhpdf_member"))
else
write (u, "(2x,A,1x,A)" "LHAPDF file      =", "[undefined]")
end if
end if
if (beams%contains ("lhpdf_photon")) then
s = var_list%get_sval (var_str ("$lhpdf_dir"))
if (s /= "") then
write (u, "(2x,A,1x,3A)" "LHAPDF dir      =", "'", char (s), "'")
end if
s = var_list%get_sval (var_str ("$lhpdf_photon_file"))
if (s /= "") then
write (u, "(2x,A,1x,3A)" "LHAPDF file      =", "'", char (s), "'")
write (u, "(2x,A,1x,I0)" "LHAPDF member =", &
var_list%get_ival (var_str ("lhpdf_member"))
write (u, "(2x,A,1x,I0)" "LHAPDF scheme =", &
var_list%get_ival (&
var_str ("lhpdf_photon_scheme"))
else
write (u, "(2x,A,1x,A)" "LHAPDF file      =", "[undefined]")
end if
end if
if (beams%contains ("isr")) then
write (u, "(2x,A," // FMT_19 // ")") "ISR alpha      =", &
var_list%get_rval (var_str ("isr_alpha"))
write (u, "(2x,A," // FMT_19 // ")") "ISR Q max      =", &
var_list%get_rval (var_str ("isr_q_max"))
write (u, "(2x,A," // FMT_19 // ")") "ISR mass      =", &
var_list%get_rval (var_str ("isr_mass"))
write (u, "(2x,A,1x,I0)" "ISR order      =", &
var_list%get_ival (var_str ("isr_order"))
write (u, "(2x,A,1x,L1)" "ISR recoil      =", &
var_list%get_lval (var_str ("?isr_recoil"))
write (u, "(2x,A,1x,L1)" "ISR energy cons. =", &

```

```

        var_list%get_lval (var_str ("?isr_keep_energy"))
end if
if (beams%contains ("epa")) then
    write (u, "(2x,A," // FMT_19 // ")") "EPA alpha          =", &
        var_list%get_rval (var_str ("epa_alpha"))
    write (u, "(2x,A," // FMT_19 // ")") "EPA x min          =", &
        var_list%get_rval (var_str ("epa_x_min"))
    write (u, "(2x,A," // FMT_19 // ")") "EPA Q min          =", &
        var_list%get_rval (var_str ("epa_q_min"))
    write (u, "(2x,A," // FMT_19 // ")") "EPA Q max          =", &
        var_list%get_rval (var_str ("epa_q_max"))
    write (u, "(2x,A," // FMT_19 // ")") "EPA mass           =", &
        var_list%get_rval (var_str ("epa_mass"))
    write (u, "(2x,A,1x,L1)") "EPA recoil          =", &
        var_list%get_lval (var_str ("?epa_recoil"))
    write (u, "(2x,A,1x,L1)") "EPA energy cons. =", &
        var_list%get_lval (var_str ("?epa_keep_energy"))
end if
if (beams%contains ("ewa")) then
    write (u, "(2x,A," // FMT_19 // ")") "EWA x min          =", &
        var_list%get_rval (var_str ("ewa_x_min"))
    write (u, "(2x,A," // FMT_19 // ")") "EWA Pt max         =", &
        var_list%get_rval (var_str ("ewa_pt_max"))
    write (u, "(2x,A," // FMT_19 // ")") "EWA mass           =", &
        var_list%get_rval (var_str ("ewa_mass"))
    write (u, "(2x,A,1x,L1)") "EWA recoil          =", &
        var_list%get_lval (var_str ("?ewa_recoil"))
    write (u, "(2x,A,1x,L1)") "EWA energy cons. =", &
        var_list%get_lval (var_str ("ewa_keep_energy"))
end if
if (beams%contains ("circe1")) then
    write (u, "(2x,A,1x,I0)") "CIRCE1 version     =", &
        var_list%get_ival (var_str ("circe1_ver"))
    write (u, "(2x,A,1x,I0)") "CIRCE1 revision    =", &
        var_list%get_ival (var_str ("circe1_rev"))
    s = var_list%get_sval (var_str ("$circe1_acc"))
    write (u, "(2x,A,1x,A)") "CIRCE1 acceler.    =", char (s)
    write (u, "(2x,A,1x,I0)") "CIRCE1 chattin.    =", &
        var_list%get_ival (var_str ("circe1_chat"))
    write (u, "(2x,A," // FMT_19 // ")") "CIRCE1 sqrts       =", &
        var_list%get_rval (var_str ("circe1_sqrts"))
    write (u, "(2x,A," // FMT_19 // ")") "CIRCE1 epsil.     =", &
        var_list%get_rval (var_str ("circe1_eps"))
    write (u, "(2x,A,1x,L1)") "CIRCE1 phot. 1     =", &
        var_list%get_lval (var_str ("?circe1_photon1"))
    write (u, "(2x,A,1x,L1)") "CIRCE1 phot. 2     =", &
        var_list%get_lval (var_str ("?circe1_photon2"))
    write (u, "(2x,A,1x,L1)") "CIRCE1 generat.    =", &
        var_list%get_lval (var_str ("?circe1_generate"))
    write (u, "(2x,A,1x,L1)") "CIRCE1 mapping     =", &
        var_list%get_lval (var_str ("?circe1_map"))
    write (u, "(2x,A," // FMT_19 // ")") "CIRCE1 map. slope =", &
        var_list%get_rval (var_str ("circe1_mapping_slope"))
    write (u, "(2x,A,1x,L1)") "CIRCE recoil photon =", &

```

```

        var_list%get_lval (var_str ("?circe1_with_radiation"))
    end if
    if (beams%contains ("circe2")) then
        s = var_list%get_sval (var_str ("$circe2_design"))
        write (u, "(2x,A,1x,A)" "CIRCE2 design   =", char (s))
        s = var_list%get_sval (var_str ("$circe2_file"))
        write (u, "(2x,A,1x,A)" "CIRCE2 file     =", char (s))
        write (u, "(2x,A,1x,L1)" "CIRCE2 polarized =", &
            var_list%get_lval (var_str ("?circe2_polarized")))
    end if
    if (beams%contains ("gaussian")) then
        write (u, "(2x,A,1x," // FMT_12 // ")") "Gaussian spread 1   =", &
            var_list%get_rval (var_str ("gaussian_spread1"))
        write (u, "(2x,A,1x," // FMT_12 // ")") "Gaussian spread 2   =", &
            var_list%get_rval (var_str ("gaussian_spread2"))
    end if
    if (beams%contains ("beam_events")) then
        s = var_list%get_sval (var_str ("$beam_events_file"))
        write (u, "(2x,A,1x,A)" "Beam events file   =", char (s))
        write (u, "(2x,A,1x,L1)" "Beam events EOF warn =", &
            var_list%get_lval (var_str ("?beam_events_warn_eof")))
    end if
end associate
end subroutine rt_data_show_beams

```

Return the collision energy as determined by the current beam settings. Without beam setup, this is the `sqrts` variable.

If the value is meaningless for a setup, the function returns zero.

```

<RT data: rt data: TBP>+≡
    procedure :: get_sqrts => rt_data_get_sqrts

<RT data: procedures>+≡
    function rt_data_get_sqrts (rt_data) result (sqrts)
        class(rt_data_t), intent(in) :: rt_data
        real(default) :: sqrts
        sqrts = rt_data%var_list%get_rval (var_str ("sqrts"))
    end function rt_data_get_sqrts

```

For testing purposes, the `rt_data_t` contents can be pacified to suppress numerical fluctuations in (constant) test matrix elements.

```

<RT data: rt data: TBP>+≡
    procedure :: pacify => rt_data_pacify

<RT data: procedures>+≡
    subroutine rt_data_pacify (rt_data, efficiency_reset, error_reset)
        class(rt_data_t), intent(inout) :: rt_data
        logical, intent(in), optional :: efficiency_reset, error_reset
        type(process_entry_t), pointer :: process
        process => rt_data%process_stack%first
        do while (associated (process))
            call process%pacify (efficiency_reset, error_reset)
            process => process%next
        end do
    end subroutine rt_data_pacify

```

```

<RT data: rt data: TBP>+≡
    procedure :: set_event_callback => rt_data_set_event_callback

<RT data: procedures>+≡
    subroutine rt_data_set_event_callback (global, callback)
        class(rt_data_t), intent(inout) :: global
        class(event_callback_t), intent(in) :: callback
        if (allocated (global%event_callback)) deallocate (global%event_callback)
        allocate (global%event_callback, source = callback)
    end subroutine rt_data_set_event_callback

<RT data: rt data: TBP>+≡
    procedure :: has_event_callback => rt_data_has_event_callback
    procedure :: get_event_callback => rt_data_get_event_callback

<RT data: procedures>+≡
    function rt_data_has_event_callback (global) result (flag)
        class(rt_data_t), intent(in) :: global
        logical :: flag
        flag = allocated (global%event_callback)
    end function rt_data_has_event_callback

    function rt_data_get_event_callback (global) result (callback)
        class(rt_data_t), intent(in) :: global
        class(event_callback_t), allocatable :: callback
        if (allocated (global%event_callback)) then
            allocate (callback, source = global%event_callback)
        end if
    end function rt_data_get_event_callback

```

Force system-dependent objects to well-defined values. Some of the variables are locked and therefore must be addressed directly.

This is, of course, only required for testing purposes. In principle, the `real_specimen` variables could be set to their values in `rt_data_t`, but this depends on the precision again, so we set them to some dummy values.

```

<RT data: public>+≡
    public :: fix_system_dependencies

<RT data: procedures>+≡
    subroutine fix_system_dependencies (global)
        class(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list

        var_list => global%get_var_list_ptr ()
        call var_list%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true., force=.true.)
        call var_list%set_log (var_str ("?openmp_is_active"), &
            .false., is_known = .true., force=.true.)
        call var_list%set_int (var_str ("openmp_num_threads_default"), &
            1, is_known = .true., force=.true.)
        call var_list%set_int (var_str ("openmp_num_threads"), &
            1, is_known = .true., force=.true.)

```

```

call var_list%set_int (var_str ("real_range"), &
307, is_known = .true., force=.true.)
call var_list%set_int (var_str ("real_precision"), &
15, is_known = .true., force=.true.)
call var_list%set_real (var_str ("real_epsilon"), &
1.e-16_default, is_known = .true., force=.true.)
call var_list%set_real (var_str ("real_tiny"), &
1.e-300_default, is_known = .true., force=.true.)

```

```

global%os_data%fc = "Fortran-compiler"
global%os_data%fcflags = "Fortran-flags"
global%os_data%fclibs = "Fortran-libs"

```

```

end subroutine fix_system_dependencies

```

<RT data: public>+≡

```

public :: show_description_of_string

```

<RT data: procedures>+≡

```

subroutine show_description_of_string (string)
type(string_t), intent(in) :: string
type(rt_data_t), target :: global
call global%global_init ()
call global%show_description_of_string (string, ascii_output=.true.)
end subroutine show_description_of_string

```

<RT data: public>+≡

```

public :: show_tex_descriptions

```

<RT data: procedures>+≡

```

subroutine show_tex_descriptions ()
type(rt_data_t), target :: global
call global%global_init ()
call fix_system_dependencies (global)
call global%set_int (var_str ("seed"), 0, is_known=.true.)
call global%var_list%sort ()
call global%write_var_descriptions ()
end subroutine show_tex_descriptions

```

33.2.14 Unit Tests

Test module, followed by the corresponding implementation module.

<rt_data_ut.f90>≡

<File header>

```

module rt_data_ut
use unit_tests
use rt_data_util

```

<Standard module head>

<RT data: public test>

```

contains

  <RT data: test driver>

end module rt_data_ut

<rt_data_util.f90>≡
  <File header>

  module rt_data_util

    <Use kinds>
    <Use strings>
    use format_defs, only: FMT_19
    use ifiles
    use lexers
    use parser
    use flavors
    use variables, only: var_list_t, var_entry_t, var_entry_init_int
    use eval_trees
    use models
    use prclib_stacks

    use rt_data

    <Standard module head>

    <RT data: test declarations>

contains

  <RT data: test auxiliary>

  <RT data: tests>

end module rt_data_util
API: driver for the unit tests below.
<RT data: public test>≡
  public :: rt_data_test
<RT data: test driver>≡
  subroutine rt_data_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <RT data: execute tests>
  end subroutine rt_data_test

```

Initial content

Display the RT data in the state just after (global) initialization.

```

<RT data: execute tests>≡
  call test (rt_data_1, "rt_data_1", &

```

```

        "initialize", &
        u, results)
<RT data: test declarations>≡
    public :: rt_data_1
<RT data: tests>≡
    subroutine rt_data_1 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global

        write (u, "(A)")  "* Test output: rt_data_1"
        write (u, "(A)")  "*   Purpose: initialize global runtime data"
        write (u, "(A)")

        call global%global_init (logfile = var_str ("rt_data.log"))
        call fix_system_dependencies (global)

        call global%set_int (var_str ("seed"), 0, is_known=.true.)

        call global%it_list%init ([2, 3], [5000, 20000])

        call global%write (u)

        call global%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: rt_data_1"

    end subroutine rt_data_1

```

Fill values

Fill in empty slots in the runtime data block.

```

<RT data: execute tests>+≡
    call test (rt_data_2, "rt_data_2", &
        "fill", &
        u, results)
<RT data: test declarations>+≡
    public :: rt_data_2
<RT data: tests>+≡
    subroutine rt_data_2 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        type(flavor_t), dimension(2) :: flv
        type(string_t) :: cut_expr_text
        type(ifile_t) :: ifile
        type(stream_t) :: stream
        type(parse_tree_t) :: parse_tree

        write (u, "(A)")  "* Test output: rt_data_2"
        write (u, "(A)")  "*   Purpose: initialize global runtime data &
            &and fill contents"

```

```

write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call fix_system_dependencies (global)

call global%select_model (var_str ("Test"))

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)
call flv%init ([25,25], global%model)

call global%set_string (var_str ("$_run_id"), &
    var_str ("run1"), is_known = .true.)
call global%set_real (var_str ("luminosity"), &
    33._default, is_known = .true.)

call syntax_pexpr_init ()
cut_expr_text = "all Pt > 100 [s]"
call ifile_append (ifile, cut_expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (parse_tree, stream, .true.)
global%pn%cuts_lexpr => parse_tree%get_root_ptr ()

allocate (global%sample_fmt (2))
global%sample_fmt(1) = "foo_fmt"
global%sample_fmt(2) = "bar_fmt"

call global%write (u)

call parse_tree_final (parse_tree)
call stream_final (stream)
call ifile_final (ifile)
call syntax_pexpr_final ()

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_2"

end subroutine rt_data_2

```

Save and restore

Set up a local runtime data block, change some contents, restore the global block.

```

<RT data: execute tests>+=
call test (rt_data_3, "rt_data_3", &

```



```

        "save/restore", &
        u, results)
<RT data: test declarations>+≡
    public :: rt_data_3
<RT data: tests>+≡
    subroutine rt_data_3 (u)
        use event_base, only: event_callback_nop_t
        integer, intent(in) :: u
        type(rt_data_t), target :: global, local
        type(flavor_t), dimension(2) :: flv
        type(string_t) :: cut_expr_text
        type(ifile_t) :: ifile
        type(stream_t) :: stream
        type(parse_tree_t) :: parse_tree
        type(prclib_entry_t), pointer :: lib
        type(event_callback_nop_t) :: event_callback_nop

        write (u, "(A)")  "* Test output: rt_data_3"
        write (u, "(A)")  "* Purpose: initialize global runtime data &
            &and fill contents;"
        write (u, "(A)")  "* copy to local block and back"
        write (u, "(A)")

        write (u, "(A)")  "* Init global data"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()
        call fix_system_dependencies (global)

        call global%set_int (var_str ("seed"), &
            0, is_known=.true.)

        call global%select_model (var_str ("Test"))

        call global%set_real (var_str ("sqrts"),&
            1000._default, is_known = .true.)
        call flv%init ([25,25], global%model)

        call global%beam_structure%init_sf (flv%get_name (), [1])
        call global%beam_structure%set_sf (1, 1, var_str ("pdf_builtin"))

        call global%set_string (var_str ("$run_id"), &
            var_str ("run1"), is_known = .true.)
        call global%set_real (var_str ("luminosity"), &
            33._default, is_known = .true.)

        call syntax_pexpr_init ()
        cut_expr_text = "all Pt > 100 [s]"
        call ifile_append (ifile, cut_expr_text)
        call stream_init (stream, ifile)
        call parse_tree_init_lexpr (parse_tree, stream, .true.)

```

```

global%pn%cuts_lexpr => parse_tree%get_root_ptr ()

allocate (global%sample_fmt (2))
global%sample_fmt(1) = "foo_fmt"
global%sample_fmt(2) = "bar_fmt"

allocate (lib)
call lib%init (var_str ("library_1"))
call global%add_prclib (lib)

write (u, "(A)")  "* Init and modify local data"
write (u, "(A)")

call local%local_init (global)
call local%append_string (var_str ("integration_method"), intrinsic=.true.)
call local%append_string (var_str ("phs_method"), intrinsic=.true.)

call local%activate ()

write (u, "(1x,A,L1)") "model associated  = ", associated (local%model)
write (u, "(1x,A,L1)") "library associated = ", associated (local%prclib)
write (u, *)

call local%model_set_real (var_str ("ms"), 150._default)
call local%set_string (var_str ("integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call local%set_string (var_str ("phs_method"), &
    var_str ("single"), is_known = .true.)

local%os_data%fc = "Local compiler"

allocate (lib)
call lib%init (var_str ("library_2"))
call local%add_prclib (lib)

call local%set_event_callback (event_callback_nop)

call local%write (u)

write (u, "(A)")
write (u, "(A)")  "* Restore global data"
write (u, "(A)")

call local%deactivate (global)

write (u, "(1x,A,L1)") "model associated  = ", associated (global%model)
write (u, "(1x,A,L1)") "library associated = ", associated (global%prclib)
write (u, *)

call global%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call parse_tree_final (parse_tree)
call stream_final (stream)
call ifile_final (ifile)
call syntax_pexpr_final ()

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_3"

end subroutine rt_data_3

```

Show variables

Display selected variables in the global record.

```

<RT data: execute tests>+≡
call test (rt_data_4, "rt_data_4", &
  "show variables", &
  u, results)

<RT data: test declarations>+≡
public :: rt_data_4

<RT data: tests>+≡
subroutine rt_data_4 (u)
  integer, intent(in) :: u
  type(rt_data_t), target :: global

  type(string_t), dimension(0) :: empty_string_array

  write (u, "(A)")  "* Test output: rt_data_4"
  write (u, "(A)")  "* Purpose: display selected variables"
  write (u, "(A)")

  call global%global_init ()

  write (u, "(A)")  "* No variables:"
  write (u, "(A)")

  call global%write_vars (u, empty_string_array)

  write (u, "(A)")  "* Two variables:"
  write (u, "(A)")

  call global%write_vars (u, &
    [var_str ("?unweighted"), var_str ("phs_method")])

  write (u, "(A)")
  write (u, "(A)")  "* Display whole record with selected variables"
  write (u, "(A)")

  call global%write (u, &
    vars = [var_str ("?unweighted"), var_str ("phs_method")])

```

```

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_4"

end subroutine rt_data_4

```

Show parts

Display only selected parts in the state just after (global) initialization.

```

<RT data: execute tests>+≡
call test (rt_data_5, "rt_data_5", &
  "show parts", &
  u, results)

<RT data: test declarations>+≡
public :: rt_data_5

<RT data: tests>+≡
subroutine rt_data_5 (u)
  integer, intent(in) :: u
  type(rt_data_t), target :: global

  write (u, "(A)")  "* Test output: rt_data_5"
  write (u, "(A)")  "* Purpose: display parts of rt data"
  write (u, "(A)")

  call global%global_init ()
  call global%write_libraries (u)

  write (u, "(A)")

  call global%write_beams (u)

  write (u, "(A)")

  call global%write_process_stack (u)

  call global%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: rt_data_5"

end subroutine rt_data_5

```

Local Model

Locally modify a model and restore the global one. We need an auxiliary function to determine the status of a model particle:

```

<RT data: test auxiliary>≡
function is_stable (pdg, global) result (flag)

```

```

integer, intent(in) :: pdg
type(rt_data_t), intent(in) :: global
logical :: flag
type(flavor_t) :: flv
call flv%init (pdg, global%model)
flag = flv%is_stable ()
end function is_stable

function is_polarized (pdg, global) result (flag)
integer, intent(in) :: pdg
type(rt_data_t), intent(in) :: global
logical :: flag
type(flavor_t) :: flv
call flv%init (pdg, global%model)
flag = flv%is_polarized ()
end function is_polarized

<RT data: execute tests>+≡
call test (rt_data_6, "rt_data_6", &
          "local model", &
          u, results)

<RT data: test declarations>+≡
public :: rt_data_6

<RT data: tests>+≡
subroutine rt_data_6 (u)
integer, intent(in) :: u
type(rt_data_t), target :: global, local
type(var_list_t), pointer :: model_vars
type(string_t) :: var_name

write (u, "(A)")  "* Test output: rt_data_6"
write (u, "(A)")  "* Purpose: apply and keep local modifications to model"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%select_model (var_str ("Test"))

write (u, "(A)")  "* Original model"
write (u, "(A)")

call global%write_model_list (u)
write (u, *)
write (u, "(A,L1)")  "s is stable      = ", is_stable (25, global)
write (u, "(A,L1)")  "f is polarized = ", is_polarized (6, global)

write (u, *)

var_name = "ff"

write (u, "(A)", advance="no")  "Global model variable: "
model_vars => global%model%get_var_list_ptr ()

```

```

call model_vars%write_var (var_name, u)

write (u, "(A)")
write (u, "(A)")  "* Apply local modifications: unstable"
write (u, "(A)")

call local%local_init (global)
call local%activate ()

call local%model_set_real (var_name, 0.4_default)
call local%modify_particle (25, stable = .false., decay = [var_str ("d1")])
call local%modify_particle (6, stable = .false., &
    decay = [var_str ("f1")], isotropic_decay = .true.)
call local%modify_particle (-6, stable = .false., &
    decay = [var_str ("f2"), var_str ("f3")], diagonal_decay = .true.)

call local%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Further modifications"
write (u, "(A)")

call local%modify_particle (6, stable = .false., &
    decay = [var_str ("f1")], &
    diagonal_decay = .true., isotropic_decay = .false.)
call local%modify_particle (-6, stable = .false., &
    decay = [var_str ("f2"), var_str ("f3")], &
    diagonal_decay = .false., isotropic_decay = .true.)
call local%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Further modifications: f stable but polarized"
write (u, "(A)")

call local%modify_particle (6, stable = .true., polarized = .true.)
call local%modify_particle (-6, stable = .true.)
call local%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Global model"
write (u, "(A)")

call global%model%write (u)
write (u, *)
write (u, "(A,L1)")  "s is stable      = ", is_stable (25, global)
write (u, "(A,L1)")  "f is polarized = ", is_polarized (6, global)

write (u, "(A)")
write (u, "(A)")  "* Local model"
write (u, "(A)")

call local%model%write (u)
write (u, *)
write (u, "(A,L1)")  "s is stable      = ", is_stable (25, local)

```

```

write (u, "(A,L1)") "f is polarized = ", is_polarized (6, local)

write (u, *)

write (u, "(A)", advance="no") "Global model variable: "
model_vars => global%model%get_var_list_ptr ()
call model_vars%write_var (var_name, u)

write (u, "(A)", advance="no") "Local model variable: "
associate (model_var_list_ptr => local%model%get_var_list_ptr())
  call model_var_list_ptr%write_var (var_name, u)
end associate

write (u, "(A)")
write (u, "(A)")  "** Restore global"

call local%deactivate (global, keep_local = .true.)

write (u, "(A)")
write (u, "(A)")  "** Global model"
write (u, "(A)")

call global%model%write (u)
write (u, *)
write (u, "(A,L1)") "s is stable      = ", is_stable (25, global)
write (u, "(A,L1)") "f is polarized = ", is_polarized (6, global)

write (u, "(A)")
write (u, "(A)")  "** Local model"
write (u, "(A)")

call local%model%write (u)
write (u, *)
write (u, "(A,L1)") "s is stable      = ", is_stable (25, local)
write (u, "(A,L1)") "f is polarized = ", is_polarized (6, local)

write (u, *)

write (u, "(A)", advance="no") "Global model variable: "
model_vars => global%model%get_var_list_ptr ()
call model_vars%write_var (var_name, u)

write (u, "(A)", advance="no") "Local model variable: "
associate (model_var_list_ptr => local%model%get_var_list_ptr())
  call model_var_list_ptr%write_var (var_name, u)
end associate

write (u, "(A)")
write (u, "(A)")  "** Cleanup"

call local%model%final ()
deallocate (local%model)

call global%final ()

```

```

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_6"

end subroutine rt_data_6

```

Result variables

Initialize result variables and check that they are accessible via the global variable list.

```

<RT data: execute tests>+≡
call test (rt_data_7, "rt_data_7", &
  "result variables", &
  u, results)

<RT data: test declarations>+≡
public :: rt_data_7

<RT data: tests>+≡
subroutine rt_data_7 (u)
  integer, intent(in) :: u
  type(rt_data_t), target :: global

  write (u, "(A)")  "* Test output: rt_data_7"
  write (u, "(A)")  "* Purpose: set and access result variables"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize process variables"
  write (u, "(A)")

  call global%global_init ()
  call global%process_stack%init_result_vars (var_str ("testproc"))

  call global%var_list%write_var (&
    var_str ("integral(testproc)"), u, defined=.true.)
  call global%var_list%write_var (&
    var_str ("error(testproc)"), u, defined=.true.)

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

  call global%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: rt_data_7"

end subroutine rt_data_7

```

Beam energy

If beam parameters are set, the variable `sqrts` is not necessarily the collision energy. The method `get_sqrts` fetches the correct value.


```

<RT data: execute tests>+≡
    call test (rt_data_8, "rt_data_8", &
               "beam energy", &
               u, results)

<RT data: test declarations>+≡
    public :: rt_data_8

<RT data: tests>+≡
    subroutine rt_data_8 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global

        write (u, "(A)")  "* Test output: rt_data_8"
        write (u, "(A)")  "*   Purpose: get correct collision energy"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize"
        write (u, "(A)")

        call global%global_init ()

        write (u, "(A)")  "* Set sqrts"
        write (u, "(A)")

        call global%set_real (var_str ("sqrts"), &
                              1000._default, is_known = .true.)
        write (u, "(1x,A," // FMT_19 // ")")  "sqrts =", global%get_sqrts ()

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

        call global%final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: rt_data_8"

    end subroutine rt_data_8

```

Local variable modifications

```

<RT data: execute tests>+≡
    call test (rt_data_9, "rt_data_9", &
               "local variables", &
               u, results)

<RT data: test declarations>+≡
    public :: rt_data_9

<RT data: tests>+≡
    subroutine rt_data_9 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global, local
        type(var_list_t), pointer :: var_list

```

```

write (u, "(A)")  "* Test output: rt_data_9"
write (u, "(A)")  "* Purpose: handle local variables"
write (u, "(A)")

call syntax_model_file_init ()

write (u, "(A)")  "* Initialize global record and set some variables"
write (u, "(A)")

call global%global_init ()
call global%select_model (var_str ("Test"))

call global%set_real (var_str ("sqrts"), 17._default, is_known = .true.)
call global%set_real (var_str ("luminosity"), 2._default, is_known = .true.)
call global%model_set_real (var_str ("ff"), 0.5_default)
call global%model_set_real (var_str ("gy"), 1.2_default)

var_list => global%get_var_list_ptr ()

call var_list%write_var (var_str ("sqrts"), u, defined=.true.)
call var_list%write_var (var_str ("luminosity"), u, defined=.true.)
call var_list%write_var (var_str ("ff"), u, defined=.true.)
call var_list%write_var (var_str ("gy"), u, defined=.true.)
call var_list%write_var (var_str ("mf"), u, defined=.true.)
call var_list%write_var (var_str ("x"), u, defined=.true.)

write (u, "(A)")

write (u, "(1x,A,1x,F5.2)") "sqrts      = ", &
    global%get_rval (var_str ("sqrts"))
write (u, "(1x,A,1x,F5.2)") "luminosity = ", &
    global%get_rval (var_str ("luminosity"))
write (u, "(1x,A,1x,F5.2)") "ff          = ", &
    global%get_rval (var_str ("ff"))
write (u, "(1x,A,1x,F5.2)") "gy          = ", &
    global%get_rval (var_str ("gy"))
write (u, "(1x,A,1x,F5.2)") "mf          = ", &
    global%get_rval (var_str ("mf"))
write (u, "(1x,A,1x,F5.2)") "x           = ", &
    global%get_rval (var_str ("x"))

write (u, "(A)")
write (u, "(A)")  "* Create local record with local variables"
write (u, "(A)")

call local%local_init (global)

call local%append_real (var_str ("luminosity"), intrinsic = .true.)
call local%append_real (var_str ("x"), user = .true.)

call local%activate ()

var_list => local%get_var_list_ptr ()

```

```

call var_list%write_var (var_str ("sqrts"), u)
call var_list%write_var (var_str ("luminosity"), u)
call var_list%write_var (var_str ("ff"), u)
call var_list%write_var (var_str ("gy"), u)
call var_list%write_var (var_str ("mf"), u)
call var_list%write_var (var_str ("x"), u, defined=.true.)

write (u, "(A)")

write (u, "(1x,A,1x,F5.2)" "sqrts      = ", &
      local%get_rval (var_str ("sqrts")))
write (u, "(1x,A,1x,F5.2)" "luminosity = ", &
      local%get_rval (var_str ("luminosity")))
write (u, "(1x,A,1x,F5.2)" "ff          = ", &
      local%get_rval (var_str ("ff")))
write (u, "(1x,A,1x,F5.2)" "gy          = ", &
      local%get_rval (var_str ("gy")))
write (u, "(1x,A,1x,F5.2)" "mf          = ", &
      local%get_rval (var_str ("mf")))
write (u, "(1x,A,1x,F5.2)" "x            = ", &
      local%get_rval (var_str ("x")))

write (u, "(A)")
write (u, "(A)") "* Modify some local variables"
write (u, "(A)")

call local%set_real (var_str ("luminosity"), 42._default, is_known=.true.)
call local%set_real (var_str ("x"), 6.66_default, is_known=.true.)
call local%model_set_real (var_str ("ff"), 0.7_default)

var_list => local%get_var_list_ptr ()

call var_list%write_var (var_str ("sqrts"), u)
call var_list%write_var (var_str ("luminosity"), u)
call var_list%write_var (var_str ("ff"), u)
call var_list%write_var (var_str ("gy"), u)
call var_list%write_var (var_str ("mf"), u)
call var_list%write_var (var_str ("x"), u, defined=.true.)

write (u, "(A)")

write (u, "(1x,A,1x,F5.2)" "sqrts      = ", &
      local%get_rval (var_str ("sqrts")))
write (u, "(1x,A,1x,F5.2)" "luminosity = ", &
      local%get_rval (var_str ("luminosity")))
write (u, "(1x,A,1x,F5.2)" "ff          = ", &
      local%get_rval (var_str ("ff")))
write (u, "(1x,A,1x,F5.2)" "gy          = ", &
      local%get_rval (var_str ("gy")))
write (u, "(1x,A,1x,F5.2)" "mf          = ", &
      local%get_rval (var_str ("mf")))
write (u, "(1x,A,1x,F5.2)" "x            = ", &
      local%get_rval (var_str ("x")))

```

```

write (u, "(A)")
write (u, "(A)")  "* Restore globals"
write (u, "(A)")

call local%deactivate (global)

var_list => global%get_var_list_ptr ()

call var_list%write_var (var_str ("sqrts"), u)
call var_list%write_var (var_str ("luminosity"), u)
call var_list%write_var (var_str ("ff"), u)
call var_list%write_var (var_str ("gy"), u)
call var_list%write_var (var_str ("mf"), u)
call var_list%write_var (var_str ("x"), u, defined=.true.)

write (u, "(A)")

write (u, "(1x,A,1x,F5.2)") "sqrts      = ", &
    global%get_rval (var_str ("sqrts"))
write (u, "(1x,A,1x,F5.2)") "luminosity = ", &
    global%get_rval (var_str ("luminosity"))
write (u, "(1x,A,1x,F5.2)") "ff          = ", &
    global%get_rval (var_str ("ff"))
write (u, "(1x,A,1x,F5.2)") "gy          = ", &
    global%get_rval (var_str ("gy"))
write (u, "(1x,A,1x,F5.2)") "mf          = ", &
    global%get_rval (var_str ("mf"))
write (u, "(1x,A,1x,F5.2)") "x           = ", &
    global%get_rval (var_str ("x"))

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call local%local_final ()

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_9"

end subroutine rt_data_9

```

Descriptions

```

<RT data: execute tests>+≡
    call test(rt_data_10, "rt_data_10", &
        "descriptions", u, results)

<RT data: test declarations>+≡
    public :: rt_data_10

<RT data: tests>+≡
    subroutine rt_data_10 (u)

```

```

integer, intent(in) :: u
type(rt_data_t) :: global
! type(var_list_t) :: var_list
write (u, "(A)")  "* Test output: rt_data_10"
write (u, "(A)")  "* Purpose: display descriptions"
write (u, "(A)")

call global%var_list%append_real (var_str ("sqrts"), &
    intrinsic=.true., &
    description=var_str ('Real variable in order to set the center-of-mass ' // &
        'energy for the collisions.'))
call global%var_list%append_real (var_str ("luminosity"), 0._default, &
    intrinsic=.true., &
    description=var_str ('This specifier \ttt{luminosity = {\em ' // &
        '<num>}} sets the integrated luminosity (in inverse femtobarns, ' // &
        'fb$^{-1}$) for the event generation of the processes in the ' // &
        '\sindarin\ input files.'))
call global%var_list%append_int (var_str ("seed"), 1234, &
    intrinsic=.true., &
    description=var_str ('Integer variable \ttt{seed = {\em <num>}} ' // &
        'that allows to set a specific random seed \ttt{num}.'))
call global%var_list%append_string (var_str ("method"), var_str ("omega"), &
    intrinsic=.true., &
    description=var_str ('This string variable specifies the method ' // &
        'for the matrix elements to be used in the evaluation.'))
call global%var_list%append_log (var_str ("?read_color_factors"), .true., &
    intrinsic=.true., &
    description=var_str ('This flag decides whether to read QCD ' // &
        'color factors from the matrix element provided by each method, ' // &
        'or to try and calculate the color factors in \whizard\ internally.'))

call global%var_list%sort ()

call global%write_var_descriptions (u)
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: rt_data_10"
end subroutine rt_data_10

```

Export objects

Export objects are variables or other data that should be copied or otherwise applied to corresponding objects in the outer scope.

We test appending and retrieval for the export list.

```

<RT data: execute tests>+≡
    call test(rt_data_11, "rt_data_11", &
        "export objects", u, results)

<RT data: test declarations>+≡
    public :: rt_data_11

```

```

<RT data: tests>+≡
subroutine rt_data_11 (u)
  integer, intent(in) :: u
  type(rt_data_t) :: global
  type(string_t), dimension(:), allocatable :: exports
  integer :: i

  write (u, "(A)")  "* Test output: rt_data_11"
  write (u, "(A)")  "* Purpose: handle export object list"
  write (u, "(A)")

  write (u, "(A)")  "* Empty export list"
  write (u, "(A)")

  call global%write_exports (u)

  write (u, "(A)")  "* Add an entry"
  write (u, "(A)")

  allocate (exports (1))
  exports(1) = var_str ("results")
  do i = 1, size (exports)
    write (u, "('+ ',A)") char (exports(i))
  end do
  write (u, *)

  call global%append_exports (exports)
  call global%write_exports (u)

  write (u, "(A)")
  write (u, "(A)")  "* Add more entries, including doubler"
  write (u, "(A)")

  deallocate (exports)
  allocate (exports (3))
  exports(1) = var_str ("foo")
  exports(2) = var_str ("results")
  exports(3) = var_str ("bar")
  do i = 1, size (exports)
    write (u, "('+ ',A)") char (exports(i))
  end do
  write (u, *)

  call global%append_exports (exports)
  call global%write_exports (u)

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

  call global%final ()

  write (u, "(A)")
  write (u, "(A)")  "* Test output end: rt_data_11"
end subroutine rt_data_11

```


33.3 Select implementations

For abstract types (process core, integrator, phase space, etc.), we need a way to dynamically select a concrete type, using either data given by the user or a previous selection of a concrete type. This is done by subroutines in the current module.

We would like to put this in the `me_methods` folder but it also depends on `gosam` and `openloops`, so it is unclear where to put it.

```
<dispatch_me_methods.f90>≡  
  <File header>  
  
  module dispatch_me_methods  
  
    <Use strings>  
    <Use debug>  
    use physics_defs, only: BORN  
    use diagnostics  
    use sm_qcd  
    use variables, only: var_list_t  
    use models  
    use model_data  
  
    use prc_core_def  
    use prc_core  
    use prc_test_core  
    use prc_template_me  
    use prc_test  
    use prc_omega  
    use prc_external  
    use prc_gosam  
    use prc_openloops  
    use prc_recola  
    use prc_threshold  
  
    <Standard module head>  
  
    <Dispatch me methods: public>  
  
    contains  
  
    <Dispatch me methods: procedures>  
  
  end module dispatch_me_methods
```

33.3.1 Process Core Definition

The `prc_core_def_t` abstract type can be instantiated by providing a `$method` string variable.

```
<Dispatch me methods: public>≡  
  public :: dispatch_core_def  
  
<Dispatch me methods: procedures>≡  
  subroutine dispatch_core_def (core_def, prt_in, prt_out, &
```



```

        model, var_list, id, nlo_type, method)
class(prc_core_def_t), allocatable, intent(out) :: core_def
type(string_t), dimension(:), intent(in) :: prt_in
type(string_t), dimension(:), intent(in) :: prt_out
type(model_t), pointer, intent(in) :: model
type(var_list_t), intent(in) :: var_list
type(string_t), intent(in), optional :: id
integer, intent(in), optional :: nlo_type
type(string_t), intent(in), optional :: method
type(string_t) :: model_name, meth
type(string_t) :: ufo_path
type(string_t) :: restrictions
logical :: ufo
logical :: cms_scheme
logical :: openmp_support
logical :: report_progress
logical :: diags, diags_color
logical :: write_phs_output
type(string_t) :: extra_options, correction_type
integer :: nlo
integer :: alpha_power
integer :: alphas_power
if (present (method)) then
    meth = method
else
    meth = var_list%get_sval (var_str ("$method"))
end if
if (debug_on) call msg_debug2 (D_CORE, "dispatch_core_def")
if (associated (model)) then
    model_name = model%get_name ()
    cms_scheme = model%get_scheme () == "Complex_Mass_Scheme"
    ufo = model%is_ufo_model ()
    ufo_path = model%get_ufo_path ()
else
    model_name = ""
    cms_scheme = .false.
    ufo = .false.
end if
restrictions = var_list%get_sval (&
    var_str ("$restrictions"))
diags = var_list%get_lval (&
    var_str ("?vis_diags"))
diags_color = var_list%get_lval (&
    var_str ("?vis_diags_color"))
openmp_support = var_list%get_lval (&
    var_str ("?omega_openmp"))
report_progress = var_list%get_lval (&
    var_str ("?report_progress"))
write_phs_output = var_list%get_lval (&
    var_str ("?omega_write_phs_output"))
extra_options = var_list%get_sval (&
    var_str ("$omega_flags"))
nlo = BORN; if (present (nlo_type)) nlo = nlo_type
alpha_power = var_list%get_ival (var_str ("alpha_power"))

```

```

alphas_power = var_list%get_ival (var_str ("alphas_power"))
correction_type = var_list%get_sval (var_str ("nlo_correction_type"))
if (debug_on) call msg_debug2 (D_CORE, "dispatching core method: ", meth)
select case (char (meth))
case ("unit_test")
  allocate (prc_test_def_t :: core_def)
  select type (core_def)
  type is (prc_test_def_t)
    call core_def%init (model_name, prt_in, prt_out)
  end select
case ("template")
  allocate (template_me_def_t :: core_def)
  select type (core_def)
  type is (template_me_def_t)
    call core_def%init (model, prt_in, prt_out, unity = .false.)
  end select
case ("template_unity")
  allocate (template_me_def_t :: core_def)
  select type (core_def)
  type is (template_me_def_t)
    call core_def%init (model, prt_in, prt_out, unity = .true.)
  end select
case ("omega")
  allocate (omega_def_t :: core_def)
  select type (core_def)
  type is (omega_def_t)
    call core_def%init (model_name, prt_in, prt_out, &
      .false., ufo, ufo_path, &
      restrictions, cms_scheme, &
      openmp_support, report_progress, write_phs_output, &
      extra_options, diags, diags_color)
  end select
case ("ovm")
  allocate (omega_def_t :: core_def)
  select type (core_def)
  type is (omega_def_t)
    call core_def%init (model_name, prt_in, prt_out, &
      .true., .false., var_str (""), &
      restrictions, cms_scheme, &
      openmp_support, report_progress, write_phs_output, &
      extra_options, diags, diags_color)
  end select
case ("gosam")
  allocate (gosam_def_t :: core_def)
  select type (core_def)
  type is (gosam_def_t)
    if (present (id)) then
      call core_def%init (id, model_name, prt_in, &
        prt_out, nlo, restrictions, var_list)
    else
      call msg_fatal ("Dispatch GoSam def: No id!")
    end if
  end select
case ("openloops")

```

```

allocate (openloops_def_t :: core_def)
select type (core_def)
type is (openloops_def_t)
  if (present (id)) then
    call core_def%init (id, model_name, prt_in, &
      prt_out, nlo, restrictions, var_list)
  else
    call msg_fatal ("Dispatch OpenLoops def: No id!")
  end if
end select
case ("recola")
  call abort_if_recola_not_active ()
  allocate (recola_def_t :: core_def)
  select type (core_def)
  type is (recola_def_t)
    if (present (id)) then
      call core_def%init (id, model_name, prt_in, prt_out, &
        nlo, alpha_power, alphas_power, correction_type, &
        restrictions)
    else
      call msg_fatal ("Dispatch RECOLA def: No id!")
    end if
  end select
case ("dummy")
  allocate (prc_external_test_def_t :: core_def)
  select type (core_def)
  type is (prc_external_test_def_t)
    if (present (id)) then
      call core_def%init (id, model_name, prt_in, prt_out)
    else
      call msg_fatal ("Dispatch User-Defined Test def: No id!")
    end if
  end select
case ("threshold")
  allocate (threshold_def_t :: core_def)
  select type (core_def)
  type is (threshold_def_t)
    if (present (id)) then
      call core_def%init (id, model_name, prt_in, prt_out, &
        nlo, restrictions)
    else
      call msg_fatal ("Dispatch Threshold def: No id!")
    end if
  end select
case default
  call msg_fatal ("Process configuration: method '" &
    // char (meth) // "' not implemented")
end select
end subroutine dispatch_core_def

```

33.3.2 Process core allocation

Here we allocate an object of abstract type `prc_core_t` with a concrete type that matches a process definition. The `prc_omega_t` extension will require the current parameter set, so we take the opportunity to grab it from the model.

```

(Dispatch me methods: public)+≡
    public :: dispatch_core

(Dispatch me methods: procedures)+≡
    subroutine dispatch_core (core, core_def, model, &
        helicity_selection, qcd, use_color_factors, has_beam_pol)
        class(prc_core_t), allocatable, intent(inout) :: core
        class(prc_core_def_t), intent(in) :: core_def
        class(model_data_t), intent(in), target, optional :: model
        type(helicity_selection_t), intent(in), optional :: helicity_selection
        type(qcd_t), intent(in), optional :: qcd
        logical, intent(in), optional :: use_color_factors
        logical, intent(in), optional :: has_beam_pol
        select type (core_def)
            type is (prc_test_def_t)
                allocate (test_t :: core)
            type is (template_me_def_t)
                allocate (prc_template_me_t :: core)
                select type (core)
                    type is (prc_template_me_t)
                        call core%set_parameters (model)
                end select
        class is (omega_def_t)
            if (.not. allocated (core)) allocate (prc_omega_t :: core)
            select type (core)
                type is (prc_omega_t)
                    call core%set_parameters (model, &
                        helicity_selection, qcd, use_color_factors)
            end select
        type is (gosam_def_t)
            if (.not. allocated (core)) allocate (prc_gosam_t :: core)
            select type (core)
                type is (prc_gosam_t)
                    call core%set_parameters (qcd)
            end select
        type is (openloops_def_t)
            if (.not. allocated (core)) allocate (prc_openloops_t :: core)
            select type (core)
                type is (prc_openloops_t)
                    call core%set_parameters (qcd)
            end select
        type is (recola_def_t)
            if (.not. allocated (core)) allocate (prc_recola_t :: core)
            select type (core)
                type is (prc_recola_t)
                    call core%set_parameters (qcd, model)
            end select
        type is (prc_external_test_def_t)
            if (.not. allocated (core)) allocate (prc_external_test_t :: core)
            select type (core)

```

```

        type is (prc_external_test_t)
            call core%set_parameters (qcd, model)
        end select
    type is (threshold_def_t)
        if (.not. allocated (core)) allocate (prc_threshold_t :: core)
        select type (core)
            type is (prc_threshold_t)
                call core%set_parameters (qcd, model)
                call core%set_beam_pol (has_beam_pol)
            end select
        class default
            call msg_bug ("Process core: unexpected process definition type")
        end select
    end subroutine dispatch_core

```

33.3.3 Process core update and restoration

Here we take an existing object of abstract type `prc_core_t` and update the parameters as given by the current state of `model`. Optionally, we can save the previous state as `saved_core`. The second routine restores the original from the save.

(In the test case, there is no possible update.)

<Dispatch me methods: public>+≡

```

    public :: dispatch_core_update
    public :: dispatch_core_restore

```

<Dispatch me methods: procedures>+≡

```

    subroutine dispatch_core_update &
        (core, model, helicity_selection, qcd, saved_core)

        class(prc_core_t), allocatable, intent(inout) :: core
        class(model_data_t), intent(in), optional, target :: model
        type(helicity_selection_t), intent(in), optional :: helicity_selection
        type(qcd_t), intent(in), optional :: qcd
        class(prc_core_t), allocatable, intent(inout), optional :: saved_core

        if (present (saved_core)) then
            allocate (saved_core, source = core)
        end if
        select type (core)
            type is (test_t)
            type is (prc_omega_t)
                call core%set_parameters (model, helicity_selection, qcd)
                call core%activate_parameters ()
            class is (prc_external_t)
                call msg_message ("Updating user defined cores is not implemented yet.")
            class default
                call msg_bug ("Process core update: unexpected process definition type")
            end select
    end subroutine dispatch_core_update

    subroutine dispatch_core_restore (core, saved_core)

```

```

class(prc_core_t), allocatable, intent(inout) :: core
class(prc_core_t), allocatable, intent(inout) :: saved_core

call move_alloc (from = saved_core, to = core)
select type (core)
type is (test_t)
type is (prc_omega_t)
    call core%activate_parameters ()
class default
    call msg_bug ("Process core restore: unexpected process definition type")
end select
end subroutine dispatch_core_restore

```

33.3.4 Unit Tests

Test module, followed by the corresponding implementation module.

<dispatch_ut.f90>≡
<File header>

```

module dispatch_ut
    use unit_tests
    use dispatch_uti

```

<Standard module head>

<Dispatch: public test>

<Dispatch: public test auxiliary>

contains

<Dispatch: test driver>

```

end module dispatch_ut

```

<dispatch_uti.f90>≡
<File header>

```

module dispatch_uti
    <Use kinds>
    <Use strings>
    use os_interface, only: os_data_t
    use physics_defs, only: ELECTRON, PROTON
    use sm_qcd, only: qcd_t
    use flavors, only: flavor_t
    use interactions, only: reset_interaction_counter
    use pdg_arrays, only: pdg_array_t, assignment(=)
    use prc_core_def, only: prc_core_def_t
    use prc_test_core, only: test_t
    use prc_core, only: prc_core_t
    use prc_test, only: prc_test_def_t
    use prc_omega, only: omega_def_t, prc_omega_t

```

```

use sf_mappings, only: sf_channel_t
use sf_base, only: sf_data_t, sf_config_t
use phs_base, only: phs_channel_collection_t
use variables, only: var_list_t
use model_data, only: model_data_t
use models, only: syntax_model_file_init, syntax_model_file_final
use rt_data, only: rt_data_t

use dispatch_phase_space, only: dispatch_sf_channels
use dispatch_beams, only: sf_prop_t, dispatch_qcd
use dispatch_beams, only: dispatch_sf_config, dispatch_sf_data
use dispatch_me_methods, only: dispatch_core_def, dispatch_core
use dispatch_me_methods, only: dispatch_core_update, dispatch_core_restore

use sf_base_ut, only: sf_test_data_t

```

⟨Standard module head⟩

⟨Dispatch: public test auxiliary⟩

⟨Dispatch: test declarations⟩

contains

⟨Dispatch: tests⟩

⟨Dispatch: test auxiliary⟩

end module dispatch_ut

API: driver for the unit tests below.

⟨Dispatch: public test⟩≡

```
public :: dispatch_test
```

⟨Dispatch: test driver⟩≡

```
subroutine dispatch_test (u, results)
  integer, intent(in) :: u
  type(test_results_t), intent(inout) :: results
```

⟨Dispatch: execute tests⟩

```
end subroutine dispatch_test
```

Select type: process definition

⟨Dispatch: execute tests⟩≡

```
call test (dispatch_1, "dispatch_1", &
  "process configuration method", &
  u, results)
```

⟨Dispatch: test declarations⟩≡

```
public :: dispatch_1
```

⟨Dispatch: tests⟩≡

```
subroutine dispatch_1 (u)
  integer, intent(in) :: u
```

```

type(string_t), dimension(2) :: prt_in, prt_out
type(rt_data_t), target :: global
class(prc_core_def_t), allocatable :: core_def

write (u, "(A)")  "* Test output: dispatch_1"
write (u, "(A)")  "* Purpose: select process configuration method"
write (u, "(A)")

call global%global_init ()

call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)

prt_in = [var_str ("a"), var_str ("b")]
prt_out = [var_str ("c"), var_str ("d")]

write (u, "(A)")  "* Allocate core_def as prc_test_def"

call global%set_string (var_str ("method"), &
    var_str ("unit_test"), is_known = .true.)
call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)
select type (core_def)
type is (prc_test_def_t)
    call core_def%write (u)
end select

deallocate (core_def)

write (u, "(A)")
write (u, "(A)")  "* Allocate core_def as omega_def"
write (u, "(A)")

call global%set_string (var_str ("method"), &
    var_str ("omega"), is_known = .true.)
call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)
select type (core_def)
type is (omega_def_t)
    call core_def%write (u)
end select

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_1"

end subroutine dispatch_1

```

Select type: process core

```

(Dispatch: execute tests) +=
call test (dispatch_2, "dispatch_2", &
    "process core", &
    u, results)

```



```

<Dispatch: test declarations>+≡
    public :: dispatch_2

<Dispatch: tests>+≡
    subroutine dispatch_2 (u)
        integer, intent(in) :: u
        type(string_t), dimension(2) :: prt_in, prt_out
        type(rt_data_t), target :: global
        class(prc_core_def_t), allocatable :: core_def
        class(prc_core_t), allocatable :: core

        write (u, "(A)")  "* Test output: dispatch_2"
        write (u, "(A)")  "*   Purpose: select process configuration method"
        write (u, "(A)")  "               and allocate process core"
        write (u, "(A)")

        call syntax_model_file_init ()
        call global%global_init ()

        prt_in = [var_str ("a"), var_str ("b")]
        prt_out = [var_str ("c"), var_str ("d")]

        write (u, "(A)")  "* Allocate core as test_t"
        write (u, "(A)")

        call global%set_string (var_str ("method"), &
                                var_str ("unit_test"), is_known = .true.)
        call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)
        call dispatch_core (core, core_def)
        select type (core)
            type is (test_t)
                call core%write (u)
        end select

        deallocate (core)
        deallocate (core_def)

        write (u, "(A)")
        write (u, "(A)")  "* Allocate core as prc_omega_t"
        write (u, "(A)")

        call global%set_string (var_str ("method"), &
                                var_str ("omega"), is_known = .true.)
        call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)

        call global%select_model (var_str ("Test"))

        call global%set_log (&
            var_str ("?helicity_selection_active"), &
            .true., is_known = .true.)
        call global%set_real (&
            var_str ("helicity_selection_threshold"), &
            1e9_default, is_known = .true.)
        call global%set_int (&
            var_str ("helicity_selection_cutoff"), &

```

```

10, is_known = .true.)

call dispatch_core (core, core_def, &
    global%model, &
    global%get_helicity_selection ())
call core_def%allocate_driver (core%driver, var_str (""))

select type (core)
type is (prc_omega_t)
    call core%write (u)
end select

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_2"

end subroutine dispatch_2

```

Select type: structure-function data

This is an extra dispatcher that enables the test structure functions. This procedure should be assigned to the `dispatch_sf_data_extra` hook before any tests are executed.

(Dispatch: public test auxiliary)≡

```
public :: dispatch_sf_data_test
```

(Dispatch: test auxiliary)≡

```

subroutine dispatch_sf_data_test (data, sf_method, i_beam, sf_prop, &
    var_list, var_list_global, model, os_data, sqrts, pdg_in, pdg_prc, polarized)
    class(sf_data_t), allocatable, intent(inout) :: data
    type(string_t), intent(in) :: sf_method
    integer, dimension(:), intent(in) :: i_beam
    type(var_list_t), intent(in) :: var_list
    type(var_list_t), intent(inout) :: var_list_global
    class(model_data_t), target, intent(in) :: model
    type(os_data_t), intent(in) :: os_data
    real(default), intent(in) :: sqrts
    type(pdg_array_t), dimension(:), intent(inout) :: pdg_in
    type(pdg_array_t), dimension(:, :), intent(in) :: pdg_prc
    type(sf_prop_t), intent(inout) :: sf_prop
    logical, intent(in) :: polarized
    select case (char (sf_method))
    case ("sf_test_0", "sf_test_1")
        allocate (sf_test_data_t :: data)
        select type (data)
        type is (sf_test_data_t)
            select case (char (sf_method))
            case ("sf_test_0"); call data%init (model, pdg_in(i_beam(1)))
            case ("sf_test_1"); call data%init (model, pdg_in(i_beam(1)), &
                mode = 1)
            end select
        end select
    end select

```

```

        end select
    end select
end subroutine dispatch_sf_data_test

```

The actual test. We can't move this to beams as it depends on `model_features` for the `model_list_t`.

```

<Dispatch: execute tests>+≡
    call test (dispatch_7, "dispatch_7", &
        "structure-function data", &
        u, results)

<Dispatch: test declarations>+≡
    public :: dispatch_7

<Dispatch: tests>+≡
    subroutine dispatch_7 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        type(os_data_t) :: os_data
        type(string_t) :: prt, sf_method
        type(sf_prop_t) :: sf_prop
        class(sf_data_t), allocatable :: data
        type(pdg_array_t), dimension(1) :: pdg_in
        type(pdg_array_t), dimension(1,1) :: pdg_prc
        type(pdg_array_t), dimension(1) :: pdg_out
        integer, dimension(:), allocatable :: pdg1

        write (u, "(A)")  "* Test output: dispatch_7"
        write (u, "(A)")  "* Purpose: select and configure &
            &structure function data"
        write (u, "(A)")

        call global%global_init ()

        call os_data%init ()
        call syntax_model_file_init ()
        call global%select_model (var_str ("QCD"))

        call reset_interaction_counter ()
        call global%set_real (var_str ("sqrts"), &
            14000._default, is_known = .true.)
        prt = "p"
        call global%beam_structure%init_sf ([prt, prt], [1])
        pdg_in = 2212

        write (u, "(A)")  "* Allocate data as sf_pdf_builtin_t"
        write (u, "(A)")

        sf_method = "pdf_builtin"
        call dispatch_sf_data (data, sf_method, [1], sf_prop, &
            global%get_var_list_ptr (), global%var_list, &
            global%model, global%os_data, global%get_sqrts (), &
            pdg_in, pdg_prc, .false.)
        call data%write (u)
    end subroutine dispatch_7

```

```

call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(A)")
write (u, "(1x,A,99(1x,I0))") "PDG(out) = ", pdg1

deallocate (data)

write (u, "(A)")
write (u, "(A)")  "* Allocate data for different PDF set"
write (u, "(A)")

pdg_in = 2212

call global%set_string (var_str ("pdf_builtin_set"), &
    var_str ("CTEQ6M"), is_known = .true.)
sf_method = "pdf_builtin"
call dispatch_sf_data (data, sf_method, [1], sf_prop, &
    global%get_var_list_ptr (), global%var_list, &
    global%model, global%os_data, global%get_sqrts (), &
    pdg_in, pdg_prc, .false.)
call data%write (u)

call data%get_pdg_out (pdg_out)
pdg1 = pdg_out(1)
write (u, "(A)")
write (u, "(1x,A,99(1x,I0))") "PDG(out) = ", pdg1

deallocate (data)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_7"

end subroutine dispatch_7

```

Beam structure

The actual test. We can't move this to beams as it depends on `model_features` for the `model_list_t`.

```

<Dispatch: execute tests>+≡
    call test (dispatch_8, "dispatch_8", &
        "beam structure", &
        u, results)

<Dispatch: test declarations>+≡
    public :: dispatch_8

<Dispatch: tests>+≡
    subroutine dispatch_8 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global

```

```

type(os_data_t) :: os_data
type(flavor_t), dimension(2) :: flv
type(sf_config_t), dimension(:), allocatable :: sf_config
type(sf_prop_t) :: sf_prop
type(sf_channel_t), dimension(:), allocatable :: sf_channel
type(phs_channel_collection_t) :: coll
type(string_t) :: sf_string
integer :: i
type(pdg_array_t), dimension (2,1) :: pdg_prc

write (u, "(A)")  "* Test output: dispatch_8"
write (u, "(A)")  "* Purpose: configure a structure-function chain"
write (u, "(A)")

call global%global_init ()

call os_data%init ()
call syntax_model_file_init ()
call global%select_model (var_str ("QCD"))

write (u, "(A)")  "* Allocate LHC beams with PDF builtin"
write (u, "(A)")

call flv(1)%init (PROTON, global%model)
call flv(2)%init (PROTON, global%model)

call reset_interaction_counter ()
call global%set_real (var_str ("sqrts"), &
    14000._default, is_known = .true.)

call global%beam_structure%init_sf (flv%get_name (), [1])
call global%beam_structure%set_sf (1, 1, var_str ("pdf_builtin"))

call dispatch_sf_config (sf_config, sf_prop, global%beam_structure, &
    global%get_var_list_ptr (), global%var_list, &
    global%model, global%os_data, global%get_sqrts (), pdg_prc)
do i = 1, size (sf_config)
    call sf_config(i)%write (u)
end do

call dispatch_sf_channels (sf_channel, sf_string, sf_prop, coll, &
    global%var_list, global%get_sqrts(), global%beam_structure)
write (u, "(1x,A)") "Mapping configuration:"
do i = 1, size (sf_channel)
    write (u, "(2x)", advance = "no")
    call sf_channel(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)")  "* Allocate ILC beams with CIRCE1"
write (u, "(A)")

call global%select_model (var_str ("QED"))
call flv(1)%init ( ELECTRON, global%model)

```

```

call flv(2)%init (-ELECTRON, global%model)

call reset_interaction_counter ()
call global%set_real (var_str ("sqrts"), &
    500._default, is_known = .true.)
call global%set_log (var_str ("?circe1_generate"), &
    .false., is_known = .true.)

call global%beam_structure%init_sf (flv%get_name (), [1])
call global%beam_structure%set_sf (1, 1, var_str ("circe1"))

call dispatch_sf_config (sf_config, sf_prop, global%beam_structure, &
    global%get_var_list_ptr (), global%var_list, &
    global%model, global%os_data, global%get_sqrts (), pdg_prc)
do i = 1, size (sf_config)
    call sf_config(i)%write (u)
end do

call dispatch_sf_channels (sf_channel, sf_string, sf_prop, coll, &
    global%var_list, global%get_sqrts(), global%beam_structure)
write (u, "(1x,A)") "Mapping configuration:"
do i = 1, size (sf_channel)
    write (u, "(2x)", advance = "no")
    call sf_channel(i)%write (u)
end do

write (u, "(A)")
write (u, "(A)") "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)") "* Test output end: dispatch_8"

end subroutine dispatch_8

```

Update process core parameters

This test dispatches a process core, temporarily modifies parameters, then restores the original.

```

<Dispatch: execute tests>+≡
    call test (dispatch_10, "dispatch_10", &
        "process core update", &
        u, results)

<Dispatch: test declarations>+≡
    public :: dispatch_10

<Dispatch: tests>+≡
    subroutine dispatch_10 (u)
        integer, intent(in) :: u
        type(string_t), dimension(2) :: prt_in, prt_out

```

```

type(rt_data_t), target :: global
class(prc_core_def_t), allocatable :: core_def
class(prc_core_t), allocatable :: core, saved_core
type(var_list_t), pointer :: model_vars

write (u, "(A)")  "* Test output: dispatch_10"
write (u, "(A)")  "* Purpose: select process configuration method,"
write (u, "(A)")  "          allocate process core,"
write (u, "(A)")  "          temporarily reset parameters"
write (u, "(A)")

call syntax_model_file_init ()
call global%global_init ()

prt_in = [var_str ("a"), var_str ("b")]
prt_out = [var_str ("c"), var_str ("d")]

write (u, "(A)")  "* Allocate core as prc_omega_t"
write (u, "(A)")

call global%set_string (var_str ("method"), &
    var_str ("omega"), is_known = .true.)
call dispatch_core_def (core_def, prt_in, prt_out, global%model, global%var_list)

call global%select_model (var_str ("Test"))

call dispatch_core (core, core_def, global%model)
call core_def%allocate_driver (core%driver, var_str (""))

select type (core)
type is (prc_omega_t)
    call core%write (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Update core with modified model and helicity selection"
write (u, "(A)")

model_vars => global%model%get_var_list_ptr ()

call model_vars%set_real (var_str ("gy"), 2._default, &
    is_known = .true.)
call global%model%update_parameters ()

call global%set_log (&
    var_str ("?helicity_selection_active"), &
    .true., is_known = .true.)
call global%set_real (&
    var_str ("helicity_selection_threshold"), &
    2e10_default, is_known = .true.)
call global%set_int (&
    var_str ("helicity_selection_cutoff"), &
    5, is_known = .true.)

```

```

call dispatch_core_update (core, &
    global%model, &
    global%get_helicity_selection (), &
    saved_core = saved_core)
select type (core)
type is (prc_omega_t)
    call core%write (u)
end select

write (u, "(A)")
write (u, "(A)")  "* Restore core from save"
write (u, "(A)")

call dispatch_core_restore (core, saved_core)
select type (core)
type is (prc_omega_t)
    call core%write (u)
end select

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_10"

end subroutine dispatch_10

```

QCD Coupling

This test dispatches an qcd object, which is used to compute the (running) coupling by one of several possible methods.

We can't move this to `beams` as it depends on `model_features` for the `model_list_t`.

```

<Dispatch: execute tests>+≡
    call test (dispatch_11, "dispatch_11", &
        "QCD coupling", &
        u, results)

<Dispatch: test declarations>+≡
    public :: dispatch_11

<Dispatch: tests>+≡
    subroutine dispatch_11 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        type(var_list_t), pointer :: model_vars
        type(qcd_t) :: qcd

        write (u, "(A)")  "* Test output: dispatch_11"
        write (u, "(A)")  "* Purpose: select QCD coupling formula"
        write (u, "(A)")

        call syntax_model_file_init ()

```



```

call global%global_init ()
call global%select_model (var_str ("SM"))
model_vars => global%get_var_list_ptr ()

write (u, "(A)")  "* Allocate alpha_s as fixed"
write (u, "(A)")

call global%set_log (var_str ("?alphas_is_fixed"), &
    .true., is_known = .true.)
call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
call qcd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Allocate alpha_s as running (built-in)"
write (u, "(A)")

call global%set_log (var_str ("?alphas_is_fixed"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?alphas_from_mz"), &
    .true., is_known = .true.)
call global%set_int &
    (var_str ("alphas_order"), 1, is_known = .true.)
call model_vars%set_real (var_str ("alphas"), 0.1234_default, &
    is_known=.true.)
call model_vars%set_real (var_str ("mZ"), 91.234_default, &
    is_known=.true.)
call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
call qcd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Allocate alpha_s as running (built-in, Lambda defined)"
write (u, "(A)")

call global%set_log (var_str ("?alphas_from_mz"), &
    .false., is_known = .true.)
call global%set_log (&
    var_str ("?alphas_from_lambda_qcd"), &
    .true., is_known = .true.)
call global%set_real &
    (var_str ("lambda_qcd"), 250.e-3_default, &
    is_known=.true.)
call global%set_int &
    (var_str ("alphas_order"), 2, is_known = .true.)
call global%set_int &
    (var_str ("alphas_nf"), 4, is_known = .true.)
call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
call qcd%write (u)

write (u, "(A)")
write (u, "(A)")  "* Allocate alpha_s as running (using builtin PDF set)"
write (u, "(A)")

call global%set_log (&
    var_str ("?alphas_from_lambda_qcd"), &

```

```

        .false., is_known = .true.)
call global%set_log &
    (var_str ("?alphas_from_pdf_builtin"), &
     .true., is_known = .true.)
call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
call qcd%write (u)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: dispatch_11"

end subroutine dispatch_11

```

33.4 Process Configuration

This module communicates between the toplevel command structure with its runtime data set and the process-library handling modules which collect the definition of individual processes. Its primary purpose is to select from the available matrix-element generating methods and configure the entry in the process library accordingly.

```
<process_configurations.f90>≡  
  <File header>  
  
  module process_configurations  
  
    <Use strings>  
    <Use debug>  
    use diagnostics  
    use io_units  
    use physics_defs, only: BORN, NLO_VIRTUAL, NLO_REAL, NLO_DGLAP, &  
      NLO_SUBTRACTION, NLO_MISMATCH  
    use models  
    use prc_core_def  
    use particle_specifiers  
    use process_libraries  
    use rt_data  
    use variables, only: var_list_t  
  
    use dispatch_me_methods, only: dispatch_core_def  
    use prc_external, only: prc_external_def_t  
  
    <Standard module head>  
  
    <Process configurations: public>  
  
    <Process configurations: types>  
  
    contains  
  
    <Process configurations: procedures>  
  
  end module process_configurations
```

33.4.1 Data Type

```
<Process configurations: public>≡  
  public :: process_configuration_t  
  
<Process configurations: types>≡  
  type :: process_configuration_t  
    type(process_def_entry_t), pointer :: entry => null ()  
    type(string_t) :: id  
    integer :: num_id = 0  
  contains  
    <Process configurations: process configuration: TBP>  
  end type process_configuration_t
```

Output (for unit tests).

```

(Process configurations: process configuration: TBP)≡
  procedure :: write => process_configuration_write

(Process configurations: procedures)≡
  subroutine process_configuration_write (config, unit)
    class(process_configuration_t), intent(in) :: config
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
    write (u, "(A)") "Process configuration:"
    if (associated (config%entry)) then
      call config%entry%write (u)
    else
      write (u, "(1x,3A)") "ID      = '", char (config%id), "'"
      write (u, "(1x,A,1x,IO)") "num ID =", config%num_id
      write (u, "(2x,A)") "[no entry]"
    end if
  end subroutine process_configuration_write

```

Initialize a process. We only need the name, the number of incoming particles, and the number of components.

```

(Process configurations: process configuration: TBP)+≡
  procedure :: init => process_configuration_init

(Process configurations: procedures)+≡
  subroutine process_configuration_init &
    (config, prc_name, n_in, n_components, model, var_list, &
     nlo_process, negative_sf)
    class(process_configuration_t), intent(out) :: config
    type(string_t), intent(in) :: prc_name
    integer, intent(in) :: n_in
    integer, intent(in) :: n_components
    type(model_t), intent(in), pointer :: model
    type(var_list_t), intent(in) :: var_list
    logical, intent(in), optional :: nlo_process, negative_sf
    logical :: nlo_proc, neg_sf
    logical :: requires_resonances
    if (debug_on) call msg_debug (D_CORE, "process_configuration_init")
    config%id = prc_name
    if (present (nlo_process)) then
      nlo_proc = nlo_process
    else
      nlo_proc = .false.
    end if
    if (present (negative_sf)) then
      neg_sf = negative_sf
    else
      neg_sf = .false.
    end if
    requires_resonances = var_list%get_lval (var_str ("?resonance_history"))

    if (debug_on) call msg_debug (D_CORE, "nlo_process", nlo_proc)
    allocate (config%entry)

```

```

if (var_list%is_known (var_str ("process_num_id"))) then
  config%num_id = &
    var_list%get_ival (var_str ("process_num_id"))
  call config%entry%init (prc_name, &
    model = model, n_in = n_in, n_components = n_components, &
    num_id = config%num_id, &
    nlo_process = nlo_proc, &
    negative_sf = neg_sf, &
    requires_resonances = requires_resonances)
else
  call config%entry%init (prc_name, &
    model = model, n_in = n_in, n_components = n_components, &
    nlo_process = nlo_proc, &
    negative_sf = neg_sf, &
    requires_resonances = requires_resonances)
end if
end subroutine process_configuration_init

```

Initialize a process component. The details depend on the process method, which determines the type of the process component core. We set the incoming and outgoing particles (as strings, to be interpreted by the process driver). All other information is taken from the variable list.

The dispatcher gets only the names of the particles. The process component definition gets the complete specifiers which contains a polarization flag and names of decay processes, where applicable.

(Process configurations: process configuration: TBP)+≡

```

procedure :: setup_component => process_configuration_setup_component

```

(Process configurations: procedures)+≡

```

subroutine process_configuration_setup_component &
  (config, i_component, prt_in, prt_out, model, var_list, &
   nlo_type, can_be_integrated)
class(process_configuration_t), intent(inout) :: config
integer, intent(in) :: i_component
type(prt_spec_t), dimension(:), intent(in) :: prt_in
type(prt_spec_t), dimension(:), intent(in) :: prt_out
type(model_t), pointer, intent(in) :: model
type(var_list_t), intent(in) :: var_list
integer, intent(in), optional :: nlo_type
logical, intent(in), optional :: can_be_integrated
type(string_t), dimension(:), allocatable :: prt_str_in
type(string_t), dimension(:), allocatable :: prt_str_out
class(prc_core_def_t), allocatable :: core_def
type(string_t) :: method
type(string_t) :: born_me_method
type(string_t) :: real_tree_me_method
type(string_t) :: loop_me_method
type(string_t) :: correlation_me_method
type(string_t) :: dglap_me_method
integer :: i
if (debug_on) call msg_debug2 (D_CORE, "process_configuration_setup_component")
allocate (prt_str_in (size (prt_in)))
allocate (prt_str_out (size (prt_out)))

```

```

forall (i = 1:size (prt_in)) prt_str_in(i) = prt_in(i)% get_name ()
forall (i = 1:size (prt_out)) prt_str_out(i) = prt_out(i)%get_name ()

method = var_list%get_sval (var_str ("$method"))
if (present (nlo_type)) then
  select case (nlo_type)
    case (BORN)
      born_me_method = var_list%get_sval (var_str ("$born_me_method"))
      if (born_me_method /= var_str ("")) then
        method = born_me_method
      end if
    case (NLO_VIRTUAL)
      loop_me_method = var_list%get_sval (var_str ("$loop_me_method"))
      if (loop_me_method /= var_str ("")) then
        method = loop_me_method
      end if
    case (NLO_REAL)
      real_tree_me_method = &
        var_list%get_sval (var_str ("$real_tree_me_method"))
      if (real_tree_me_method /= var_str ("")) then
        method = real_tree_me_method
      end if
    case (NLO_DGLAP)
      dglap_me_method = &
        var_list%get_sval (var_str ("$dglap_me_method"))
      if (dglap_me_method /= var_str ("")) then
        method = dglap_me_method
      end if
    case (NLO_SUBTRACTION,NLO_MISMATCH)
      correlation_me_method = &
        var_list%get_sval (var_str ("$correlation_me_method"))
      if (correlation_me_method /= var_str ("")) then
        method = correlation_me_method
      end if
    case default
  end select
end if
call dispatch_core_def (core_def, prt_str_in, prt_str_out, &
  model, var_list, config%id, nlo_type, method)
select type (core_def)
class is (prc_external_def_t)
  if (present (can_be_integrated)) then
    call core_def%set_active_writer (can_be_integrated)
  else
    call msg_fatal ("Cannot decide if external core is integrated!")
  end if
end select

if (debug_on) call msg_debug2 (D_CORE, "import_component with method ", method)
call config%entry%import_component (i_component, &
  n_out = size (prt_out), &
  prt_in = prt_in, &
  prt_out = prt_out, &
  method = method, &

```

```

        variant = core_def, &
        nlo_type = nlo_type, &
        can_be_integrated = can_be_integrated)
end subroutine process_configuration_setup_component

```

```

<Process configurations: process configuration: TBP>+≡
  procedure :: set_fixed_emitter => process_configuration_set_fixed_emitter

```

```

<Process configurations: procedures>+≡
  subroutine process_configuration_set_fixed_emitter (config, i, emitter)
    class(process_configuration_t), intent(inout) :: config
    integer, intent(in) :: i, emitter
    call config%entry%set_fixed_emitter (i, emitter)
  end subroutine process_configuration_set_fixed_emitter

```

```

<Process configurations: process configuration: TBP>+≡
  procedure :: set_coupling_powers => process_configuration_set_coupling_powers

```

```

<Process configurations: procedures>+≡
  subroutine process_configuration_set_coupling_powers &
    (config, alpha_power, alphas_power)
    class(process_configuration_t), intent(inout) :: config
    integer, intent(in) :: alpha_power, alphas_power
    call config%entry%set_coupling_powers (alpha_power, alphas_power)
  end subroutine process_configuration_set_coupling_powers

```

```

<Process configurations: process configuration: TBP>+≡
  procedure :: set_component_associations => &
    process_configuration_set_component_associations

```

```

<Process configurations: procedures>+≡
  subroutine process_configuration_set_component_associations &
    (config, i_list, remnant, use_real_finite, mismatch)
    class(process_configuration_t), intent(inout) :: config
    integer, dimension(:), intent(in) :: i_list
    logical, intent(in) :: remnant, use_real_finite, mismatch
    integer :: i_component
    do i_component = 1, config%entry%get_n_components ()
      if (any (i_list == i_component)) then
        call config%entry%set_associated_components (i_component, &
          i_list, remnant, use_real_finite, mismatch)
      end if
    end do
  end subroutine process_configuration_set_component_associations

```

Record a process configuration: append it to the currently selected process definition library.

```

<Process configurations: process configuration: TBP>+≡
  procedure :: record => process_configuration_record

```

```

<Process configurations: procedures>+≡
  subroutine process_configuration_record (config, global)
    class(process_configuration_t), intent(inout) :: config
    type(rt_data_t), intent(inout) :: global
    if (associated (global%prclib)) then
      call global%prclib%open ()
      call global%prclib%append (config%entry)
      if (config%num_id /= 0) then
        write (msg_buffer, "(5A,I0,A)" "Process library '", &
              char (global%prclib%get_name ()), &
              "' : recorded process '", char (config%id), "' (" , &
              config%num_id, ")")
      else
        write (msg_buffer, "(5A)" "Process library '", &
              char (global%prclib%get_name ()), &
              "' : recorded process '", char (config%id), "'")
      end if
      call msg_message ()
    else
      call msg_fatal ("Recording process '" // char (config%id) &
                     // "' : active process library undefined")
    end if
  end subroutine process_configuration_record

```

33.4.2 Unit Tests

Test module, followed by the corresponding implementation module.

```

<process_configurations_ut.f90>≡
  <File header>

  module process_configurations_ut
    use unit_tests
    use process_configurations_uti

    <Standard module head>

    <Process configurations: public test>

    <Process configurations: public test auxiliary>

    contains

    <Process configurations: test driver>

  end module process_configurations_ut

<process_configurations_uti.f90>≡
  <File header>

  module process_configurations_uti

    <Use strings>
    use particle_specifiers, only: new_prt_spec

```



```

    use prclib_stacks
    use models
    use rt_data

    use process_configurations

    <Standard module head>

    <Process configurations: test declarations>

    <Process configurations: public test auxiliary>

    contains

    <Process configurations: test auxiliary>

    <Process configurations: tests>

    end module process_configurations_util

```

API: driver for the unit tests below.

```

<Process configurations: public test>≡
    public :: process_configurations_test

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

```

Minimal setup

The workflow for setting up a minimal process configuration with the test matrix element method.

We wrap this in a public procedure, so we can reuse it in later modules. The procedure prepares a process definition list for two processes (one `prc_test` and one `omega` type) and appends this to the process library stack in the global data set.

The `mode` argument determines which processes to build.

The `procname` argument replaces the predefined `procname(s)`.

This is re-exported by the UT module.

```

<Process configurations: public test auxiliary>≡
    public :: prepare_test_library

<Process configurations: test auxiliary>≡
    subroutine prepare_test_library (global, libname, mode, procname)
        type(rt_data_t), intent(inout), target :: global
        type(string_t), intent(in) :: libname
        integer, intent(in) :: mode
        type(string_t), intent(in), dimension(:), optional :: procname
        type(prclib_entry_t), pointer :: lib

```

```

type(string_t) :: prc_name
type(string_t), dimension(:), allocatable :: prt_in, prt_out
integer :: n_components
type(process_configuration_t) :: prc_config

if (.not. associated (global%prclib_stack%get_first_ptr ())) then
    allocate (lib)
    call lib%init (libname)
    call global%add_prclib (lib)
end if

if (btest (mode, 0)) then

    call global%select_model (var_str ("Test"))

    if (present (procname)) then
        prc_name = procname(1)
    else
        prc_name = "prc_config_a"
    end if
    n_components = 1
    allocate (prt_in (2), prt_out (2))
    prt_in = [var_str ("s"), var_str ("s")]
    prt_out = [var_str ("s"), var_str ("s")]

    call global%set_string (var_str ("method"), &
        var_str ("unit_test"), is_known = .true.)

    call prc_config%init (prc_name, &
        size (prt_in), n_components, &
        global%model, global%var_list)
    call prc_config%setup_component (1, &
        new_prt_spec (prt_in), new_prt_spec (prt_out), &
        global%model, global%var_list)
    call prc_config%record (global)

    deallocate (prt_in, prt_out)

end if

if (btest (mode, 1)) then

    call global%select_model (var_str ("QED"))

    if (present (procname)) then
        prc_name = procname(2)
    else
        prc_name = "prc_config_b"
    end if
    n_components = 1
    allocate (prt_in (2), prt_out (2))
    prt_in = [var_str ("e+"), var_str ("e-")]
    prt_out = [var_str ("m+"), var_str ("m-")]

```

```

call global%set_string (var_str ("$method"),&
    var_str ("omega"), is_known = .true.)

call prc_config%init (prc_name, &
    size (prt_in), n_components, &
    global%model, global%var_list)
call prc_config%setup_component (1, &
    new_prt_spec (prt_in), new_prt_spec (prt_out), &
    global%model, global%var_list)
call prc_config%record (global)

deallocate (prt_in, prt_out)

end if

if (btest (mode, 2)) then

    call global%select_model (var_str ("Test"))

    if (present (procname)) then
        prc_name = procname(1)
    else
        prc_name = "prc_config_a"
    end if
    n_components = 1
    allocate (prt_in (1), prt_out (2))
    prt_in = [var_str ("s")]
    prt_out = [var_str ("f"), var_str ("fbar")]

    call global%set_string (var_str ("$method"),&
        var_str ("unit_test"), is_known = .true.)

    call prc_config%init (prc_name, &
        size (prt_in), n_components, &
        global%model, global%var_list)
    call prc_config%setup_component (1, &
        new_prt_spec (prt_in), new_prt_spec (prt_out), &
        global%model, global%var_list)
    call prc_config%record (global)

    deallocate (prt_in, prt_out)

end if

end subroutine prepare_test_library

```

The actual test: the previous procedure with some prelude and postlude. In the global variable list, just before printing we reset the variables where the value may depend on the system and run environment.

(Process configurations: execute tests)≡

```

call test (process_configurations_1, "process_configurations_1", &
    "test processes", &
    u, results)

```

```

<Process configurations: test declarations>≡
  public :: process_configurations_1

<Process configurations: tests>≡
  subroutine process_configurations_1 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global

    write (u, "(A)")  "* Test output: process_configurations_1"
    write (u, "(A)")  "*   Purpose: configure test processes"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)

    write (u, "(A)")  "* Configure processes as prc_test, model Test"
    write (u, "(A)")  "*                               and omega, model QED"
    write (u, *)

    call global%set_int (var_str ("process_num_id"), &
      42, is_known = .true.)
    call prepare_test_library (global, var_str ("prc_config_lib_1"), 3)

    global%os_data%fc = "Fortran-compiler"
    global%os_data%fcflags = "Fortran-flags"
    global%os_data%fclibs = "Fortran-libs"

    call global%write_libraries (u)

    call global%final ()
    call syntax_model_file_final ()

    write (u, "(A)")
    write (u, "(A)")  "* Test output end: process_configurations_1"

  end subroutine process_configurations_1

```

O'MEGA options

Slightly extended example where we pass O'MEGA options to the library. The `prepare_test_library` contents are spelled out.

```

<Process configurations: execute tests>+≡
  call test (process_configurations_2, "process_configurations_2", &
    "omega options", &
    u, results)

<Process configurations: test declarations>+≡
  public :: process_configurations_2

<Process configurations: tests>+≡
  subroutine process_configurations_2 (u)

```

```

integer, intent(in) :: u
type(rt_data_t), target :: global

type(string_t) :: libname
type(prclib_entry_t), pointer :: lib
type(string_t) :: prc_name
type(string_t), dimension(:), allocatable :: prt_in, prt_out
integer :: n_components
type(process_configuration_t) :: prc_config

write (u, "(A)")  "* Test output: process_configurations_2"
write (u, "(A)")  "* Purpose: configure test processes with options"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()

write (u, "(A)")  "* Configure processes as omega, model QED"
write (u, *)

libname = "prc_config_lib_2"

allocate (lib)
call lib%init (libname)
call global%add_prclib (lib)

call global%select_model (var_str ("QED"))

prc_name = "prc_config_c"
n_components = 2
allocate (prt_in (2), prt_out (2))
prt_in = [var_str ("e+"), var_str ("e-")]
prt_out = [var_str ("m+"), var_str ("m-")]

call global%set_string (var_str ("$method"), &
    var_str ("omega"), is_known = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)

call prc_config%init (prc_name, size (prt_in), n_components, &
    global%model, global%var_list)

call global%set_log (var_str ("?report_progress"), &
    .true., is_known = .true.)
call prc_config%setup_component (1, &
    new_prt_spec (prt_in), new_prt_spec (prt_out), global%model, global%var_list)

call global%set_log (var_str ("?report_progress"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .true., is_known = .true.)
call global%set_string (var_str ("$restrictions"), &
    var_str ("3+4~A"), is_known = .true.)

```

```

call global%set_string (var_str ("$omega_flags"), &
    var_str ("-fusion:progress_file omega_prc_config.log"), &
    is_known = .true.)
call prc_config%setup_component (2, &
    new_prt_spec (prt_in), new_prt_spec (prt_out), global%model, global%var_list)

call prc_config%record (global)

deallocate (prt_in, prt_out)

global%os_data%fc = "Fortran-compiler"
global%os_data%fcflags = "Fortran-flags"
global%os_data%fclibs = "Fortran-libs"

call global%write_vars (u, [ &
    var_str ("$model_name"), &
    var_str ("$method"), &
    var_str ("?report_progress"), &
    var_str ("$restrictions"), &
    var_str ("$omega_flags")])
write (u, "(A)")
call global%write_libraries (u)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: process_configurations_2"

end subroutine process_configurations_2

```

33.5 Compilation

This module manages compilation and loading of process libraries. It is needed as a separate module because integration depends on it.

```
<compilations.f90>≡  
  <File header>  
  
  module compilations  
  
    <Use strings>  
    use io_units  
    use system_defs, only: TAB  
    use system_dependencies, only: OS_IS_DARWIN  
    use diagnostics  
    use os_interface  
    use variables, only: var_list_t  
    use model_data  
    use process_libraries  
    use prclib_stacks  
    use rt_data  
  
    <Standard module head>  
  
    <Compilations: public>  
  
    <Compilations: types>  
  
    <Compilations: parameters>  
  
    contains  
  
    <Compilations: procedures>  
  
  end module compilations
```

33.5.1 The data type

The compilation item handles the compilation and loading of a single process library.

```
<Compilations: public>≡  
  public :: compilation_item_t  
  
<Compilations: types>≡  
  type :: compilation_item_t  
  private  
  type(string_t) :: libname  
  type(string_t) :: static_external_tag  
  type(process_library_t), pointer :: lib => null ()  
  logical :: recompile_library = .false.  
  logical :: verbose = .false.  
  logical :: use_workspace = .false.  
  type(string_t) :: workspace  
  contains  
  <Compilations: compilation item: TBP>
```

```
end type compilation_item_t
```

Initialize.

Set flags and global properties of the library. Establish the workspace name, if defined.

<Compilations: compilation item: TBP>≡

```
procedure :: init => compilation_item_init
```

<Compilations: procedures>≡

```
subroutine compilation_item_init (comp, libname, stack, var_list)
  class(compilation_item_t), intent(out) :: comp
  type(string_t), intent(in) :: libname
  type(prclib_stack_t), intent(inout) :: stack
  type(var_list_t), intent(in) :: var_list
  comp%libname = libname
  comp%lib => stack%get_library_ptr (comp%libname)
  if (.not. associated (comp%lib)) then
    call msg_fatal ("Process library '" // char (comp%libname) &
      // "' has not been declared.")
  end if
  comp%recompile_library = &
    var_list%get_lval (var_str ("?recompile_library"))
  comp%verbose = &
    var_list%get_lval (var_str ("?me_verbose"))
  comp%use_workspace = &
    var_list%is_known (var_str ("$_compile_workspace"))
  if (comp%use_workspace) then
    comp%workspace = &
      var_list%get_sval (var_str ("$_compile_workspace"))
    if (comp%workspace == "") comp%use_workspace = .false.
  else
    comp%workspace = ""
  end if
end subroutine compilation_item_init
```

Compile the current library. The force flag has the effect that we first delete any previous files, as far as accessible by the current makefile. It also guarantees that previous files not accessible by a makefile will be overwritten.

<Compilations: compilation item: TBP>+≡

```
procedure :: compile => compilation_item_compile
```

<Compilations: procedures>+≡

```
subroutine compilation_item_compile (comp, model, os_data, force, recompile)
  class(compilation_item_t), intent(inout) :: comp
  class(model_data_t), intent(in), target :: model
  type(os_data_t), intent(in) :: os_data
  logical, intent(in) :: force, recompile
  if (associated (comp%lib)) then
    if (comp%use_workspace) call setup_workspace (comp%workspace, os_data)
    call msg_message ("Process library '" &
      // char (comp%libname) // "': compiling ...")
    call comp%lib%configure (os_data)
    if (signal_is_pending ()) return
```



```

call comp%lib%compute_md5sum (model)
call comp%lib%write_makefile &
    (os_data, force, verbose=comp%verbose, workspace=comp%workspace)
if (signal_is_pending ()) return
if (force) then
    call comp%lib%clean &
        (os_data, distclean = .false., workspace=comp%workspace)
    if (signal_is_pending ()) return
end if
call comp%lib%write_driver (force, workspace=comp%workspace)
if (signal_is_pending ()) return
if (recompile) then
    call comp%lib%load &
        (os_data, keep_old_source = .true., workspace=comp%workspace)
    if (signal_is_pending ()) return
end if
call comp%lib%update_status (os_data, workspace=comp%workspace)
end if
end subroutine compilation_item_compile

```

The workspace directory is created if it does not exist. (Applies only if the use has set the workspace directory.)

<Compilations: parameters>+≡

```

character(*), parameter :: ALLOWED_IN_DIRNAME = &
    "abcdefghijklmnopqrstuvwxyz&
    &ABCDEFGHIJKLMNOPQRSTUVWXYZ&
    &1234567890&
    &.,_-= "

```

<Compilations: procedures>+≡

```

subroutine setup_workspace (workspace, os_data)
    type(string_t), intent(in) :: workspace
    type(os_data_t), intent(in) :: os_data
    if (verify (workspace, ALLOWED_IN_DIRNAME) == 0) then
        call msg_message ("Compile: preparing workspace directory '" &
            // char (workspace) // "'")
        call os_system_call ("mkdir -p '" // workspace // "'")
    else
        call msg_fatal ("compile: workspace name '" &
            // char (workspace) // "' contains illegal characters")
    end if
end subroutine setup_workspace

```

Load the current library, just after compiling it.

<Compilations: compilation item: TBP>+≡

```

procedure :: load => compilation_item_load

```

<Compilations: procedures>+≡

```

subroutine compilation_item_load (comp, os_data)
    class(compilation_item_t), intent(inout) :: comp
    type(os_data_t), intent(in) :: os_data
    if (associated (comp%lib)) then
        call comp%lib%load (os_data, workspace=comp%workspace)
    end if

```

```
end subroutine compilation_item_load
```

Message as a separate call:

```
<Compilations: compilation item: TBP>+≡
  procedure :: success => compilation_item_success

<Compilations: procedures>+≡
  subroutine compilation_item_success (comp)
    class(compilation_item_t), intent(in) :: comp
    if (associated (comp%lib)) then
      call msg_message ("Process library '" // char (comp%libname) &
        // "' : ... success.")
    else
      call msg_fatal ("Process library '" // char (comp%libname) &
        // "' : ... failure.")
    end if
  end subroutine compilation_item_success
```

33.5.2 API for library compilation and loading

This is a shorthand for compiling and loading a single library. The `compilation_item` object is used only internally.

The `global` data set may actually be local to the caller. The compilation affects the library specified by its name if it is on the stack, but it does not reset the currently selected library.

```
<Compilations: public>+≡
  public :: compile_library

<Compilations: procedures>+≡
  subroutine compile_library (libname, global)
    type(string_t), intent(in) :: libname
    type(rt_data_t), intent(inout), target :: global
    type(compilation_item_t) :: comp
    logical :: force, recompile
    force = &
      global%var_list%get_lval (var_str ("?rebuild_library"))
    recompile = &
      global%var_list%get_lval (var_str ("?recompile_library"))
    if (associated (global%model)) then
      call comp%init (libname, global%prclib_stack, global%var_list)
      call comp%compile (global%model, global%os_data, force, recompile)
      if (signal_is_pending ()) return
      call comp%load (global%os_data)
      if (signal_is_pending ()) return
    else
      call msg_fatal ("Process library compilation: " &
        // " model is undefined.")
    end if
    call comp%success ()
  end subroutine compile_library
```

33.5.3 Compiling static executable

This object handles the creation of a static executable which should contain a set of static process libraries.

```
<Compilations: public>+≡
    public :: compilation_t
<Compilations: types>+≡
    type :: compilation_t
        private
            type(string_t) :: exe_name
            type(string_t), dimension(:), allocatable :: lib_name
        contains
            <Compilations: compilation: TBP>
        end type compilation_t
```

Output.

```
<Compilations: compilation: TBP>≡
    procedure :: write => compilation_write
<Compilations: procedures>+≡
    subroutine compilation_write (object, unit)
        class(compilation_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u, i
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Compilation object:"
        write (u, "(3x,3A)") "executable      = '", &
            char (object%exe_name), "'"
        write (u, "(3x,A)", advance="no") "process libraries ="
        do i = 1, size (object%lib_name)
            write (u, "(1x,3A)", advance="no") " '", char (object%lib_name(i)), "'"
        end do
        write (u, *)
    end subroutine compilation_write
```

Initialize: we know the names of the executable and of the libraries. Optionally, we may provide a workspace directory.

```
<Compilations: compilation: TBP>+≡
    procedure :: init => compilation_init
<Compilations: procedures>+≡
    subroutine compilation_init (compilation, exe_name, lib_name)
        class(compilation_t), intent(out) :: compilation
        type(string_t), intent(in) :: exe_name
        type(string_t), dimension(:), intent(in) :: lib_name
        compilation%exe_name = exe_name
        allocate (compilation%lib_name (size (lib_name)))
        compilation%lib_name = lib_name
    end subroutine compilation_init
```

Write the dispatcher subroutine for the compiled libraries. Also write a subroutine which returns the names of the compiled libraries.

```
<Compilations: compilation: TBP>+≡
```

```

procedure :: write_dispatcher => compilation_write_dispatcher
{Compilations: procedures}+=
subroutine compilation_write_dispatcher (compilation)
  class(compilation_t), intent(in) :: compilation
  type(string_t) :: file
  integer :: u, i
  file = compilation%exe_name // "_prclib_dispatcher.f90"
  call msg_message ("Static executable '" // char (compilation%exe_name) &
    // "' : writing library dispatcher")
  u = free_unit ()
  open (u, file = char (file), status="replace", action="write")
  write (u, "(3A)" " ! Whizard: process libraries for executable '", &
    char (compilation%exe_name), "'")
  write (u, "(A)" " ! Automatically generated file, do not edit")
  write (u, "(A)" " subroutine dispatch_prclib_static " // &
    "(driver, basename, modellibs_ldflags)"
  write (u, "(A)" " use iso_varying_string, string_t => varying_string"
  write (u, "(A)" " use prclib_interfaces"
  do i = 1, size (compilation%lib_name)
    associate (lib_name => compilation%lib_name(i))
      write (u, "(A)" " use " // char (lib_name) // "_driver"
    end associate
  end do
  write (u, "(A)" " implicit none"
  write (u, "(A)" " class(prclib_driver_t), intent(inout), allocatable &
    &:: driver"
  write (u, "(A)" " type(string_t), intent(in) :: basename"
  write (u, "(A)" " logical, intent(in), optional :: " // &
    "modellibs_ldflags"
  write (u, "(A)" " select case (char (basename))"
  do i = 1, size (compilation%lib_name)
    associate (lib_name => compilation%lib_name(i))
      write (u, "(3A)" " case ('', char (lib_name), '')"
      write (u, "(3A)" " allocate (" , char (lib_name), "_driver_t &
        &:: driver)"
    end associate
  end do
  write (u, "(A)" " end select"
  write (u, "(A)" "end subroutine dispatch_prclib_static"
  write (u, *)
  write (u, "(A)" "subroutine get_prclib_static (libname)"
  write (u, "(A)" " use iso_varying_string, string_t => varying_string"
  write (u, "(A)" " implicit none"
  write (u, "(A)" " type(string_t), dimension(:), intent(inout), &
    &allocatable :: libname"
  write (u, "(A,IO,A)" " allocate (libname (" , &
    size (compilation%lib_name), ")")
  do i = 1, size (compilation%lib_name)
    associate (lib_name => compilation%lib_name(i))
      write (u, "(A,IO,A,A,A)" " libname(" , i, ") = '", &
        char (lib_name), "'")
    end associate
  end do
  write (u, "(A)" "end subroutine get_prclib_static"

```

```

        close (u)
    end subroutine compilation_write_dispatcher

```

Write the Makefile subroutine for the compiled libraries.

```

<Compilations: compilation: TBP>+≡
    procedure :: write_makefile => compilation_write_makefile

<Compilations: procedures>+≡
    subroutine compilation_write_makefile &
        (compilation, os_data, ext_libtag, verbose, overwrite_os)
        class(compilation_t), intent(in) :: compilation
        type(os_data_t), intent(in) :: os_data
        logical, intent(in) :: verbose
        logical, intent(in), optional :: overwrite_os
        logical :: overwrite
        type(string_t), intent(in), optional :: ext_libtag
        type(string_t) :: file, ext_tag
        integer :: u, i
        overwrite = .false.
        if (present (overwrite_os)) overwrite = overwrite_os
        if (present (ext_libtag)) then
            ext_tag = ext_libtag
        else
            ext_tag = ""
        end if
        file = compilation%exe_name // ".makefile"
        call msg_message ("Static executable '" // char (compilation%exe_name) &
            // "' : writing makefile")
        u = free_unit ()
        open (u, file = char (file), status="replace", action="write")
        write (u, "(3A)") "# WHIZARD: Makefile for executable '", &
            char (compilation%exe_name), "'"
        write (u, "(A)") "# Automatically generated file, do not edit"
        write (u, "(A)") ""
        write (u, "(A)") "# Executable name"
        write (u, "(A)") "EXE = " // char (compilation%exe_name)
        write (u, "(A)") ""
        write (u, "(A)") "# Compiler"
        write (u, "(A)") "FC = " // char (os_data%fc)
        write (u, "(A)") "CXX = " // char (os_data%cxx)
        write (u, "(A)") ""
        write (u, "(A)") "# Included libraries"
        write (u, "(A)") "FCINCL = " // char (os_data%whizard_includes)
        write (u, "(A)") ""
        write (u, "(A)") "# Compiler flags"
        write (u, "(A)") "FCFLAGS = " // char (os_data%fcflags)
        write (u, "(A)") "FCLIBS = " // char (os_data%fclibs)
        write (u, "(A)") "CXXFLAGS = " // char (os_data%cxxflags)
        write (u, "(A)") "CXXLIBSS = " // char (os_data%cxxlibs)
        write (u, "(A)") "LDLFLAGS = " // char (os_data%ldflags)
        write (u, "(A)") "LDLFLAGS_STATIC = " // char (os_data%ldflags_static)
        write (u, "(A)") "LDLFLAGS_HEPMC = " // char (os_data%ldflags_hePMC)
        write (u, "(A)") "LDLFLAGS_LCIO = " // char (os_data%ldflags_lcio)
        write (u, "(A)") "LDLFLAGS_HOPPET = " // char (os_data%ldflags_hoppet)

```

```

write (u, "(A)") "LDFLAGS_LOOPTOOLS = " // char (os_data%ldflags_looptools)
write (u, "(A)") "LDWHIZARD = " // char (os_data%whizard_ldflags)
write (u, "(A)") ""
write (u, "(A)") "# Libtool"
write (u, "(A)") "LIBTOOL = " // char (os_data%whizard_libtool)
if (verbose) then
  write (u, "(A)") "FCOMPILE = $(LIBTOOL) --tag=FC --mode=compile"
  if (OS_IS_DARWIN .and. .not. overwrite) then
    write (u, "(A)") "LINK = $(LIBTOOL) --tag=CXX --mode=link"
  else
    write (u, "(A)") "LINK = $(LIBTOOL) --tag=FC --mode=link"
  end if
else
  write (u, "(A)") "FCOMPILE = @$(LIBTOOL) --silent --tag=FC --mode=compile"
  if (OS_IS_DARWIN .and. .not. overwrite) then
    write (u, "(A)") "LINK = @$(LIBTOOL) --silent --tag=CXX --mode=link"
  else
    write (u, "(A)") "LINK = @$(LIBTOOL) --silent --tag=FC --mode=link"
  end if
end if
write (u, "(A)") ""
write (u, "(A)") "# Compile commands (default)"
write (u, "(A)") "LTF_COMPILE = $(FCOMPILE) $(FC) -c $(FCINCL) $(FCFLAGS)"
write (u, "(A)") ""
write (u, "(A)") "# Default target"
write (u, "(A)") "all: link"
write (u, "(A)") ""
write (u, "(A)") "# Libraries"
do i = 1, size (compilation%lib_name)
  associate (lib_name => compilation%lib_name(i))
    write (u, "(A)") "LIBRARIES += " // char (lib_name) // ".la"
    write (u, "(A)") char (lib_name) // ".la:"
    write (u, "(A)") TAB // "$(MAKE) -f " // char (lib_name) // ".makefile"
  end associate
end do
write (u, "(A)") ""
write (u, "(A)") "# Library dispatcher"
write (u, "(A)") "DISP = $(EXE)_prclib_dispatcher"
write (u, "(A)") "$(DISP).lo: $(DISP).f90 $(LIBRARIES)"
if (.not. verbose) then
  write (u, "(A)") TAB // '@echo " FC " $@"
end if
write (u, "(A)") TAB // "$(LTF_COMPILE) $<"
write (u, "(A)") ""
write (u, "(A)") "# Executable"
write (u, "(A)") "$(EXE): $(DISP).lo $(LIBRARIES)"
if (.not. verbose) then
  if (OS_IS_DARWIN .and. .not. overwrite) then
    write (u, "(A)") TAB // '@echo " CXXLD " $@"
  else
    write (u, "(A)") TAB // '@echo " FCLD " $@"
  end if
end if
if (OS_IS_DARWIN .and. .not. overwrite) then

```

```

        write (u, "(A)") TAB // "$ (LINK) $(CXX) -static $(CXXFLAGS) \"
    else
        write (u, "(A)") TAB // "$ (LINK) $(FC) -static $(FCFLAGS) \"
    end if
    write (u, "(A)") TAB // "    $(LDWHIZARD) $(LDFLAGS) \"
    write (u, "(A)") TAB // "    -o $(EXE) $^ \"
    write (u, "(A)") TAB // "    $(LDFLAGS_HEPMC) $(LDFLAGS_LCIO) $(LDFLAGS_HOPPET) \"
    if (OS_IS_DARWIN .and. .not. overwrite) then
        write (u, "(A)") TAB // "    $(LDFLAGS_LOOPTOOLS) $(LDFLAGS_STATIC) \"
        write (u, "(A)") TAB // "    $(CXXLIBS) $(FCLIBS)\" // char (ext_tag)
    else
        write (u, "(A)") TAB // "    $(LDFLAGS_LOOPTOOLS) $(LDFLAGS_STATIC)\" // char (ext_tag)
    end if
    write (u, "(A)") ""
    write (u, "(A)") "# Main targets"
    write (u, "(A)") "link: compile $(EXE)"
    write (u, "(A)") "compile: $(LIBRARIES) $(DISP).lo"
    write (u, "(A)") ".PHONY: link compile"
    write (u, "(A)") ""
    write (u, "(A)") "# Cleanup targets"
    write (u, "(A)") "clean-exe:"
    write (u, "(A)") TAB // "rm -f $(EXE)"
    write (u, "(A)") "clean-objects:"
    write (u, "(A)") TAB // "rm -f $(DISP).lo"
    write (u, "(A)") "clean-source:"
    write (u, "(A)") TAB // "rm -f $(DISP).f90"
    write (u, "(A)") "clean-makefile:"
    write (u, "(A)") TAB // "rm -f $(EXE).makefile"
    write (u, "(A)") ""
    write (u, "(A)") "clean: clean-exe clean-objects clean-source"
    write (u, "(A)") "distclean: clean clean-makefile"
    write (u, "(A)") ".PHONY: clean distclean"
    close (u)
end subroutine compilation_write_makefile

```

Compile the dispatcher source code.

```

<Compilations: compilation: TBP>+≡
    procedure :: make_compile => compilation_make_compile

<Compilations: procedures>+≡
    subroutine compilation_make_compile (compilation, os_data)
        class(compilation_t), intent(in) :: compilation
        type(os_data_t), intent(in) :: os_data
        call os_system_call ("make compile " // os_data%makeflags &
            // " -f " // compilation%exe_name // ".makefile")
    end subroutine compilation_make_compile

```

Link the dispatcher together with all matrix-element code and the WHIZARD and O'MEGA main libraries, to generate a static executable.

```

<Compilations: compilation: TBP>+≡
    procedure :: make_link => compilation_make_link

<Compilations: procedures>+≡
    subroutine compilation_make_link (compilation, os_data)

```

```

class(compilation_t), intent(in) :: compilation
type(os_data_t), intent(in) :: os_data
call os_system_call ("make link " // os_data%makeflags &
// " -f " // compilation%exe_name // ".makefile")
end subroutine compilation_make_link

```

Cleanup.

```

<Compilations: compilation: TBP>+≡
  procedure :: make_clean_exe => compilation_make_clean_exe

<Compilations: procedures>+≡
  subroutine compilation_make_clean_exe (compilation, os_data)
    class(compilation_t), intent(in) :: compilation
    type(os_data_t), intent(in) :: os_data
    call os_system_call ("make clean-exe " // os_data%makeflags &
// " -f " // compilation%exe_name // ".makefile")
  end subroutine compilation_make_clean_exe

```

33.5.4 API for executable compilation

This is a shorthand for compiling and loading an executable, including the enclosed libraries. The `compilation` object is used only internally.

The global data set may actually be local to the caller. The compilation affects the library specified by its name if it is on the stack, but it does not reset the currently selected library.

```

<Compilations: public>+≡
  public :: compile_executable

<Compilations: procedures>+≡
  subroutine compile_executable (exename, libname, global)
    type(string_t), intent(in) :: exename
    type(string_t), dimension(:), intent(in) :: libname
    type(rt_data_t), intent(inout), target :: global
    type(compilation_t) :: compilation
    type(compilation_item_t) :: item
    type(string_t) :: ext_libtag
    logical :: force, recompile, verbose
    integer :: i
    ext_libtag = ""
    force = &
      global%var_list%get_lval (var_str ("?rebuild_library"))
    recompile = &
      global%var_list%get_lval (var_str ("?recompile_library"))
    verbose = &
      global%var_list%get_lval (var_str ("?me_verbose"))
    call compilation%init (exename, [libname])
    if (signal_is_pending ()) return
    call compilation%write_dispatcher ()
    if (signal_is_pending ()) return
    do i = 1, size (libname)
      call item%init (libname(i), global%prclib_stack, global%var_list)
      call item%compile (global%model, global%os_data, &

```



```

        force=force, recompile=recompile)
    ext_libtag = "" // item%lib%get_static_modelname (global%os_data)
    if (signal_is_pending ()) return
    call item%success ()
end do
call compilation%write_makefile &
    (global%os_data, ext_libtag=ext_libtag, verbose=verbose)
if (signal_is_pending ()) return
call compilation%make_compile (global%os_data)
if (signal_is_pending ()) return
call compilation%make_link (global%os_data)
end subroutine compile_executable

```

33.5.5 Unit Tests

Test module, followed by the stand-alone unit-test procedures.

`<compilations_ut.f90>`≡

<File header>

```

module compilations_ut
  use unit_tests
  use compilations_util

```

<Standard module head>

<Compilations: public test>

`contains`

<Compilations: test driver>

```

end module compilations_ut

```

`<compilations_util.f90>`≡

<File header>

```

module compilations_util

```

<Use strings>

```

  use io_units
  use models
  use rt_data
  use process_configurations_ut, only: prepare_test_library

```

```

  use compilations

```

<Standard module head>

<Compilations: test declarations>

`contains`

<Compilations: tests>

```
end module compilations_util
```

API: driver for the unit tests below.

```
<Compilations: public test>≡
  public :: compilations_test

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

Intrinsic Matrix Element

Compile an intrinsic test matrix element (`prc_test` type).

Note: In this and the following test, we reset the Fortran compiler and flag variables immediately before they are printed, so the test is portable.

```
<Compilations: execute tests>≡
  call test (compilations_1, "compilations_1", &
    "intrinsic test processes", &
    u, results)

<Compilations: test declarations>≡
  public :: compilations_1

<Compilations: tests>≡
  subroutine compilations_1 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global

    write (u, "(A)")  "* Test output: compilations_1"
    write (u, "(A)")  "* Purpose: configure and compile test process"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()

    libname = "compilation_1"
    procname = "prc_comp_1"
    call prepare_test_library (global, libname, 1, [procname])

    call compile_library (libname, global)

    call global%write_libraries (u)

    call global%final ()
    call syntax_model_file_final ()

    write (u, "(A)")
```

```

        write (u, "(A)")  "* Test output end: compilations_1"

    end subroutine compilations_1

```

External Matrix Element

Compile an external test matrix element (omega type)

```

<Compilations: execute tests>+≡
    call test (compilations_2, "compilations_2", &
        "external process (omega)", &
        u, results)

<Compilations: test declarations>+≡
    public :: compilations_2

<Compilations: tests>+≡
    subroutine compilations_2 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global

        write (u, "(A)")  "* Test output: compilations_2"
        write (u, "(A)")  "* Purpose: configure and compile test process"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()
        call global%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true.)

        libname = "compilation_2"
        procname = "prc_comp_2"
        call prepare_test_library (global, libname, 2, [procname,procname])

        call compile_library (libname, global)

        call global%write_libraries (u, libpath = .false.)

        call global%final ()
        call syntax_model_file_final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: compilations_2"

    end subroutine compilations_2

```

External Matrix Element

Compile an external test matrix element (omega type) and create driver files for a static executable.

```

<Compilations: execute tests>+≡

```

```

call test (compilations_3, "compilations_3", &
  "static executable: driver", &
  u, results)
<Compilations: test declarations>+≡
  public :: compilations_3
<Compilations: tests>+≡
  subroutine compilations_3 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname, exename
    type(rt_data_t), target :: global
    type(compilation_t) :: compilation
    integer :: u_file
    character(80) :: buffer

    write (u, "(A)")  "* Test output: compilations_3"
    write (u, "(A)")  "* Purpose: make static executable"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize library"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)

    libname = "compilations_3_lib"
    procname = "prc_comp_3"
    exename = "compilations_3"

    call prepare_test_library (global, libname, 2, [procname,procname])

    call compilation%init (exename, [libname])
    call compilation%write (u)

    write (u, "(A)")
    write (u, "(A)")  "* Write dispatcher"
    write (u, "(A)")

    call compilation%write_dispatcher ()

    u_file = free_unit ()
    open (u_file, file = char (exename) // "_prclib_dispatcher.f90", &
      status = "old", action = "read")
    do
      read (u_file, "(A)", end = 1) buffer
      write (u, "(A)") trim (buffer)
    end do
1  close (u_file)

    write (u, "(A)")
    write (u, "(A)")  "* Write Makefile"

```

```

write (u, "(A)")

associate (os_data => global%os_data)
  os_data%fc = "fortran-compiler"
  os_data%cxx = "c++-compiler"
  os_data%whizard_includes = "my-includes"
  os_data%fcflags = "my-fcflags"
  os_data%fclibs = "my-fclibs"
  os_data%cxxflags = "my-cxxflags"
  os_data%cxxlibs = "my-cxxlibs"
  os_data%ldflags = "my-ldflags"
  os_data%ldflags_static = "my-ldflags-static"
  os_data%ldflags_hepmc = "my-ldflags-hepmc"
  os_data%ldflags_lcio = "my-ldflags-lcio"
  os_data%ldflags_hoppet = "my-ldflags-hoppet"
  os_data%ldflags_looptools = "my-ldflags-looptools"
  os_data%whizard_ldflags = "my-ldwhizard"
  os_data%whizard_libtool = "my-libtool"
end associate

call compilation%write_makefile &
  (global%os_data, verbose = .true., overwrite_os = .true.)

open (u_file, file = char (exename) // ".makefile", &
      status = "old", action = "read")
do
  read (u_file, "(A)", end = 2) buffer
  write (u, "(A)") trim (buffer)
end do
2  close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: compilations_3"

end subroutine compilations_3

```

33.5.6 Test static build

The tests for building a static executable are separate, since they should be skipped if the WHIZARD build itself has static libraries disabled.

```

<Compilations: public test>+≡
  public :: compilations_static_test

<Compilations: test driver>+≡
  subroutine compilations_static_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results

```

```

    <Compilations: static tests>
end subroutine compilations_static_test

```

External Matrix Element

Compile an external test matrix element (omega type) and incorporate this in a new static WHIZARD executable.

```

<Compilations: static tests>≡
    call test (compilations_static_1, "compilations_static_1", &
        "static executable: compilation", &
        u, results)

<Compilations: test declarations>+≡
    public :: compilations_static_1

<Compilations: tests>+≡
    subroutine compilations_static_1 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname, exename
        type(rt_data_t), target :: global
        type(compilation_item_t) :: item
        type(compilation_t) :: compilation
        logical :: exist

        write (u, "(A)")  "* Test output: compilations_static_1"
        write (u, "(A)")  "* Purpose: make static executable"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize library"

        call syntax_model_file_init ()

        call global%global_init ()
        call global%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true.)

        libname = "compilations_static_1_lib"
        procname = "prc_comp_stat_1"
        exename = "compilations_static_1"

        call prepare_test_library (global, libname, 2, [procname,procname])

        call compilation%init (exename, [libname])

        write (u, "(A)")
        write (u, "(A)")  "* Write dispatcher"

        call compilation%write_dispatcher ()

        write (u, "(A)")
        write (u, "(A)")  "* Write Makefile"

        call compilation%write_makefile (global%os_data, verbose = .true.)

```

```

write (u, "(A)")
write (u, "(A)")  "* Build libraries"

call item%init (libname, global%prclib_stack, global%var_list)
call item%compile &
      (global%model, global%os_data, force=.true., recompile=.false.)
call item%success ()

write (u, "(A)")
write (u, "(A)")  "* Check executable (should be absent)"
write (u, "(A)")

call compilation%make_clean_exe (global%os_data)
inquire (file = char (exename), exist = exist)
write (u, "(A,A,L1)") char (exename), " exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Build executable"
write (u, "(A)")

call compilation%make_compile (global%os_data)
call compilation%make_link (global%os_data)

write (u, "(A)")  "* Check executable (should be present)"
write (u, "(A)")

inquire (file = char (exename), exist = exist)
write (u, "(A,A,L1)") char (exename), " exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call compilation%make_clean_exe (global%os_data)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: compilations_static_1"

end subroutine compilations_static_1

```

External Matrix Element

Compile an external test matrix element (ω type) and incorporate this in a new static WHIZARD executable. In this version, we use the wrapper `compile_executable` procedure.

```

<Compilations: static tests>+=
  call test (compilations_static_2, "compilations_static_2", &
    "static executable: shortcut", &
    u, results)

```

```

<Compilations: test declarations>+≡
    public :: compilations_static_2

<Compilations: tests>+≡
    subroutine compilations_static_2 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname, exename
        type(rt_data_t), target :: global
        logical :: exist
        integer :: u_file

        write (u, "(A)")  "* Test output: compilations_static_2"
        write (u, "(A)")  "*   Purpose: make static executable"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize library and compile"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()
        call global%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true.)

        libname = "compilations_static_2_lib"
        procname = "prc_comp_stat_2"
        exename = "compilations_static_2"

        call prepare_test_library (global, libname, 2, [procname,procname])

        call compile_executable (exename, [libname], global)

        write (u, "(A)")  "* Check executable (should be present)"
        write (u, "(A)")

        inquire (file = char (exename), exist = exist)
        write (u, "(A,A,L1)")  char (exename), " exists = ", exist

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

        u_file = free_unit ()
        open (u_file, file = char (exename), status = "old", action = "write")
        close (u_file, status = "delete")

        call global%final ()
        call syntax_model_file_final ()

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: compilations_static_2"

    end subroutine compilations_static_2

```


33.6 Integration

This module manages phase space setup, matrix-element evaluation and integration, as far as it is not done by lower-level routines, in particular in the `processes` module.

`<integrations.f90>`≡

<File header>

```
module integrations
```

```
<Use kinds>
```

```
<Use strings>
```

```
<Use debug>
```

```
  use io_units
```

```
  use diagnostics
```

```
  use os_interface
```

```
  use cputime
```

```
  use sm_qcd
```

```
  use physics_defs
```

```
  use model_data
```

```
  use pdg_arrays
```

```
  use variables, only: var_list_t
```

```
  use eval_trees
```

```
  use sf_mappings
```

```
  use sf_base
```

```
  use phs_base
```

```
  use rng_base
```

```
  use mci_base
```

```
  use process_libraries
```

```
  use prc_core
```

```
  use process_config, only: COMP_MASTER, COMP_REAL_FIN, &  
    COMP_MISMATCH, COMP_PDF, COMP_REAL, COMP_SUB, COMP_VIRT, &  
    COMP_REAL_SING
```

```
  use process
```

```
  use pcm_base, only: pcm_t
```

```
  use instances
```

```
  use process_stacks
```

```
  use models
```

```
  use iterations
```

```
  use rt_data
```

```
  use dispatch_me_methods, only: dispatch_core
```

```
  use dispatch_beams, only: dispatch_qcd, sf_prop_t, dispatch_sf_config
```

```
  use dispatch_phase_space, only: dispatch_sf_channels
```

```
  use dispatch_phase_space, only: dispatch_phs
```

```
  use dispatch_mci, only: dispatch_mci_s, setup_grid_path
```

```
  use dispatch_transforms, only: dispatch_evt_shower_hook
```

```
  use compilations, only: compile_library
```

```
  use dispatch_fks, only: dispatch_fks_s
```

```
  use nlo_data
```

```
<Use mpi f08>
```

```

    <Standard module head>

    <Integrations: public>

    <Integrations: types>

contains

    <Integrations: procedures>

end module integrations

```

33.6.1 The integration type

This type holds all relevant data, the integration methods operates on this. In contrast to the `simulation_t` introduced later, the `integration_t` applies to a single process.

```

<Integrations: public>≡
    public :: integration_t

<Integrations: types>≡
    type :: integration_t
        private
            type(string_t) :: process_id
            type(string_t) :: run_id
            type(process_t), pointer :: process => null ()
            logical :: rebuild_phs = .false.
            logical :: ignore_phs_mismatch = .false.
            logical :: phs_only = .false.
            logical :: process_has_me = .true.
            integer :: n_calls_test = 0
            logical :: vis_history = .true.
            type(string_t) :: history_filename
            type(string_t) :: log_filename
            type(helicity_selection_t) :: helicity_selection
            logical :: use_color_factors = .false.
            logical :: has_beam_pol = .false.
            logical :: combined_integration = .false.
            type(iteration_multipliers_t) :: iteration_multipliers
            type(nlo_settings_t) :: nlo_settings
        contains
            <Integrations: integration: TBP>
    end type integration_t

```

33.6.2 Initialization

Initialization, first part: Create a process entry. Push it on the stack if the global environment is supplied.

```

<Integrations: integration: TBP>≡
    procedure :: create_process => integration_create_process

```

```

<Integrations: procedures>≡
subroutine integration_create_process (intg, process_id, global)
  class(integration_t), intent(out) :: intg
  type(rt_data_t), intent(inout), optional, target :: global
  type(string_t), intent(in) :: process_id
  type(process_entry_t), pointer :: process_entry
  if (debug_on) call msg_debug (D_CORE, "integration_create_process")
  intg%process_id = process_id
  if (present (global)) then
    allocate (process_entry)
    intg%process => process_entry%process_t
    call global%process_stack%push (process_entry)
  else
    allocate (process_t :: intg%process)
  end if
end subroutine integration_create_process

```

Initialization, second part: Initialize the process object, using the local environment. We allocate a RNG factory and a QCD object. We also fetch a pointer to the model that the process uses. The process initializer will create a snapshot of that model.

This procedure does not modify the local stack directly. The intent(inout) attribute for the local data set is due to the random generator seed which may be incremented during initialization.

NOTE: Changes to model parameters within the current context are respected only if the process model coincides with the current model. This is the usual case. If not, we read the model from the global model library, which has default parameters. To become more flexible, we should implement a local model library which records local changes to currently inactive models.

```

<Integrations: integration: TBP>+≡
  procedure :: init_process => integration_init_process

<Integrations: procedures>+≡
subroutine integration_init_process (intg, local)
  class(integration_t), intent(inout) :: intg
  type(rt_data_t), intent(inout), target :: local
  type(string_t) :: model_name
  type(model_t), pointer :: model
  class(model_data_t), pointer :: model_instance
  type(var_list_t), pointer :: var_list
  if (debug_on) call msg_debug (D_CORE, "integration_init_process")
  if (.not. local%prclib%contains (intg%process_id)) then
    call msg_fatal ("Process '" // char (intg%process_id) // "' not found" &
      // " in library '" // char (local%prclib%get_name ()) // "'")
    return
  end if
  model_name = local%prclib%get_model_name (intg%process_id)
  if (local%get_sval (var_str ("$model_name")) == model_name) then
    model => local%model
  else
    model => local%model_list%get_model_ptr (model_name)
  end if
  var_list => local%get_var_list_ptr ()

```

```

call intg%process%init (intg%process_id, &
    local%prclib, &
    local%os_data, &
    model, &
    var_list, &
    local%beam_structure)
intg%run_id = intg%process%get_run_id ()
end subroutine integration_init_process

```

Initialization, third part: complete process configuration.

<Integrations: integration: TBP>+≡

```

procedure :: setup_process => integration_setup_process

```

<Integrations: procedures>+≡

```

subroutine integration_setup_process (intg, local, verbose, init_only)
    class(integration_t), intent(inout) :: intg
    type(rt_data_t), intent(inout), target :: local
    logical, intent(in), optional :: verbose
    logical, intent(in), optional :: init_only

    type(var_list_t), pointer :: var_list
    class(mci_t), allocatable :: mci_template
    type(sf_config_t), dimension(:), allocatable :: sf_config
    type(sf_prop_t) :: sf_prop
    type(sf_channel_t), dimension(:), allocatable :: sf_channel
    type(phs_channel_collection_t) :: phs_channel_collection
    logical :: sf_trace
    logical :: verb, initialize_only
    type(string_t) :: sf_string
    type(string_t) :: workspace
    real(default) :: sqrts

    verb = .true.; if (present (verbose)) verb = verbose

    initialize_only = .false.
    if (present (init_only)) initialize_only = init_only

    call display_init_message (verb)

    var_list => local%get_var_list_ptr ()
    call setup_log_and_history ()

    associate (process => intg%process)
        call set_intg_parameters (process)

        call process%setup_cores (dispatch_core, &
            intg%helicity_selection, intg%use_color_factors, intg%has_beam_pol)

        call process%init_phs_config ()
        call process%init_components ()

        call process%record_inactive_components ()
        intg%process_has_me = process%has_matrix_element ()
        if (.not. intg%process_has_me) then

```

```

        call msg_warning ("Process '" &
            // char (intg%process_id) // "' : matrix element vanishes")
    end if

    call setup_beams ()
    call setup_structure_functions ()

    workspace = var_list%get_sval (var_str ("$integrate_workspace"))
    if (workspace == "") then
        call process%configure_phs &
            (intg%rebuild_phs, &
            intg%ignore_phs_mismatch, &
            intg%combined_integration)
    else
        call setup_grid_path (workspace)
        call process%configure_phs &
            (intg%rebuild_phs, &
            intg%ignore_phs_mismatch, &
            intg%combined_integration, &
            workspace)
    end if

    call process%complete_pcm_setup ()

    call process%prepare_blha_cores ()
    call process%create_blha_interface ()
    call process%prepare_any_external_code ()

    call process%setup_terms (with_beams = intg%has_beam_pol)
    call process%check_masses ()
    call process%optimize_nlo_singular_regions ()

    if (verb) then
        call process%write (screen = .true.)
        call process%print_phs_startup_message ()
    end if

    if (intg%process_has_me) then
        if (size (sf_config) > 0) then
            call process%collect_channels (phs_channel_collection)
        else if (.not. initialize_only &
            .and. process%contains_trivial_component ()) then
            call msg_fatal ("Integrate: 2 -> 1 process can't be handled &
                &with fixed-energy beams")
        end if
        if (local%beam_structure%asymmetric ()) then
            sqrts = process%get_sqrts ()
        else
            sqrts = local%get_sqrts ()
        end if
        call dispatch_sf_channels &
            (sf_channel, sf_string, sf_prop, phs_channel_collection, &
            local%var_list, sqrts, local%beam_structure)
        if (allocated (sf_channel)) then

```

```

        if (size (sf_channel) > 0) then
            call process%set_sf_channel (sf_channel)
        end if
    end if
    call phs_channel_collection%final ()
    if (verb) call process%sf_startup_message (sf_string)
end if

call process%setup_mci (dispatch_mci_s)

call setup_expressions ()

call process%compute_md5sum ()
end associate

contains

subroutine setup_log_and_history ()
    if (intg%run_id /= "") then
        intg%history_filename = intg%process_id // "." // intg%run_id &
            // ".history"
        intg%log_filename = intg%process_id // "." // intg%run_id // ".log"
    else
        intg%history_filename = intg%process_id // ".history"
        intg%log_filename = intg%process_id // ".log"
    end if
    intg%vis_history = &
        var_list%get_lval (var_str ("?vis_history"))
end subroutine setup_log_and_history

subroutine set_intg_parameters (process)
    type(process_t), intent(in) :: process
    intg%n_calls_test = &
        var_list%get_ival (var_str ("n_calls_test"))
    intg%combined_integration = &
        var_list%get_lval (var_str ('?combined_nlo_integration')) &
        .and. process%is_nlo_calculation ()
    intg%use_color_factors = &
        var_list%get_lval (var_str ("?read_color_factors"))
    intg%has_beam_pol = &
        local%beam_structure%has_polarized_beams ()
    intg%helicity_selection = &
        local%get_helicity_selection ()
    intg%rebuild_phs = &
        var_list%get_lval (var_str ("?rebuild_phase_space"))
    intg%ignore_phs_mismatch = &
        .not. var_list%get_lval (var_str ("?check_phs_file"))
    intg%phs_only = &
        var_list%get_lval (var_str ("?phs_only"))
end subroutine set_intg_parameters

subroutine display_init_message (verb)
    logical, intent(in) :: verb
    if (verb) then

```

```

        call msg_message ("Initializing integration for process " &
            // char (intg%process_id) // ":")
        if (intg%run_id /= "") &
            call msg_message ("Run ID = " // '"" // char (intg%run_id) // '""')
        end if
end subroutine display_init_message

subroutine setup_beams ()
    real(default) :: sqrts
    logical :: decay_rest_frame
    sqrts = local%get_sqrts ()
    decay_rest_frame = &
        var_list%get_lval (var_str ("?decay_rest_frame"))
    if (intg%process_has_me) then
        call intg%process%setup_beams_beam_structure &
            (local%beam_structure, sqrts, decay_rest_frame)
    end if
    if (verb .and. intg%process_has_me) then
        call intg%process%beams_startup_message &
            (beam_structure = local%beam_structure)
    end if
end subroutine setup_beams

subroutine setup_structure_functions ()
    integer :: n_in
    type(pdg_array_t), dimension(:,:), allocatable :: pdg_prc
    type(string_t) :: sf_trace_file
    if (intg%process_has_me) then
        call intg%process%get_pdg_in (pdg_prc)
    else
        n_in = intg%process%get_n_in ()
        allocate (pdg_prc (n_in, intg%process%get_n_components ()))
        pdg_prc = 0
    end if
    call dispatch_sf_config (sf_config, sf_prop, local%beam_structure, &
        local%get_var_list_ptr (), local%var_list, &
        local%model, local%os_data, local%get_sqrts (), pdg_prc)

    sf_trace = &
        var_list%get_lval (var_str ("?sf_trace"))
    sf_trace_file = &
        var_list%get_sval (var_str ("$sf_trace_file"))
    if (sf_trace) then
        call intg%process%init_sf_chain (sf_config, sf_trace_file)
    else
        call intg%process%init_sf_chain (sf_config)
    end if
end subroutine setup_structure_functions

subroutine setup_expressions ()
    type(eval_tree_factory_t) :: expr_factory
    if (associated (local%pn%cuts_lexpr)) then
        if (verb) call msg_message ("Applying user-defined cuts.")
        call expr_factory%init (local%pn%cuts_lexpr)
    end if
end subroutine setup_expressions

```

```

        call intg%process%set_cuts (expr_factory)
    else
        if (verb) call msg_warning ("No cuts have been defined.")
    end if
    if (associated (local%pn%scale_expr)) then
        if (verb) call msg_message ("Using user-defined general scale.")
        call expr_factory%init (local%pn%scale_expr)
        call intg%process%set_scale (expr_factory)
    end if
    if (associated (local%pn%fac_scale_expr)) then
        if (verb) call msg_message ("Using user-defined factorization scale.")
        call expr_factory%init (local%pn%fac_scale_expr)
        call intg%process%set_fac_scale (expr_factory)
    end if
    if (associated (local%pn%ren_scale_expr)) then
        if (verb) call msg_message ("Using user-defined renormalization scale.")
        call expr_factory%init (local%pn%ren_scale_expr)
        call intg%process%set_ren_scale (expr_factory)
    end if
    if (associated (local%pn%weight_expr)) then
        if (verb) call msg_message ("Using user-defined reweighting factor.")
        call expr_factory%init (local%pn%weight_expr)
        call intg%process%set_weight (expr_factory)
    end if
end subroutine setup_expressions
end subroutine integration_setup_process

```

33.6.3 Integration

Integrate: do the final integration. Here, we do a multi-iteration integration. Again, we skip iterations that are already on file. Record the results in the global variable list.

```

<Integrations: integration: TBP>+≡
    procedure :: evaluate => integration_evaluate

<Integrations: procedures>+≡
    subroutine integration_evaluate &
        (intg, process_instance, i_mci, pass, it_list, pacify)
    class(integration_t), intent(inout) :: intg
    type(process_instance_t), intent(inout), target :: process_instance
    integer, intent(in) :: i_mci
    integer, intent(in) :: pass
    type(iterations_list_t), intent(in) :: it_list
    logical, intent(in), optional :: pacify
    integer :: n_calls, n_it
    logical :: adapt_grids, adapt_weights, final
    n_it = it_list%get_n_it (pass)
    n_calls = it_list%get_n_calls (pass)
    adapt_grids = it_list%adapt_grids (pass)
    adapt_weights = it_list%adapt_weights (pass)
    final = pass == it_list%get_n_pass ()
    call process_instance%integrate ( &
        i_mci, n_it, n_calls, adapt_grids, adapt_weights, &

```



```

        final, pacify)
    end subroutine integration_evaluate

```

In case the user has not provided a list of iterations, make a reasonable default. This can depend on the process. The usual approach is to define two distinct passes, one for adaptation and one for integration.

```

<Integrations: integration: TBP>+≡
    procedure :: make_iterations_list => integration_make_iterations_list

<Integrations: procedures>+≡
    subroutine integration_make_iterations_list (intg, it_list)
        class(integration_t), intent(in) :: intg
        type(iterations_list_t), intent(out) :: it_list
        integer :: pass, n_pass
        integer, dimension(:), allocatable :: n_it, n_calls
        logical, dimension(:), allocatable :: adapt_grids, adapt_weights
        n_pass = intg%process%get_n_pass_default ()
        allocate (n_it (n_pass), n_calls (n_pass))
        allocate (adapt_grids (n_pass), adapt_weights (n_pass))
        do pass = 1, n_pass
            n_it(pass)      = intg%process%get_n_it_default (pass)
            n_calls(pass)   = intg%process%get_n_calls_default (pass)
            adapt_grids(pass) = intg%process%adapt_grids_default (pass)
            adapt_weights(pass) = intg%process%adapt_weights_default (pass)
        end do
        call it_list%init (n_it, n_calls, &
            adapt_grids = adapt_grids, adapt_weights = adapt_weights)
    end subroutine integration_make_iterations_list

```

In NLO calculations, the individual components might scale very differently with the number of calls. This especially applies to the real-subtracted component, which usually fluctuates more than the Born and virtual component, making it a bottleneck of the calculation. Thus, the calculation is throttled twice, first by the number of calls for the real component, second by the number of surplus calls of computation-intense virtual matrix elements. Therefore, we want to set a different number of calls for each component, which is done by the subroutine `integration.apply.call_multipliers`.

```

<Integrations: integration: TBP>+≡
    procedure :: init_iteration_multipliers => integration_init_iteration_multipliers

<Integrations: procedures>+≡
    subroutine integration_init_iteration_multipliers (intg, local)
        class(integration_t), intent(inout) :: intg
        type(rt_data_t), intent(in) :: local
        integer :: n_pass, pass
        type(iterations_list_t) :: it_list
        n_pass = local%it_list%get_n_pass ()
        if (n_pass == 0) then
            call intg%make_iterations_list (it_list)
            n_pass = it_list%get_n_pass ()
        end if
        associate (it_multipliers => intg%iteration_multipliers)
            allocate (it_multipliers%n_calls0 (n_pass))
        end associate
    end subroutine

```

```

do pass = 1, n_pass
  it_multipliers%n_calls0(pass) = local%it_list%get_n_calls (pass)
end do
it_multipliers%mult_real = local%var_list%get_rval &
  (var_str ("mult_call_real"))
it_multipliers%mult_virt = local%var_list%get_rval &
  (var_str ("mult_call_virt"))
it_multipliers%mult_dglap = local%var_list%get_rval &
  (var_str ("mult_call_dglap"))
end associate
end subroutine integration_init_iteration_multipliers

```

<Integrations: integration: TBP>+≡

```

procedure :: apply_call_multipliers => integration_apply_call_multipliers

```

<Integrations: procedures>+≡

```

subroutine integration_apply_call_multipliers (intg, n_pass, i_component, it_list)
  class(integration_t), intent(in) :: intg
  integer, intent(in) :: n_pass, i_component
  type(iterations_list_t), intent(inout) :: it_list
  integer :: nlo_type
  integer :: n_calls0, n_calls
  integer :: pass
  real(default) :: multiplier
  nlo_type = intg%process%get_component_nlo_type (i_component)
  do pass = 1, n_pass
    associate (multipliers => intg%iteration_multipliers)
      select case (nlo_type)
        case (NLO_REAL)
          multiplier = multipliers%mult_real
        case (NLO_VIRTUAL)
          multiplier = multipliers%mult_virt
        case (NLO_DGLAP)
          multiplier = multipliers%mult_dglap
        case default
          return
      end select
    end associate
    if (n_pass <= size (intg%iteration_multipliers%n_calls0)) then
      n_calls0 = intg%iteration_multipliers%n_calls0 (pass)
      n_calls = floor (multiplier * n_calls0)
      call it_list%set_n_calls (pass, n_calls)
    end if
  end do
end subroutine integration_apply_call_multipliers

```

33.6.4 API for integration objects

This initializer does everything except assigning cuts/scale/weight expressions.

<Integrations: integration: TBP>+≡

```

procedure :: init => integration_init

```

<Integrations: procedures>+≡

```

subroutine integration_init &
    (intg, process_id, local, global, local_stack, init_only)
    class(integration_t), intent(out) :: intg
    type(string_t), intent(in) :: process_id
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    logical, intent(in), optional :: init_only
    logical, intent(in), optional :: local_stack
    logical :: use_local
    use_local = .false.; if (present (local_stack)) use_local = local_stack
    if (present (global)) then
        call intg%create_process (process_id, global)
    else if (use_local) then
        call intg%create_process (process_id, local)
    else
        call intg%create_process (process_id)
    end if
    call intg%init_process (local)
    call intg%setup_process (local, init_only = init_only)
    call intg%init_iteration_multipliers (local)
end subroutine integration_init

```

Do the integration for a single process, both warmup and final evaluation. The `eff_reset` flag is to suppress numerical noise in the graphical output of the integration history.

<Integrations: integration: TBP>+≡

```

procedure :: integrate => integration_integrate

```

<Integrations: procedures>+≡

```

subroutine integration_integrate (intg, local, eff_reset)
    class(integration_t), intent(inout) :: intg
    type(rt_data_t), intent(in), target :: local
    logical, intent(in), optional :: eff_reset
    type(string_t) :: log_filename
    type(var_list_t), pointer :: var_list
    type(process_instance_t), allocatable, target :: process_instance
    type(iterations_list_t) :: it_list
    logical :: pacify
    integer :: pass, i_mci, n_mci, n_pass
    integer :: i_component
    integer :: nlo_type
    logical :: display_summed
    logical :: nlo_active
    type(string_t) :: component_output

    allocate (process_instance)
    call process_instance%init (intg%process)

    var_list => intg%process%get_var_list_ptr ()
    call openmp_set_num_threads_verbose &
        (var_list%get_ival (var_str ("openmp_num_threads")), &
         var_list%get_lval (var_str ("?openmp_logging")))
    pacify = var_list%get_lval (var_str ("?pacify"))

```

```

display_summed = .true.
n_mci = intg%process%get_n_mci ()
if (n_mci == 1) then
    write (msg_buffer, "(A,A,A)") &
        "Starting integration for process '", &
        char (intg%process%get_id ()), "'"
    call msg_message ()
end if

call setup_hooks ()

nlo_active = any (intg%process%get_component_nlo_type &
    ([i_mci, i_mci = 1, n_mci]) /= BORN)
do i_mci = 1, n_mci
    i_component = intg%process%get_master_component (i_mci)
    nlo_type = intg%process%get_component_nlo_type (i_component)
    if (intg%process%component_can_be_integrated (i_component)) then
        if (n_mci > 1) then
            if (nlo_active) then
                if (intg%combined_integration .and. nlo_type == BORN) then
                    component_output = var_str ("Combined")
                else
                    component_output = component_status (nlo_type)
                end if
                write (msg_buffer, "(A,A,A,A,A)") &
                    "Starting integration for process '", &
                    char (intg%process%get_id ()), "' part '", &
                    char (component_output), "'"
            else
                write (msg_buffer, "(A,A,A,I0)") &
                    "Starting integration for process '", &
                    char (intg%process%get_id ()), "' part ", i_mci
            end if
            call msg_message ()
        end if
        n_pass = local%it_list%get_n_pass ()
        if (n_pass == 0) then
            call msg_message ("Integrate: iterations not specified, &
                &using default")
            call intg%make_iterations_list (it_list)
            n_pass = it_list%get_n_pass ()
        else
            it_list = local%it_list
        end if
        call intg%apply_call_multipliers (n_pass, i_mci, it_list)
        call msg_message ("Integrate: " // char (it_list%to_string ()))
        do pass = 1, n_pass
            call intg%evaluate (process_instance, i_mci, pass, it_list, pacify)
            if (signal_is_pending ()) return
        end do
        call intg%process%final_integration (i_mci)
        if (intg%vis_history) then
            call intg%process%display_integration_history &

```

```

        (i_mci, intg%history_filename, local%os_data, eff_reset)
    end if
    if (local%logfile == intg%log_filename) then
        if (intg%run_id /= "") then
            log_filename = intg%process_id // "." // intg%run_id // &
                ".var.log"
        else
            log_filename = intg%process_id // ".var.log"
        end if
        call msg_message ("Name clash for global logfile and process log: ", &
            arr=[var_str ("| Renaming log file from ") // local%logfile, &
                var_str ("| to ") // log_filename // var_str (" .")])
    else
        log_filename = intg%log_filename
    end if
    call intg%process%write_logfile (i_mci, log_filename)
end if
end do

if (n_mci > 1 .and. display_summed) then
    call msg_message ("Integrate: sum of all components")
    call intg%process%display_summed_results (pacify)
end if

call process_instance%final ()
deallocate (process_instance)
contains
    subroutine setup_hooks ()
        class(process_instance_hook_t), pointer :: hook
        call dispatch_evt_shower_hook (hook, var_list, process_instance)
        if (associated (hook)) then
            call process_instance%append_after_hook (hook)
        end if
    end subroutine setup_hooks
end subroutine integration_integrate

```

Do a dummy integration for a process which could not be initialized (e.g., has no matrix element). The result is zero.

```

<Integrations: integration: TBP>+≡
    procedure :: integrate_dummy => integration_integrate_dummy

<Integrations: procedures>+≡
    subroutine integration_integrate_dummy (intg)
        class(integration_t), intent(inout) :: intg
        call intg%process%integrate_dummy ()
    end subroutine integration_integrate_dummy

```

Just sample the matrix element under realistic conditions (but no cuts); throw away the results.

```

<Integrations: integration: TBP>+≡
    procedure :: sampler_test => integration_sampler_test

<Integrations: procedures>+≡
    subroutine integration_sampler_test (intg)

```

```

class(integration_t), intent(inout) :: intg
type(process_instance_t), allocatable, target :: process_instance
integer :: n_mci, i_mci
type(timer_t) :: timer_mci, timer_tot
real(default) :: t_mci, t_tot
allocate (process_instance)
call process_instance%init (intg%process)
n_mci = intg%process%get_n_mci ()
if (n_mci == 1) then
    write (msg_buffer, "(A,A,A)") &
        "Test: probing process '", &
        char (intg%process%get_id ()), "'"
    call msg_message ()
end if
call timer_tot%start ()
do i_mci = 1, n_mci
    if (n_mci > 1) then
        write (msg_buffer, "(A,A,A,IO)") &
            "Test: probing process '", &
            char (intg%process%get_id ()), "' part ", i_mci
        call msg_message ()
    end if
    call timer_mci%start ()
    call process_instance%sampler_test (i_mci, intg%n_calls_test)
    call timer_mci%stop ()
    t_mci = timer_mci
    write (msg_buffer, "(A,ES12.5)") "Test: " &
        // "time in seconds (wallclock): ", t_mci
    call msg_message ()
end do
call timer_tot%stop ()
t_tot = timer_tot
if (n_mci > 1) then
    write (msg_buffer, "(A,ES12.5)") "Test: " &
        // "total time (wallclock): ", t_tot
    call msg_message ()
end if
call process_instance%final ()
end subroutine integration_sampler_test

```

Return the process pointer (needed by simulate):

```

<Integrations: integration: TBP>+≡
    procedure :: get_process_ptr => integration_get_process_ptr

<Integrations: procedures>+≡
    function integration_get_process_ptr (intg) result (ptr)
        class(integration_t), intent(in) :: intg
        type(process_t), pointer :: ptr
        ptr => intg%process
    end function integration_get_process_ptr

```

Simply integrate, do a dummy integration if necessary. The `integration` object exists only internally.

If the `global` environment is provided, the process object is appended to the global stack. Otherwise, if `local_stack` is set, we append to the local process stack. If this is unset, the `process` object is not recorded permanently.

The `init_only` flag can be used to skip the actual integration part. We will end up with a process object that is completely initialized, including phase space configuration.

The `eff_reset` flag is to suppress numerical noise in the visualization of the integration history.

```

<Integrations: public>+=
    public :: integrate_process

<Integrations: procedures>+=
    subroutine integrate_process (process_id, local, global, local_stack, init_only, eff_reset)
        type(string_t), intent(in) :: process_id
        type(rt_data_t), intent(inout), target :: local
        type(rt_data_t), intent(inout), optional, target :: global
        logical, intent(in), optional :: local_stack, init_only, eff_reset
        type(string_t) :: prclib_name
        type(integration_t) :: intg
        character(32) :: buffer
    <Integrations: integrate process: variables>
    <Integrations: integrate process: init>
        if (.not. associated (local%prclib)) then
            call msg_fatal ("Integrate: current process library is undefined")
            return
        end if

        if (.not. local%prclib%is_active ()) then
            call msg_message ("Integrate: current process library needs compilation")
            prclib_name = local%prclib%get_name ()
            call compile_library (prclib_name, local)
            if (signal_is_pending ()) return
            call msg_message ("Integrate: compilation done")
        end if

        call intg%init (process_id, local, global, local_stack, init_only)
        if (signal_is_pending ()) return

        if (present (init_only)) then
            if (init_only) return
        end if

        if (intg%n_calls_test > 0) then
            write (buffer, "(I0)") intg%n_calls_test
            call msg_message ("Integrate: test (" // trim (buffer) // " calls) ...")
            call intg%sampler_test ()
            call msg_message ("Integrate: ... test complete.")
            if (signal_is_pending ()) return
        end if
    <Integrations: integrate process: end init>

        if (intg%phs_only) then
            call msg_message ("Integrate: phase space only, skipping integration")
        else

```

```

        if (intg%process_has_me) then
            call intg%integrate (local, eff_reset)
        else
            call intg%integrate_dummy ()
        end if
    end if
end subroutine integrate_process

```

<Integrations: integrate process: variables>≡

<Integrations: integrate process: init>≡

<Integrations: integrate process: end init>≡

The parallelization leads to undefined behavior while writing simultaneously to one file. The master worker has to initialize single-handed the corresponding library files and the phase space file. The slave worker will wait with a blocking MPI_BCAST until they receive a logical flag.

<MPI: Integrations: integrate process: variables>≡

```

type(var_list_t), pointer :: var_list
logical :: mpi_logging, process_init
integer :: rank, n_size

```

<MPI: Integrations: integrate process: init>≡

```

if (debug_on) call msg_debug (D_MPI, "integrate_process")
var_list => local%get_var_list_ptr ()
process_init = .false.
call mpi_get_comm_id (n_size, rank)
mpi_logging = (("vamp2" == char (var_list%get_sval (var_str ("%integration_method")))) .and. &
    & (n_size > 1)) .or. var_list%get_lval (var_str ("%mpi_logging")))
if (debug_on) call msg_debug (D_MPI, "n_size", rank)
if (debug_on) call msg_debug (D_MPI, "rank", rank)
if (debug_on) call msg_debug (D_MPI, "mpi_logging", mpi_logging)
if (rank /= 0) then
    if (mpi_logging) then
        call msg_message ("MPI: wait for master to finish process initialization ...")
    end if
    call MPI_bcast (process_init, 1, MPI_LOGICAL, 0, MPI_COMM_WORLD)
else
    process_init = .true.
end if

```

```

if (process_init) then

```

<MPI: Integrations: integrate process: end init>≡

```

if (rank == 0) then
    if (mpi_logging) then
        call msg_message ("MPI: finish process initialization, load slaves ...")
    end if
    call MPI_bcast (process_init, 1, MPI_LOGICAL, 0, MPI_COMM_WORLD)
end if
end if
call MPI_barrier (MPI_COMM_WORLD)
call mpi_set_logging (mpi_logging)

```


33.6.5 Unit Tests

Test module, followed by the stand-alone unit-test procedures.

```
<integrations_ut.f90>≡  
  <File header>  
  
  module integrations_ut  
    use unit_tests  
    use integrations_uti  
  
    <Standard module head>  
  
    <Integrations: public test>  
  
    contains  
  
    <Integrations: test driver>  
  
  end module integrations_ut  
<integrations_uti.f90>≡  
  <File header>  
  
  module integrations_uti  
  
    <Use kinds>  
    <Use strings>  
    use io_units  
    use ifiles  
    use lexers  
    use parser  
    use flavors  
    use interactions, only: reset_interaction_counter  
    use phs_forests  
    use eval_trees  
    use models  
    use rt_data  
    use process_configurations_ut, only: prepare_test_library  
    use compilations, only: compile_library  
  
    use integrations  
  
    use phs_wood_ut, only: write_test_phs_file  
  
    <Standard module head>  
  
    <Integrations: test declarations>  
  
    contains  
  
    <Integrations: tests>  
  
  end module integrations_uti
```

API: driver for the unit tests below.

```

<Integrations: public test>≡
  public :: integrations_test

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

<Integrations: public test>+≡
  public :: integrations_history_test

<Integrations: test driver>+≡
  subroutine integrations_history_test (u, results)
    integer, intent(in) :: u
    type(test_results_t), intent(inout) :: results
    <Integrations: execute history tests>
  end subroutine integrations_history_test

```

Integration of test process

Compile and integrate an intrinsic test matrix element (`prc_test` type). The phase-space implementation is `phs_single` (single-particle phase space), the integrator is `mci_midpoint`.

The cross section for the $2 \rightarrow 2$ process $ss \rightarrow ss$ with its constant matrix element is given by

$$\sigma = c \times f \times \Phi_2 \times |M|^2. \quad (33.1)$$

c is the conversion constant

$$c = 0.3894 \times 10^{12} \text{ fb GeV}^2. \quad (33.2)$$

f is the flux of the incoming particles with mass $m = 125 \text{ GeV}$ and energy $\sqrt{s} = 1000 \text{ GeV}$

$$f = \frac{(2\pi)^4}{2\lambda^{1/2}(s, m^2, m^2)} = \frac{(2\pi)^4}{2\sqrt{s}\sqrt{s-4m^2}} = 8.048 \times 10^{-4} \text{ GeV}^{-2} \quad (33.3)$$

Φ_2 is the volume of the two-particle phase space

$$\Phi_2 = \frac{1}{4(2\pi)^5} = 2.5529 \times 10^{-5}. \quad (33.4)$$

The squared matrix element $|M|^2$ is unity. Combining everything, we obtain

$$\sigma = 8000 \text{ fb} \quad (33.5)$$

This number should appear as the final result.

Note: In this and the following test, we reset the Fortran compiler and flag variables immediately before they are printed, so the test is portable.

```

<Integrations: execute tests>≡
  call test (integrations_1, "integrations_1", &
    "intrinsic test process", &
    u, results)

```

```

<Integrations: test declarations>≡
    public :: integrations_1

<Integrations: tests>≡
    subroutine integrations_1 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global

        write (u, "(A)")  "* Test output: integrations_1"
        write (u, "(A)")  "* Purpose: integrate test process"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()

        libname = "integration_1"
        procname = "prc_config_a"

        call prepare_test_library (global, libname, 1)
        call compile_library (libname, global)

        call global%set_string (var_str ("$_run_id"), &
            var_str ("integrations1"), is_known = .true.)
        call global%set_string (var_str ("$_method"), &
            var_str ("unit_test"), is_known = .true.)
        call global%set_string (var_str ("$_phs_method"), &
            var_str ("single"), is_known = .true.)
        call global%set_string (var_str ("$_integration_method"), &
            var_str ("midpoint"), is_known = .true.)
        call global%set_log (var_str ("?vis_history"), &
            .false., is_known = .true.)
        call global%set_log (var_str ("?integration_timer"), &
            .false., is_known = .true.)
        call global%set_int (var_str ("seed"), &
            0, is_known=.true.)

        call global%set_real (var_str ("sqrts"), &
            1000._default, is_known = .true.)

        call global%it_list%init ([1], [1000])

        call reset_interaction_counter ()
        call integrate_process (procname, global, local_stack=.true.)

        call global%write (u, vars = [ &
            var_str ("$_method"), &
            var_str ("sqrts"), &
            var_str ("$_integration_method"), &
            var_str ("$_phs_method"), &
            var_str ("$_run_id")])

        call global%final ()
        call syntax_model_file_final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_1"

end subroutine integrations_1

```

Integration with cuts

Compile and integrate an intrinsic test matrix element (`prc_test` type) with cuts set.

```

<Integrations: execute tests>+≡
  call test (integrations_2, "integrations_2", &
    "intrinsic test process with cut", &
    u, results)

<Integrations: test declarations>+≡
  public :: integrations_2

<Integrations: tests>+≡
  subroutine integrations_2 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global

    type(string_t) :: cut_expr_text
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(parse_tree_t) :: parse_tree

    type(string_t), dimension(0) :: empty_string_array

    write (u, "(A)")  "* Test output: integrations_2"
    write (u, "(A)")  "* Purpose: integrate test process with cut"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()

    write (u, "(A)")  "* Prepare a cut expression"
    write (u, "(A)")

    call syntax_pexpr_init ()
    cut_expr_text = "all Pt > 100 [s]"
    call ifile_append (ifile, cut_expr_text)
    call stream_init (stream, ifile)
    call parse_tree_init_lexpr (parse_tree, stream, .true.)
    global%pn%cuts_lexpr => parse_tree%get_root_ptr ()

    write (u, "(A)")  "* Build and initialize a test process"
    write (u, "(A)")

    libname = "integration_3"

```

```

procname = "prc_config_a"

call prepare_test_library (global, libname, 1)
call compile_library (libname, global)

call global%set_string (var_str ("$_run_id"), &
    var_str ("integrations1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%write (u, vars = empty_string_array)

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_2"

end subroutine integrations_2

```

Standard phase space

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the default (`phs_wood`) phase-space implementation. We use an explicit phase-space configuration file with a single channel and integrate by `mci_midpoint`.

```

<Integrations: execute tests>+≡
    call test (integrations_3, "integrations_3", &
        "standard phase space", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_3

<Integrations: tests>+≡
    subroutine integrations_3 (u)

```

```

<Use kinds>
<Use strings>

use interactions, only: reset_interaction_counter
use models
use rt_data
use process_configurations_ut, only: prepare_test_library
use compilations, only: compile_library
use integrations

implicit none

integer, intent(in) :: u
type(string_t) :: libname, procname
type(rt_data_t), target :: global
integer :: u_phs

write (u, "(A)")  "* Test output: integrations_3"
write (u, "(A)")  "* Purpose: integrate test process"
write (u, "(A)")

write (u, "(A)")  "* Initialize process and parameters"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_phs_forest_init ()

call global%global_init ()

libname = "integration_3"
procname = "prc_config_a"

call prepare_test_library (global, libname, 1)
call compile_library (libname, global)

call global%set_string (var_str ("$_run_id"), &
    var_str ("integrations1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("default"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?phs_s_mapping"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

```

```

write (u, "(A)")  "* Create a scratch phase-space file"
write (u, "(A)")

u_phs = free_unit ()
open (u_phs, file = "integrations_3.phs", &
      status = "replace", action = "write")
call write_test_phs_file (u_phs, var_str ("prc_config_a_i1"))
close (u_phs)

call global%set_string (var_str ("phs_file"),&
      var_str ("integrations_3.phs"), is_known = .true.)

call global%it_list%init ([1], [1000])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%write (u, vars = [ &
      var_str ("phs_method"), &
      var_str ("phs_file")])

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_3"

end subroutine integrations_3

```

VAMP integration

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the single-channel (`phs_single`) phase-space implementation. The integration method is `vamp`.

```

<Integrations: execute tests>+≡
  call test (integrations_4, "integrations_4", &
    "VAMP integration (one iteration)", &
    u, results)

<Integrations: test declarations>+≡
  public :: integrations_4

<Integrations: tests>+≡
  subroutine integrations_4 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname

```

```

type(rt_data_t), target :: global

write (u, "(A)")  "* Test output: integrations_4"
write (u, "(A)")  "* Purpose: integrate test process using VAMP"
write (u, "(A)")

write (u, "(A)")  "* Initialize process and parameters"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()

libname = "integrations_4_lib"
procname = "integrations_4"

call prepare_test_library (global, libname, 1, [procname])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = [var_str ("integration_method")], &
    pacify = .true.)

```



```

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_4"

end subroutine integrations_4

```

Multiple iterations integration

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the single-channel (`phs_single`) phase-space implementation. The integration method is `vamp`. We launch three iterations.

```

<Integrations: execute tests>+≡
  call test (integrations_5, "integrations_5", &
    "VAMP integration (three iterations)", &
    u, results)

<Integrations: test declarations>+≡
  public :: integrations_5

<Integrations: tests>+≡
  subroutine integrations_5 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global

    write (u, "(A)")  "* Test output: integrations_5"
    write (u, "(A)")  "* Purpose: integrate test process using VAMP"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process and parameters"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()

    libname = "integrations_5_lib"
    procname = "integrations_5"

    call prepare_test_library (global, libname, 1, [procname])
    call compile_library (libname, global)

    call global%append_log (&
      var_str ("?rebuild_grids"), .true., intrinsic = .true.)

    call global%set_string (var_str ("$_run_id"), &
      var_str ("r1"), is_known = .true.)
    call global%set_string (var_str ("$_method"), &

```

```

        var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("integration_method"),&
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"),&
    .false., is_known = .true.)
call global%set_log (var_str ("?vis_history"),&
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"),&
    1000._default, is_known = .true.)

call global%it_list%init ([3], [1000])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = [var_str ("integration_method")], &
    pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_5"

end subroutine integrations_5

```

Multiple passes integration

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the single-channel (`phs_single`) phase-space implementation. The integration method is `vamp`. We launch three passes with three iterations each.

```

<Integrations: execute tests>+≡
    call test (integrations_6, "integrations_6", &
        "VAMP integration (three passes)", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_6

```

```

<Integrations: tests>+=
subroutine integrations_6 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname
  type(rt_data_t), target :: global
  type(string_t), dimension(0) :: no_vars

  write (u, "(A)")  "* Test output: integrations_6"
  write (u, "(A)")  "* Purpose: integrate test process using VAMP"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize process and parameters"
  write (u, "(A)")

  call syntax_model_file_init ()

  call global%global_init ()

  libname = "integrations_6_lib"
  procname = "integrations_6"

  call prepare_test_library (global, libname, 1, [procname])
  call compile_library (libname, global)

  call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)

  call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
  call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
  call global%set_string (var_str ("$_phs_method"), &
    var_str ("single"), is_known = .true.)
  call global%set_string (var_str ("$_integration_method"), &
    var_str ("vamp"), is_known = .true.)
  call global%set_log (var_str ("?use_vamp_equivalences"), &
    .false., is_known = .true.)
  call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
  call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
  call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

  call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

  call global%it_list%init ([3, 3, 3], [1000, 1000, 1000], &
    adapt = [.true., .true., .false.], &
    adapt_code = [var_str ("wg"), var_str ("g"), var_str ("")])

  write (u, "(A)")  "* Integrate"
  write (u, "(A)")

```

```

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = no_vars, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_6"

end subroutine integrations_6

```

VAMP and default phase space

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the default (`phs_wood`) phase-space implementation. The integration method is `vamp`. We launch three passes with three iterations each. We enable channel equivalences and groves.

```

<Integrations: execute tests>+≡
  call test (integrations_7, "integrations_7", &
    "VAMP integration with wood phase space", &
    u, results)

<Integrations: test declarations>+≡
  public :: integrations_7

<Integrations: tests>+≡
  subroutine integrations_7 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global
    type(string_t), dimension(0) :: no_vars
    integer :: iostat, u_phs
    character(95) :: buffer
    type(string_t) :: phs_file
    logical :: exist

    write (u, "(A)")  "* Test output: integrations_7"
    write (u, "(A)")  "* Purpose: integrate test process using VAMP"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process and parameters"
    write (u, "(A)")

    call syntax_model_file_init ()
    call syntax_phs_forest_init ()

    call global%global_init ()

```

```

libname = "integrations_7_lib"
procname = "integrations_7"

call prepare_test_library (global, libname, 1, [procname])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?phs_s_mapping"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([3, 3, 3], [1000, 1000, 1000], &
    adapt = [.true., .true., .false.], &
    adapt_code = [var_str ("wg"), var_str ("g"), var_str ("")])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = no_vars, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

```

```

write (u, "(A)")
write (u, "(A)")  "* Generated phase-space file"
write (u, "(A)")

phs_file = procname // ".r1.i1.phs"
inquire (file = char (phs_file), exist = exist)
if (exist) then
  u_phs = free_unit ()
  open (u_phs, file = char (phs_file), action = "read", status = "old")
  iostat = 0
  do while (iostat == 0)
    read (u_phs, "(A)", iostat = iostat)  buffer
    if (iostat == 0) write (u, "(A)")  trim (buffer)
  end do
  close (u_phs)
else
  write (u, "(A)")  "[file is missing]"
end if

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_7"

end subroutine integrations_7

```

Structure functions

Compile and integrate an intrinsic test matrix element (`prc_test` type) using the default (`phs_wood`) phase-space implementation. The integration method is `vamp`. There is a structure function of type `unit_test`.

We use a test structure function $f(x) = x$ for both beams. Together with the $1/x_1 x_2$ factor from the phase-space flux and a unit matrix element, we should get the same result as previously for the process without structure functions. There is a slight correction due to the m_s mass which we set to zero here.

```

<Integrations: execute tests>+≡
  call test (integrations_8, "integrations_8", &
    "integration with structure function", &
    u, results)

<Integrations: test declarations>+≡
  public :: integrations_8

<Integrations: tests>+≡
  subroutine integrations_8 (u)
    <Use kinds>
    <Use strings>
    use interactions, only: reset_interaction_counter
    use phs_forests
    use models
    use rt_data
    use process_configurations_ut, only: prepare_test_library
    use compilations, only: compile_library
    use integrations

```

```

implicit none

integer, intent(in) :: u
type(string_t) :: libname, procname
type(rt_data_t), target :: global
type(flavor_t) :: flv
type(string_t) :: name

write (u, "(A)")  "* Test output: integrations_8"
write (u, "(A)")  "* Purpose: integrate test process using VAMP &
    &with structure function"
write (u, "(A)")

write (u, "(A)")  "* Initialize process and parameters"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_phs_forest_init ()

call global%global_init ()

libname = "integrations_8_lib"
procname = "integrations_8"

call prepare_test_library (global, libname, 1, [procname])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?phs_s_mapping"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), 0._default)

```

```

call reset_interaction_counter ()

call flv%init (25, global%model)

name = flv%get_name ()
call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call global%it_list%init ([1], [1000])
call integrate_process (procname, global, local_stack=.true.)

call global%write (u, vars = [var_str ("ms")])

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_8"

end subroutine integrations_8

```

Integration with sign change

Compile and integrate an intrinsic test matrix element (`prc_test` type). The phase-space implementation is `phs_single` (single-particle phase space), the integrator is `mci_midpoint`. The weight that is applied changes the sign in half of phase space. The weight is -3 and 1 , respectively, so the total result is equal to the original, but negative sign.

The efficiency should (approximately) become the average of 1 and $1/3$, that is $2/3$.

```

<Integrations: execute tests>+≡
  call test (integrations_9, "integrations_9", &
    "handle sign change", &
    u, results)

<Integrations: test declarations>+≡
  public :: integrations_9

<Integrations: tests>+≡
  subroutine integrations_9 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname
    type(rt_data_t), target :: global

    type(string_t) :: wgt_expr_text

```



```

type(ifile_t) :: ifile
type(stream_t) :: stream
type(parse_tree_t) :: parse_tree

write (u, "(A)")  "* Test output: integrations_9"
write (u, "(A)")  "* Purpose: integrate test process"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()

write (u, "(A)")  "* Prepare a weight expression"
write (u, "(A)")

call syntax_pexpr_init ()
wgt_expr_text = "eval 2 * sgn (Pz) - 1 [s]"
call ifile_append (ifile, wgt_expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (parse_tree, stream, .true.)
global%pn%weight_expr => parse_tree%get_root_ptr ()

write (u, "(A)")  "* Build and evaluate a test process"
write (u, "(A)")

libname = "integration_9"
procname = "prc_config_a"

call prepare_test_library (global, libname, 1)
call compile_library (libname, global)

call global%set_string (var_str ("$_run_id"), &
    var_str ("integrations1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true.)

```

```

call global%write (u, vars = [ &
    var_str ("method"), &
    var_str ("sqrts"), &
    var_str ("integration_method"), &
    var_str ("phs_method"), &
    var_str ("run_id")])

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_9"

end subroutine integrations_9

```

Integration history for VAMP integration with default phase space

This test is only run when event analysis can be done.

```

<Integrations: execute history tests>≡
    call test (integrations_history_1, "integrations_history_1", &
        "Test integration history files", &
        u, results)

<Integrations: test declarations>+≡
    public :: integrations_history_1

<Integrations: tests>+≡
    subroutine integrations_history_1 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname
        type(rt_data_t), target :: global
        type(string_t), dimension(0) :: no_vars
        integer :: iostat, u_his
        character(91) :: buffer
        type(string_t) :: his_file, ps_file, pdf_file
        logical :: exist, exist_ps, exist_pdf

        write (u, "(A)")  "* Test output: integrations_history_1"
        write (u, "(A)")  "* Purpose: test integration history files"
        write (u, "(A)")

        write (u, "(A)")  "* Initialize process and parameters"
        write (u, "(A)")

        call syntax_model_file_init ()
        call syntax_phs_forest_init ()

        call global%global_init ()

        libname = "integrations_history_1_lib"
        procname = "integrations_history_1"

        call global%set_log (var_str ("?vis_history"), &
            .true., is_known = .true.)

```

```

call global%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)
call global%set_log (var_str ("?phs_s_mapping"),&
    .false., is_known = .true.)

call prepare_test_library (global, libname, 1, [procname])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$_phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$_integration_method"),&
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"),&
    .true., is_known = .true.)
call global%set_real (var_str ("error_threshold"),&
    5E-6_default, is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known=.true.)

call global%set_real (var_str ("sqrts"),&
    1000._default, is_known = .true.)

call global%it_list%init ([2, 2, 2], [1000, 1000, 1000], &
    adapt = [.true., .true., .false.], &
    adapt_code = [var_str ("wg"), var_str ("g"), var_str ("")])

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call reset_interaction_counter ()
call integrate_process (procname, global, local_stack=.true., &
    eff_reset = .true.)

call global%pacify (efficiency_reset = .true., error_reset = .true.)
call global%write (u, vars = no_vars, pacify = .true.)

write (u, "(A)")
write (u, "(A)")  "* Generated history files"
write (u, "(A)")

his_file = procname // ".r1.history.tex"
ps_file  = procname // ".r1.history.ps"
pdf_file = procname // ".r1.history.pdf"
inquire (file = char (his_file), exist = exist)
if (exist) then

```

```

u_his = free_unit ()
open (u_his, file = char (his_file), action = "read", status = "old")
iostat = 0
do while (iostat == 0)
    read (u_his, "(A)", iostat = iostat)  buffer
    if (iostat == 0) write (u, "(A)") trim (buffer)
end do
close (u_his)
else
    write (u, "(A)") "[History LaTeX file is missing]"
end if
inquire (file = char (ps_file), exist = exist_ps)
if (exist_ps) then
    write (u, "(A)") "[History Postscript file exists and is nonempty]"
else
    write (u, "(A)") "[History Postscript file is missing/non-regular]"
end if
inquire (file = char (pdf_file), exist = exist_pdf)
if (exist_pdf) then
    write (u, "(A)") "[History PDF file exists and is nonempty]"
else
    write (u, "(A)") "[History PDF file is missing/non-regular]"
end if

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: integrations_history_1"

end subroutine integrations_history_1

```

33.7 Event Streams

This module manages I/O from/to multiple concurrent event streams. Usually, there is at most one input stream, but several output streams. For the latter, we set up an array which can hold `eio_t` (event I/O) objects of different dynamic types simultaneously. One of them may be marked as an input channel.

```
(event_streams.f90)≡  
  <File header>  
  
  module event_streams  
  
    <Use strings>  
    use io_units  
    use diagnostics  
    use events  
    use event_handles, only: event_handle_t  
    use eio_data  
    use eio_base  
    use rt_data  
  
    use dispatch_transforms, only: dispatch_eio  
  
    <Standard module head>  
  
    <Event streams: public>  
  
    <Event streams: types>  
  
    contains  
  
    <Event streams: procedures>  
  
  end module event_streams
```

33.7.1 Event Stream Array

Each entry is an `eio_t` object. Since the type is dynamic, we need a wrapper:

```
<Event streams: types>≡  
  type :: event_stream_entry_t  
    class(eio_t), allocatable :: eio  
  end type event_stream_entry_t
```

An array of event-stream entry objects. If one of the entries is an input channel, `i_in` is the corresponding index.

```
<Event streams: public>≡  
  public :: event_stream_array_t  
  
<Event streams: types>+≡  
  type :: event_stream_array_t  
    type(event_stream_entry_t), dimension(:), allocatable :: entry  
    integer :: i_in = 0  
  contains  
    <Event streams: event stream array: TBP>
```

```
end type event_stream_array_t
```

Output.

```
<Event streams: event stream array: TBP>≡
  procedure :: write => event_stream_array_write

<Event streams: procedures>≡
  subroutine event_stream_array_write (object, unit)
    class(event_stream_array_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer :: u, i
    u = given_output_unit (unit)
    write (u, "(1x,A)") "Event stream array:"
    if (allocated (object%entry)) then
      select case (size (object%entry))
        case (0)
          write (u, "(3x,A)") "[empty]"
        case default
          do i = 1, size (object%entry)
            if (i == object%i_in) write (u, "(1x,A)") "Input stream:"
            call object%entry(i)%eio%write (u)
          end do
        end select
      else
        write (u, "(3x,A)") "[undefined]"
      end if
    end subroutine event_stream_array_write
```

Check if there is content.

```
<Event streams: event stream array: TBP>+≡
  procedure :: is_valid => event_stream_array_is_valid

<Event streams: procedures>+≡
  function event_stream_array_is_valid (es_array) result (flag)
    class(event_stream_array_t), intent(in) :: es_array
    logical :: flag

    flag = allocated (es_array%entry)

  end function event_stream_array_is_valid
```

Finalize all streams.

```
<Event streams: event stream array: TBP>+≡
  procedure :: final => event_stream_array_final

<Event streams: procedures>+≡
  subroutine event_stream_array_final (es_array)
    class(event_stream_array_t), intent(inout) :: es_array
    integer :: i
    if (allocated (es_array%entry)) then
      do i = 1, size (es_array%entry)
        call es_array%entry(i)%eio%final ()
      end do
    end if
  end subroutine event_stream_array_final
```

```
end subroutine event_stream_array_final
```

Initialization. We use a generic `sample` name, open event I/O objects for all provided stream types (using the `dispatch_eio` routine), and initialize for the given list of process pointers. If there is an `input` argument, this channel is initialized as an input channel and appended to the array.

The `input_data` or, if not present, `data` may be modified. This happens if we open a stream for reading and get new information there.

(Event streams: event stream array: TBP)+≡

```
procedure :: init => event_stream_array_init
```

(Event streams: procedures)+≡

```
subroutine event_stream_array_init &
  (es_array, sample, stream_fmt, global, &
   data, input, input_sample, input_data, allow_switch, &
   checkpoint, callback, &
   error)
  class(event_stream_array_t), intent(out) :: es_array
  type(string_t), intent(in) :: sample
  type(string_t), dimension(:), intent(in) :: stream_fmt
  type(rt_data_t), intent(in) :: global
  type(event_sample_data_t), intent(inout), optional :: data
  type(string_t), intent(in), optional :: input
  type(string_t), intent(in), optional :: input_sample
  type(event_sample_data_t), intent(inout), optional :: input_data
  logical, intent(in), optional :: allow_switch
  integer, intent(in), optional :: checkpoint
  integer, intent(in), optional :: callback
  logical, intent(out), optional :: error
  type(string_t) :: sample_in
  integer :: n, i, n_output, i_input, i_checkpoint, i_callback
  logical :: success, switch
  if (present (input_sample)) then
    sample_in = input_sample
  else
    sample_in = sample
  end if
  if (present (allow_switch)) then
    switch = allow_switch
  else
    switch = .true.
  end if
  if (present (error)) then
    error = .false.
  end if
  n = size (stream_fmt)
  n_output = n
  if (present (input)) then
    n = n + 1
    i_input = n
  else
    i_input = 0
  end if
  if (present (checkpoint)) then
```

```

        n = n + 1
        i_checkpoint = n
    else
        i_checkpoint = 0
    end if
    if (present (callback)) then
        n = n + 1
        i_callback = n
    else
        i_callback = 0
    end if
    allocate (es_array%entry (n))
    if (i_checkpoint > 0) then
        call dispatch_eio &
            (es_array%entry(i_checkpoint)%eio, var_str ("checkpoint"), &
             global%var_list, global%fallback_model, &
             global%event_callback)
        call es_array%entry(i_checkpoint)%eio%init_out (sample, data)
    end if
    if (i_callback > 0) then
        call dispatch_eio &
            (es_array%entry(i_callback)%eio, var_str ("callback"), &
             global%var_list, global%fallback_model, &
             global%event_callback)
        call es_array%entry(i_callback)%eio%init_out (sample, data)
    end if
    if (i_input > 0) then
        call dispatch_eio (es_array%entry(i_input)%eio, input, &
            global%var_list, global%fallback_model, &
            global%event_callback)
        if (present (input_data)) then
            call es_array%entry(i_input)%eio%init_in &
                (sample_in, input_data, success)
        else
            call es_array%entry(i_input)%eio%init_in &
                (sample_in, data, success)
        end if
        if (success) then
            es_array%i_in = i_input
        else if (present (input_sample)) then
            if (present (error)) then
                error = .true.
            else
                call msg_fatal ("Events: &
                    &parameter mismatch in input, aborting")
            end if
        else
            call msg_message ("Events: &
                &parameter mismatch, discarding old event set")
            call es_array%entry(i_input)%eio%final ()
            if (switch) then
                call msg_message ("Events: generating new events")
                call es_array%entry(i_input)%eio%init_out (sample, data)
            end if
        end if
    end if

```



```

        end if
    end if
    do i = 1, n_output
        call dispatch_eio (es_array%entry(i)%eio, stream_fmt(i), &
            global%var_list, global%fallback_model, &
            global%event_callback)
        call es_array%entry(i)%eio%init_out (sample, data)
    end do
end subroutine event_stream_array_init

```

Switch the (only) input channel to an output channel, so further events are appended to the respective stream.

```

(Event streams: event stream array: TBP)+≡
    procedure :: switch_inout => event_stream_array_switch_inout

(Event streams: procedures)+≡
    subroutine event_stream_array_switch_inout (es_array)
        class(event_stream_array_t), intent(inout) :: es_array
        integer :: n
        if (es_array%has_input ()) then
            n = es_array%i_in
            call es_array%entry(n)%eio%switch_inout ()
            es_array%i_in = 0
        else
            call msg_bug ("Reading events: switch_inout: no input stream selected")
        end if
    end subroutine event_stream_array_switch_inout

```

Output an event (with given process number) to all output streams. If there is no output stream, do nothing.

```

(Event streams: event stream array: TBP)+≡
    procedure :: output => event_stream_array_output

(Event streams: procedures)+≡
    subroutine event_stream_array_output &
        (es_array, event, i_prc, event_index, passed, pacify, event_handle)
        class(event_stream_array_t), intent(inout) :: es_array
        type(event_t), intent(in), target :: event
        integer, intent(in) :: i_prc, event_index
        logical, intent(in), optional :: passed, pacify
        class(event_handle_t), intent(inout), optional :: event_handle
        logical :: increased
        integer :: i
        do i = 1, size (es_array%entry)
            if (i /= es_array%i_in) then
                associate (eio => es_array%entry(i)%eio)
                    if (eio%split) then
                        if (eio%split_n_evt > 0 .and. event_index > 1) then
                            if (mod (event_index, eio%split_n_evt) == 1) then
                                call eio%split_out ()
                            end if
                        else if (eio%split_n_kbytes > 0) then
                            call eio%update_split_count (increased)
                            if (increased) call eio%split_out ()
                        end if
                    end associate
                end if
            end if
        end do
    end subroutine event_stream_array_output

```

```

        end if
    end if
    call eio%output (event, i_prc, reading = es_array%i_in /= 0, &
        passed = passed, &
        pacify = pacify, &
        event_handle = event_handle)
    end associate
end if
end do
end subroutine event_stream_array_output

```

Input the `i_prc` index which selects the process for the current event. This is separated from reading the event, because it determines which event record to read. `iostat` may indicate an error or an EOF condition, as usual.

```

<Event streams: event stream array: TBP>+≡
    procedure :: input_i_prc => event_stream_array_input_i_prc

<Event streams: procedures>+≡
    subroutine event_stream_array_input_i_prc (es_array, i_prc, iostat)
        class(event_stream_array_t), intent(inout) :: es_array
        integer, intent(out) :: i_prc
        integer, intent(out) :: iostat
        integer :: n
        if (es_array%has_input ()) then
            n = es_array%i_in
            call es_array%entry(n)%eio%input_i_prc (i_prc, iostat)
        else
            call msg_fatal ("Reading events: no input stream selected")
        end if
    end subroutine event_stream_array_input_i_prc

```

Input an event from the selected input stream. `iostat` may indicate an error or an EOF condition, as usual.

```

<Event streams: event stream array: TBP>+≡
    procedure :: input_event => event_stream_array_input_event

<Event streams: procedures>+≡
    subroutine event_stream_array_input_event &
        (es_array, event, iostat, event_handle)
        class(event_stream_array_t), intent(inout) :: es_array
        type(event_t), intent(inout), target :: event
        integer, intent(out) :: iostat
        class(event_handle_t), intent(inout), optional :: event_handle
        integer :: n
        if (es_array%has_input ()) then
            n = es_array%i_in
            call es_array%entry(n)%eio%input_event (event, iostat, event_handle)
        else
            call msg_fatal ("Reading events: no input stream selected")
        end if
    end subroutine event_stream_array_input_event

```

Skip an entry of `eio_t`. Used to synchronize the event read-in for NLO events.

```

(Event streams: event stream array: TBP)+≡
  procedure :: skip_eio_entry => event_stream_array_skip_eio_entry

(Event streams: procedures)+≡
  subroutine event_stream_array_skip_eio_entry (es_array, iostat)
    class(event_stream_array_t), intent(inout) :: es_array
    integer, intent(out) :: iostat
    integer :: n
    if (es_array%has_input ()) then
      n = es_array%i_in
      call es_array%entry(n)%eio%skip (iostat)
    else
      call msg_fatal ("Reading events: no input stream selected")
    end if
  end subroutine event_stream_array_skip_eio_entry

```

Return true if there is an input channel among the event streams.

```

(Event streams: event stream array: TBP)+≡
  procedure :: has_input => event_stream_array_has_input

(Event streams: procedures)+≡
  function event_stream_array_has_input (es_array) result (flag)
    class(event_stream_array_t), intent(in) :: es_array
    logical :: flag
    flag = es_array%i_in /= 0
  end function event_stream_array_has_input

```

33.7.2 Unit Tests

Test module, followed by the stand-alone unit-test procedures.

```

(event_streams_ut.f90)≡
  <File header>

  module event_streams_ut
    use unit_tests
    use event_streams_util

    <Standard module head>

    <Event streams: public test>

    contains

    <Event streams: test driver>

  end module event_streams_ut

(event_streams_util.f90)≡
  <File header>

  module event_streams_util

```

```

<Use kinds>
<Use strings>
    use model_data
    use eio_data
    use process, only: process_t
    use instances, only: process_instance_t
    use models
    use rt_data
    use events

    use event_streams

<Standard module head>

<Event streams: test declarations>

contains

<Event streams: tests>

end module event_streams_util

```

API: driver for the unit tests below.

```

<Event streams: public test>≡
    public :: event_streams_test

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

```

Empty event stream

This should set up an empty event output stream array, including initialization, output, and finalization (which are all no-ops).

```

<Event streams: execute tests>≡
    call test (event_streams_1, "event_streams_1", &
        "empty event stream array", &
        u, results)

<Event streams: test declarations>≡
    public :: event_streams_1

<Event streams: tests>≡
    subroutine event_streams_1 (u)
        integer, intent(in) :: u
        type(event_stream_array_t) :: es_array
        type(rt_data_t) :: global
        type(event_t) :: event
        type(string_t) :: sample
        type(string_t), dimension(0) :: empty_string_array

```

```

write (u, "(A)")  "* Test output: event_streams_1"
write (u, "(A)")  "* Purpose: handle empty event stream array"
write (u, "(A)")

sample = "event_streams_1"

call es_array%init (sample, empty_string_array, global)
call es_array%output (event, 42, 1)
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: event_streams_1"

end subroutine event_streams_1

```

Nontrivial event stream

Here we generate a trivial event and choose raw output as an entry in the stream array.

```

<Event streams: execute tests>+≡
  call test (event_streams_2, "event_streams_2", &
    "nontrivial event stream array", &
    u, results)

<Event streams: test declarations>+≡
  public :: event_streams_2

<Event streams: tests>+≡
  subroutine event_streams_2 (u)
    use processes_ut, only: prepare_test_process
    integer, intent(in) :: u
    type(event_stream_array_t) :: es_array
    type(rt_data_t) :: global
    type(model_data_t), target :: model
    type(event_t), allocatable, target :: event
    type(process_t), allocatable, target :: process
    type(process_instance_t), allocatable, target :: process_instance
    type(string_t) :: sample
    type(string_t), dimension(0) :: empty_string_array
    integer :: i_prc, iostat

    write (u, "(A)")  "* Test output: event_streams_2"
    write (u, "(A)")  "* Purpose: handle empty event stream array"
    write (u, "(A)")

    call syntax_model_file_init ()
    call global%global_init ()
    call global%init_fallback_model &
      (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

    call model%init_test ()

```

```

write (u, "(A)")  "* Generate test process event"
write (u, "(A)")

allocate (process)
allocate (process_instance)
call prepare_test_process (process, process_instance, model, &
    run_id = var_str ("run_test"))
call process_instance%setup_event_data ()

allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())
call event%generate (1, [0.4_default, 0.4_default])
call event%set_index (42)
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Allocate raw eio stream and write event to file"
write (u, "(A)")

sample = "event_streams_2"

call es_array%init (sample, [var_str ("raw")], global)
call es_array%output (event, 1, 1)
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)")  "* Reallocate raw eio stream for reading"
write (u, "(A)")

sample = "foo"
call es_array%init (sample, empty_string_array, global, &
    input = var_str ("raw"), input_sample = var_str ("event_streams_2"))
call es_array%write (u)

write (u, "(A)")
write (u, "(A)")  "* Reread event"
write (u, "(A)")

call es_array%input_i_prc (i_prc, iostat)

write (u, "(1x,A,I0)")  "i_prc = ", i_prc
write (u, "(A)")
call es_array%input_event (event, iostat)
call es_array%final ()

call event%write (u)

call global%final ()

call model%final ()

```

```

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: event_streams_2"

end subroutine event_streams_2

```

Switch in/out

Here we generate an event file and test switching from writing to reading when the file is exhausted.

```

<Event streams: execute tests>+≡
call test (event_streams_3, "event_streams_3", &
  "switch input/output", &
  u, results)

<Event streams: test declarations>+≡
public :: event_streams_3

<Event streams: tests>+≡
subroutine event_streams_3 (u)
  use processes_ut, only: prepare_test_process
  integer, intent(in) :: u
  type(event_stream_array_t) :: es_array
  type(rt_data_t) :: global
  type(model_data_t), target :: model
  type(event_t), allocatable, target :: event
  type(process_t), allocatable, target :: process
  type(process_instance_t), allocatable, target :: process_instance
  type(string_t) :: sample
  type(string_t), dimension(0) :: empty_string_array
  integer :: i_prc, iostat

  write (u, "(A)")  "* Test output: event_streams_3"
  write (u, "(A)")  "* Purpose: handle in/out switching"
  write (u, "(A)")

  call syntax_model_file_init ()
  call global%global_init ()
  call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

  call model%init_test ()

  write (u, "(A)")  "* Generate test process event"
  write (u, "(A)")

  allocate (process)
  allocate (process_instance)
  call prepare_test_process (process, process_instance, model, &
    run_id = var_str ("run_test"))
  call process_instance%setup_event_data ()

```

```

allocate (event)
call event%basic_init ()
call event%connect (process_instance, process%get_model_ptr ())
call event%generate (1, [0.4_default, 0.4_default])
call event%increment_index ()
call event%evaluate_expressions ()

write (u, "(A)") "* Allocate raw eio stream and write event to file"
write (u, "(A)")

sample = "event_streams_3"

call es_array%init (sample, [var_str ("raw")], global)
call es_array%output (event, 1, 1)
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)") "* Reallocate raw eio stream for reading"
write (u, "(A)")

call es_array%init (sample, empty_string_array, global, &
    input = var_str ("raw"))
call es_array%write (u)

write (u, "(A)")
write (u, "(A)") "* Reread event"
write (u, "(A)")

call es_array%input_i_prc (i_prc, iostat)
call es_array%input_event (event, iostat)

write (u, "(A)") "* Attempt to read another event (fail), then generate"
write (u, "(A)")

call es_array%input_i_prc (i_prc, iostat)
if (iostat < 0) then
    call es_array%switch_inout ()
    call event%generate (1, [0.3_default, 0.3_default])
    call event%increment_index ()
    call event%evaluate_expressions ()
    call es_array%output (event, 1, 2)
end if
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
call event%write (u)

write (u, "(A)")
write (u, "(A)") "* Reallocate raw eio stream for reading"
write (u, "(A)")

call es_array%init (sample, empty_string_array, global, &

```



```

        input = var_str ("raw"))
    call es_array%write (u)

    write (u, "(A)")
    write (u, "(A)") "* Reread two events and display 2nd event"
    write (u, "(A)")

    call es_array%input_i_prc (i_prc, iostat)
    call es_array%input_event (event, iostat)
    call es_array%input_i_prc (i_prc, iostat)

    call es_array%input_event (event, iostat)
    call es_array%final ()

    call event%write (u)

    call global%final ()

    call model%final ()
    call syntax_model_file_final ()

    write (u, "(A)")
    write (u, "(A)") "* Test output end: event_streams_3"

end subroutine event_streams_3

```

Checksum

Here we generate an event file and repeat twice, once with identical parameters and once with modified parameters.

```

<Event streams: execute tests>+≡
    call test (event_streams_4, "event_streams_4", &
        "check MD5 sum", &
        u, results)

<Event streams: test declarations>+≡
    public :: event_streams_4

<Event streams: tests>+≡
    subroutine event_streams_4 (u)
        integer, intent(in) :: u
        type(event_stream_array_t) :: es_array
        type(rt_data_t) :: global
        type(process_t), allocatable, target :: process
        type(string_t) :: sample
        type(string_t), dimension(0) :: empty_string_array
        type(event_sample_data_t) :: data

        write (u, "(A)") "* Test output: event_streams_4"
        write (u, "(A)") "* Purpose: handle in/out switching"
        write (u, "(A)")

        write (u, "(A)") "* Generate test process event"
    end subroutine event_streams_4

```

```

write (u, "(A)")

call syntax_model_file_init ()
call global%global_init ()
call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%set_log (var_str ("?check_event_file"), &
    .true., is_known = .true.)

allocate (process)

write (u, "(A)") "* Allocate raw eio stream for writing"
write (u, "(A)")

sample = "event_streams_4"
data%md5sum_cfg = "1234567890abcdef1234567890abcdef"

call es_array%init (sample, [var_str ("raw")], global, data)
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)") "* Reallocate raw eio stream for reading"
write (u, "(A)")

call es_array%init (sample, empty_string_array, global, &
    data, input = var_str ("raw"))
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)") "* Reallocate modified raw eio stream for reading (fail)"
write (u, "(A)")

data%md5sum_cfg = "1234567890_____1234567890_____"
call es_array%init (sample, empty_string_array, global, &
    data, input = var_str ("raw"))
call es_array%write (u)
call es_array%final ()

write (u, "(A)")
write (u, "(A)") "* Repeat ignoring checksum"
write (u, "(A)")

call global%set_log (var_str ("?check_event_file"), &
    .false., is_known = .true.)
call es_array%init (sample, empty_string_array, global, &
    data, input = var_str ("raw"))
call es_array%write (u)
call es_array%final ()

call global%final ()
call syntax_model_file_final ()

```

```
write (u, "(A)")  
write (u, "(A)")  "* Test output end: event_streams_4"  
  
end subroutine event_streams_4
```

33.8 Restricted Subprocesses

This module provides an automatic means to construct restricted subprocesses of a current process object. A restricted subprocess has the same initial and final state as the current process, but a restricted set of Feynman graphs.

The actual application extracts the set of resonance histories that apply to the process and uses this to construct subprocesses that are restricted to one of those histories, respectively. The resonance histories are derived from the phase-space setup. This implies that the method is tied to the OMega matrix element generator and to the wood phase space method.

The processes are collected in a new process library that is generated on-the-fly.

The `resonant_subprocess_t` object is intended as a component of the event record, which manages all operations regarding resonance handling.

The run-time calculations are delegated to an event transform (`evt_resonance_t`), as a part of the event transform chain. The transform selects one (or none) of the resonance histories, given the momentum configuration, computes matrix elements and inserts resonances into the particle set.

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

```
module restricted_subprocesses
```

```
  <Use kinds>
```

```
  <Use strings>
```

```
  use diagnostics, only: msg_message, msg_fatal, msg_bug  
  use diagnostics, only: signal_is_pending  
  use io_units, only: given_output_unit  
  use format_defs, only: FMT_14, FMT_19  
  use string_utils, only: str  
  use lorentz, only: vector4_t  
  use particle_specifiers, only: prt_spec_t  
  use particles, only: particle_set_t  
  use resonances, only: resonance_history_t, resonance_history_set_t  
  use variables, only: var_list_t  
  use models, only: model_t  
  use process_libraries, only: process_component_def_t  
  use process_libraries, only: process_library_t  
  use process_libraries, only: STAT_ACTIVE  
  use prclib_stacks, only: prclib_entry_t  
  use event_transforms, only: evt_t  
  use resonance_insertion, only: evt_resonance_t  
  use rt_data, only: rt_data_t  
  use compilations, only: compile_library  
  use process_configurations, only: process_configuration_t  
  use process, only: process_t, process_ptr_t  
  use instances, only: process_instance_t, process_instance_ptr_t  
  use integrations, only: integrate_process
```

```
  <Use mpi f08>
```

```
  <Standard module head>
```

```

    <Restricted subprocesses: public>

    <Restricted subprocesses: types>

    <Restricted subprocesses: interfaces>

contains

    <Restricted subprocesses: procedures>

end module restricted_subprocesses

```

33.8.1 Process configuration

We extend the `process_configuration_t` by another method for initialization that takes into account a resonance history.

```

<Restricted subprocesses: public>≡
    public :: restricted_process_configuration_t

<Restricted subprocesses: types>≡
    type, extends (process_configuration_t) :: restricted_process_configuration_t
    private
    contains
    <Restricted subprocesses: restricted process configuration: TBP>
end type restricted_process_configuration_t

```

Resonance history as an argument. We use it to override the `restrictions` setting in a local variable list. Since we can construct the restricted process only by using OMega, we enforce it as the ME method. Other settings are taken from the variable list. The model will most likely be set, but we insert a safeguard just in case.

Also, the resonant subprocess should not itself spawn resonant subprocesses, so we unset `?resonance_history`.

We have to create a local copy of the model here, via pointer allocation. The reason is that the model as stored (via pointer) in the base type will be finalized and deallocated.

The current implementation will generate a LO process, the optional `nlo_process` is unset. (It is not obvious whether the construction makes sense beyond LO.)

```

<Restricted subprocesses: restricted process configuration: TBP>≡
    procedure :: init_resonant_process

<Restricted subprocesses: procedures>≡
    subroutine init_resonant_process &
        (prc_config, prc_name, prt_in, prt_out, res_history, model, var_list)
    class(restricted_process_configuration_t), intent(out) :: prc_config
    type(string_t), intent(in) :: prc_name
    type(prt_spec_t), dimension(:), intent(in) :: prt_in
    type(prt_spec_t), dimension(:), intent(in) :: prt_out
    type(resonance_history_t), intent(in) :: res_history
    type(model_t), intent(in), target :: model
    type(var_list_t), intent(in), target :: var_list
    type(model_t), pointer :: local_model

```

```

type(var_list_t) :: local_var_list
allocate (local_model)
call local_model%init_instance (model)
call local_var_list%link (var_list)
call local_var_list%append_string (var_str ("model_name"), &
    sval = local_model%get_name (), &
    intrinsic=.true.)
call local_var_list%append_string (var_str ("method"), &
    sval = var_str ("omega"), &
    intrinsic=.true.)
call local_var_list%append_string (var_str ("restrictions"), &
    sval = res_history%as_omega_string (size (prt_in)), &
    intrinsic = .true.)
call local_var_list%append_log (var_str ("?resonance_history"), &
    lval = .false., &
    intrinsic = .true.)
call prc_config%init (prc_name, size (prt_in), 1, &
    local_model, local_var_list)
call prc_config%setup_component (1, &
    prt_in, prt_out, &
    local_model, local_var_list)
end subroutine init_resonant_process

```

33.8.2 Resonant-subprocess set manager

This data type enables generation of a library of resonant subprocesses for a given master process, and it allows for convenient access. The matrix elements from the subprocesses can be used as channel weights to activate a selector, which then returns a preferred channel via some random number generator.

```

<Restricted subprocesses: public>+≡
    public :: resonant_subprocess_set_t

<Restricted subprocesses: types>+≡
    type :: resonant_subprocess_set_t
    private
    integer, dimension(:), allocatable :: n_history
    type(resonance_history_set_t), dimension(:), allocatable :: res_history_set
    logical :: lib_active = .false.
    type(string_t) :: libname
    type(string_t), dimension(:), allocatable :: proc_id
    type(process_ptr_t), dimension(:), allocatable :: subprocess
    type(process_instance_ptr_t), dimension(:), allocatable :: instance
    logical :: filled = .false.
    type(evt_resonance_t), pointer :: evt => null ()
contains
    <Restricted subprocesses: resonant subprocess set: TBP>
end type resonant_subprocess_set_t

```

Output

```

<Restricted subprocesses: resonant subprocess set: TBP>≡
    procedure :: write => resonant_subprocess_set_write

```

<Restricted subprocesses: procedures>+≡

```

subroutine resonant_subprocess_set_write (prc_set, unit, testflag)
  class(resonant_subprocess_set_t), intent(in) :: prc_set
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  logical :: truncate
  integer :: u, i
  u = given_output_unit (unit)
  truncate = .false.; if (present (testflag)) truncate = testflag
  write (u, "(1x,A)") "Resonant subprocess set:"
  if (allocated (prc_set%n_history)) then
    if (any (prc_set%n_history > 0)) then
      do i = 1, size (prc_set%n_history)
        if (prc_set%n_history(i) > 0) then
          write (u, "(1x,A,I0)") "Component #", i
          call prc_set%res_history_set(i)%write (u, indent=1)
        end if
      end do
    end if
    if (prc_set%lib_active) then
      write (u, "(3x,A,A,A)") "Process library = ', &
        char (prc_set%libname), "' "
    else
      write (u, "(3x,A)") "Process library: [inactive]"
    end if
    if (associated (prc_set%evt)) then
      if (truncate) then
        write (u, "(3x,A,1x," // FMT_14 // ")") &
          "Process sqme =", prc_set%get_master_sqme ()
      else
        write (u, "(3x,A,1x," // FMT_19 // ")") &
          "Process sqme =", prc_set%get_master_sqme ()
      end if
    end if
    if (associated (prc_set%evt)) then
      write (u, "(3x,A)") "Event transform: associated"
      write (u, "(2x)", advance="no")
      call prc_set%evt%write_selector (u, testflag)
    else
      write (u, "(3x,A)") "Event transform: not associated"
    end if
  else
    write (u, "(2x,A)") "[empty]"
  end if
else
  write (u, "(3x,A)") "[not allocated]"
end if
end subroutine resonant_subprocess_set_write

```

33.8.3 Resonance history set

Initialize subprocess set with an array of pre-created resonance history sets.

Safeguard: if there are no resonances in the input, initialize the local set as

empty, but complete.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: init => resonant_subprocess_set_init
  procedure :: fill_resonances => resonant_subprocess_set_fill_resonances

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_init (prc_set, n_component)
    class(resonant_subprocess_set_t), intent(out) :: prc_set
    integer, intent(in) :: n_component
    allocate (prc_set%res_history_set (n_component))
    allocate (prc_set%n_history (n_component), source = 0)
  end subroutine resonant_subprocess_set_init

  subroutine resonant_subprocess_set_fill_resonances (prc_set, &
    res_history_set, i_component)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(resonance_history_set_t), intent(in) :: res_history_set
    integer, intent(in) :: i_component
    prc_set%n_history(i_component) = res_history_set%get_n_history ()
    if (prc_set%n_history(i_component) > 0) then
      prc_set%res_history_set(i_component) = res_history_set
    else
      call prc_set%res_history_set(i_component)%init (initial_size = 0)
      call prc_set%res_history_set(i_component)%freeze ()
    end if
  end subroutine resonant_subprocess_set_fill_resonances

```

Return the resonance history set.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: get_resonance_history_set &
    => resonant_subprocess_set_get_resonance_history_set

<Restricted subprocesses: procedures>+≡
  function resonant_subprocess_set_get_resonance_history_set (prc_set) &
    result (res_history_set)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    type(resonance_history_set_t), dimension(:), allocatable :: res_history_set
    res_history_set = prc_set%res_history_set
  end function resonant_subprocess_set_get_resonance_history_set

```

33.8.4 Library for the resonance history set

The recommended library name: append `_R` to the process name.

```

<Restricted subprocesses: public>+≡
  public :: get_libname_res

<Restricted subprocesses: procedures>+≡
  elemental function get_libname_res (proc_id) result (libname)
    type(string_t), intent(in) :: proc_id
    type(string_t) :: libname
    libname = proc_id // "_R"
  end function get_libname_res

```


Here we scan the global process library whether any processes require resonant subprocesses to be constructed. If yes, create process objects with phase space and construct the process libraries as usual. Then append the library names to the array.

The temporary integration objects should carry the `phs_only` flag. We set this in the local environment.

Once a process object with resonance histories (derived from phase space) has been created, we extract the resonance histories and use them, together with the process definition, to create the new library.

Finally, compile the library.

```

<Restricted subprocesses: public>+=
  public :: spawn_resonant_subprocess_libraries

<Restricted subprocesses: procedures>+=
  subroutine spawn_resonant_subprocess_libraries &
    (libname, local, global, libname_res)
    type(string_t), intent(in) :: libname
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), target :: global
    type(string_t), dimension(:), allocatable, intent(inout) :: libname_res
    type(process_library_t), pointer :: lib
    type(string_t), dimension(:), allocatable :: process_id_res
    type(process_t), pointer :: process
    type(resonance_history_set_t) :: res_history_set
    type(process_component_def_t), pointer :: process_component_def
    logical :: phs_only_saved, exist
    integer :: i_proc, i_component
    lib => global%prclib_stack%get_library_ptr (libname)
    call lib%get_process_id_req_resonant (process_id_res)
    if (size (process_id_res) > 0) then
      call msg_message ("Creating resonant-subprocess libraries &
        &for library '" // char (libname) // "'")
      libname_res = get_libname_res (process_id_res)
      phs_only_saved = local%var_list%get_lval (var_str ("?phs_only"))
      call local%var_list%set_log &
        (var_str ("?phs_only"), .true., is_known=.true.)
      do i_proc = 1, size (process_id_res)
        associate (proc_id => process_id_res (i_proc))
          call msg_message ("Process '" // char (proc_id) // "': &
            &constructing phase space for resonance structure")
          call integrate_process (proc_id, local, global)
          process => global%process_stack%get_process_ptr (proc_id)
          call create_library (libname_res(i_proc), global, exist)
          if (.not. exist) then
            do i_component = 1, process%get_n_components ()
              call process%extract_resonance_history_set &
                (res_history_set, i_component = i_component)
              process_component_def &
                => process%get_component_def_ptr (i_component)
              call add_to_library (libname_res(i_proc), &
                res_history_set, &
                process_component_def%get_prt_spec_in (), &
                process_component_def%get_prt_spec_out (), &
                global)
            end do
          end if
        end associate
      end do
    end if
  end subroutine

```

```

        end do
        call msg_message ("Process library '" &
            // char (libname_res(i_proc)) &
            // "': created")
        end if
        call global%update_prclib (lib)
    end associate
end do
call local%var_list%set_log &
    (var_str ("?phs_only"), phs_only_saved, is_known=.true.)
end if
end subroutine spawn_resonant_subprocess_libraries

```

This is another version of the library constructor, bound to a restricted-subprocess set object. Create the appropriate process library, add processes, and close the library.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
    procedure :: create_library => resonant_subprocess_set_create_library
    procedure :: add_to_library => resonant_subprocess_set_add_to_library
    procedure :: freeze_library => resonant_subprocess_set_freeze_library

<Restricted subprocesses: procedures>+≡
    subroutine resonant_subprocess_set_create_library (prc_set, &
        libname, global, exist)
        class(resonant_subprocess_set_t), intent(inout) :: prc_set
        type(string_t), intent(in) :: libname
        type(rt_data_t), intent(inout), target :: global
        logical, intent(out) :: exist
        prc_set%libname = libname
        call create_library (prc_set%libname, global, exist)
    end subroutine resonant_subprocess_set_create_library

    subroutine resonant_subprocess_set_add_to_library (prc_set, &
        i_component, prt_in, prt_out, global)
        class(resonant_subprocess_set_t), intent(inout) :: prc_set
        integer, intent(in) :: i_component
        type(prt_spec_t), dimension(:), intent(in) :: prt_in
        type(prt_spec_t), dimension(:), intent(in) :: prt_out
        type(rt_data_t), intent(inout), target :: global
        call add_to_library (prc_set%libname, &
            prc_set%res_history_set(i_component), &
            prt_in, prt_out, global)
    end subroutine resonant_subprocess_set_add_to_library

    subroutine resonant_subprocess_set_freeze_library (prc_set, global)
        class(resonant_subprocess_set_t), intent(inout) :: prc_set
        type(rt_data_t), intent(inout), target :: global
        type(prclib_entry_t), pointer :: lib_entry
        type(process_library_t), pointer :: lib
        lib => global%prclib_stack%get_library_ptr (prc_set%libname)
        call lib%get_process_id_list (prc_set%proc_id)
        prc_set%lib_active = .true.
    end subroutine resonant_subprocess_set_freeze_library

```

The common parts of the procedures above: (i) create a new process library or recover it, (ii) for each history, create a process configuration and record it.

(Restricted subprocesses: procedures)+≡

```

subroutine create_library (libname, global, exist)
  type(string_t), intent(in) :: libname
  type(rt_data_t), intent(inout), target :: global
  logical, intent(out) :: exist
  type(prclib_entry_t), pointer :: lib_entry
  type(process_library_t), pointer :: lib
  type(resonance_history_t) :: res_history
  type(string_t), dimension(:), allocatable :: proc_id
  type(restricted_process_configuration_t) :: prc_config
  integer :: i
  lib => global%prclib_stack%get_library_ptr (libname)
  exist = associated (lib)
  if (.not. exist) then
    call msg_message ("Creating library for resonant subprocesses '" &
      // char (libname) // "'")
    allocate (lib_entry)
    call lib_entry%init (libname)
    lib => lib_entry%process_library_t
    call global%add_prclib (lib_entry)
  else
    call msg_message ("Using library for resonant subprocesses '" &
      // char (libname) // "'")
    call global%update_prclib (lib)
  end if
end subroutine create_library

subroutine add_to_library (libname, res_history_set, prt_in, prt_out, global)
  type(string_t), intent(in) :: libname
  type(resonance_history_set_t), intent(in) :: res_history_set
  type(prt_spec_t), dimension(:), intent(in) :: prt_in
  type(prt_spec_t), dimension(:), intent(in) :: prt_out
  type(rt_data_t), intent(inout), target :: global
  type(prclib_entry_t), pointer :: lib_entry
  type(process_library_t), pointer :: lib
  type(resonance_history_t) :: res_history
  type(string_t), dimension(:), allocatable :: proc_id
  type(restricted_process_configuration_t) :: prc_config
  integer :: n0, i
  lib => global%prclib_stack%get_library_ptr (libname)
  if (associated (lib)) then
    n0 = lib%get_n_processes ()
    allocate (proc_id (res_history_set%get_n_history ()))
    do i = 1, size (proc_id)
      proc_id(i) = libname // str (n0 + i)
      res_history = res_history_set%get_history(i)
      call prc_config%init_resonant_process (proc_id(i), &
        prt_in, prt_out, &
        res_history, &
        global%model, global%var_list)
      call msg_message ("Resonant subprocess #" &
        // char (str(n0+i)) // ": " &

```

```

        // char (res_history%as_omega_string (size (prt_in))))
        call prc_config%record (global)
        if (signal_is_pending ()) return
    end do
else
    call msg_bug ("Adding subprocesses: library '" &
        // char (libname) // "' not found")
    end if
end subroutine add_to_library

```

Compile the generated library, required settings taken from the global data set.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
    procedure :: compile_library => resonant_subprocess_set_compile_library

<Restricted subprocesses: procedures>+≡
    subroutine resonant_subprocess_set_compile_library (prc_set, global)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        type(rt_data_t), intent(inout), target :: global
        type(process_library_t), pointer :: lib
        lib => global%prclib_stack%get_library_ptr (prc_set%libname)
        if (lib%get_status () < STAT_ACTIVE) then
            call compile_library (prc_set%libname, global)
        end if
    end subroutine resonant_subprocess_set_compile_library

```

Check if the library has been created / the process has been evaluated.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
    procedure :: is_active => resonant_subprocess_set_is_active

<Restricted subprocesses: procedures>+≡
    function resonant_subprocess_set_is_active (prc_set) result (flag)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        logical :: flag
        flag = prc_set%lib_active
    end function resonant_subprocess_set_is_active

```

Return number of generated process objects, library, and process IDs.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
    procedure :: get_n_process => resonant_subprocess_set_get_n_process
    procedure :: get_libname => resonant_subprocess_set_get_libname
    procedure :: get_proc_id => resonant_subprocess_set_get_proc_id

<Restricted subprocesses: procedures>+≡
    function resonant_subprocess_set_get_n_process (prc_set) result (n)
        class(resonant_subprocess_set_t), intent(in) :: prc_set
        integer :: n
        if (prc_set%lib_active) then
            n = size (prc_set%proc_id)
        else
            n = 0
        end if
    end function resonant_subprocess_set_get_n_process

```

```

function resonant_subprocess_set_get_libname (prc_set) result (libname)
  class(resonant_subprocess_set_t), intent(in) :: prc_set
  type(string_t) :: libname
  if (prc_set%lib_active) then
    libname = prc_set%libname
  else
    libname = ""
  end if
end function resonant_subprocess_set_get_libname

function resonant_subprocess_set_get_proc_id (prc_set, i) result (proc_id)
  class(resonant_subprocess_set_t), intent(in) :: prc_set
  integer, intent(in) :: i
  type(string_t) :: proc_id
  if (allocated (prc_set%proc_id)) then
    proc_id = prc_set%proc_id(i)
  else
    proc_id = ""
  end if
end function resonant_subprocess_set_get_proc_id

```

33.8.5 Process objects and instances

Prepare process objects for all entries in the resonant-subprocesses library. The process objects are appended to the global process stack. A local environment can be used where we place temporary variable settings that affect process-object generation. We initialize the processes, such that we can evaluate matrix elements, but we do not need to integrate them.

The internal procedure `prepare_process` is an abridged version of the procedure with this name in the `simulations` module.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: prepare_process_objects &
    => resonant_subprocess_set_prepare_process_objects

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_prepare_process_objects &
    (prc_set, local, global)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    type(rt_data_t), pointer :: current
    type(process_library_t), pointer :: lib
    type(string_t) :: phs_method_saved, integration_method_saved
    type(string_t) :: proc_id, libname_cur, libname_res
    integer :: i, n
    if (.not. prc_set%is_active ()) return
    if (present (global)) then
      current => global
    else
      current => local
    end if
    libname_cur = current%prclib%get_name ()
  end subroutine

```

```

libname_res = prc_set%get_libname ()
lib => current%prclib_stack%get_library_ptr (libname_res)
if (associated (lib)) call current%update_prclib (lib)
phs_method_saved = local%get_sval (var_str ("phs_method"))
integration_method_saved = local%get_sval (var_str ("integration_method"))
call local%set_string (var_str ("phs_method"), &
    var_str ("none"), is_known = .true.)
call local%set_string (var_str ("integration_method"), &
    var_str ("none"), is_known = .true.)
n = prc_set%get_n_process ()
allocate (prc_set%subprocess (n))
do i = 1, n
    proc_id = prc_set%get_proc_id (i)
    call prepare_process (prc_set%subprocess(i)%p, proc_id)
    if (signal_is_pending ()) return
end do
call local%set_string (var_str ("phs_method"), &
    phs_method_saved, is_known = .true.)
call local%set_string (var_str ("integration_method"), &
    integration_method_saved, is_known = .true.)
lib => current%prclib_stack%get_library_ptr (libname_cur)
if (associated (lib)) call current%update_prclib (lib)
contains
subroutine prepare_process (process, process_id)
    type(process_t), pointer, intent(out) :: process
    type(string_t), intent(in) :: process_id
    call msg_message ("Simulate: initializing resonant subprocess '" &
        // char (process_id) // "'")
    if (present (global)) then
        call integrate_process (process_id, local, global, &
            init_only = .true.)
    else
        call integrate_process (process_id, local, local_stack = .true., &
            init_only = .true.)
    end if
    process => current%process_stack%get_process_ptr (process_id)
    if (.not. associated (process)) then
        call msg_fatal ("Simulate: resonant subprocess '" &
            // char (process_id) // "' could not be initialized: aborting")
    end if
end subroutine prepare_process
end subroutine resonant_subprocess_set_prepare_process_objects

```

Workspace for the resonant subprocesses.

(Restricted subprocesses: resonant subprocess set: TBP)+≡

```

procedure :: prepare_process_instances &
    => resonant_subprocess_set_prepare_process_instances

```

(Restricted subprocesses: procedures)+≡

```

subroutine resonant_subprocess_set_prepare_process_instances (prc_set, global)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    type(rt_data_t), intent(in), target :: global
    integer :: i, n
    if (.not. prc_set%is_active ()) return

```

```

n = size (prc_set%subprocess)
allocate (prc_set%instance (n))
do i = 1, n
  allocate (prc_set%instance(i)%p)
  call prc_set%instance(i)%p%init (prc_set%subprocess(i)%p)
  call prc_set%instance(i)%p%setup_event_data (global%model)
end do
end subroutine resonant_subprocess_set_prepare_process_instances

```

33.8.6 Event transform connection

The idea is that the resonance-insertion event transform has been allocated somewhere (namely, in the standard event-transform chain), but we maintain a link such that we can inject matrix-element results event by event. The event transform holds a selector, to choose one of the resonance histories (or none), and it manages resonance insertion for the particle set.

The data that the event transform requires can be provided here. The resonance history set has already been assigned with the `dispatch` initializer. Here, we supply the set of subprocess instances that we have generated (see above). The master-process instance is set when we `connect` the transform by the standard method.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: connect_transform => &
    resonant_subprocess_set_connect_transform

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_connect_transform (prc_set, evt)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    class(evt_t), intent(in), target :: evt
    select type (evt)
      type is (evt_resonance_t)
        prc_set%evt => evt
        call prc_set%evt%set_subprocess_instances (prc_set%instance)
      class default
        call msg_bug ("Resonant subprocess set: event transform has wrong type")
    end select
  end subroutine resonant_subprocess_set_connect_transform

```

Set the on-shell limit value in the connected transform.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: set_on_shell_limit => resonant_subprocess_set_on_shell_limit

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_on_shell_limit (prc_set, on_shell_limit)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    real(default), intent(in) :: on_shell_limit
    call prc_set%evt%set_on_shell_limit (on_shell_limit)
  end subroutine resonant_subprocess_set_on_shell_limit

```

Set the Gaussian turnoff parameter in the connected transform.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: set_on_shell_turnoff => resonant_subprocess_set_on_shell_turnoff

```

```

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_on_shell_turnoff &
    (prc_set, on_shell_turnoff)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    real(default), intent(in) :: on_shell_turnoff
    call prc_set%evt%set_on_shell_turnoff (on_shell_turnoff)
  end subroutine resonant_subprocess_set_on_shell_turnoff

```

Reweight (suppress) the background contribution probability, for the kinematics where a resonance history is active.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: set_background_factor &
    => resonant_subprocess_set_background_factor

```

```

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_background_factor &
    (prc_set, background_factor)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    real(default), intent(in) :: background_factor
    call prc_set%evt%set_background_factor (background_factor)
  end subroutine resonant_subprocess_set_background_factor

```

33.8.7 Wrappers for runtime calculations

All runtime calculations are delegated to the event transform. The following procedures are essentially redundant wrappers. We retain them for a unit test below.

Debugging aid:

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: dump_instances => resonant_subprocess_set_dump_instances

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_dump_instances (prc_set, unit, testflag)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: testflag
    integer :: i, n, u
    u = given_output_unit (unit)
    write (u, "(A)")  "*** Process instances of resonant subprocesses"
    write (u, *)
    n = size (prc_set%subprocess)
    do i = 1, n
      associate (instance => prc_set%instance(i)%p)
        call instance%write (u, testflag)
        write (u, *)
        write (u, *)
      end associate
    end do
  end subroutine resonant_subprocess_set_dump_instances

```


Inject the current kinematics configuration, reading from the previous event transform or from the process instance.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: fill_momenta => resonant_subprocess_set_fill_momenta

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_fill_momenta (prc_set)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    integer :: i, n
    call prc_set%evt%fill_momenta ()
  end subroutine resonant_subprocess_set_fill_momenta

```

Determine the indices of the resonance histories that can be considered on-shell for the current kinematics.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: determine_on_shell_histories &
    => resonant_subprocess_set_determine_on_shell_histories

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_determine_on_shell_histories &
    (prc_set, i_component, index_array)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    integer, intent(in) :: i_component
    integer, dimension(:), allocatable, intent(out) :: index_array
    call prc_set%evt%determine_on_shell_histories (index_array)
  end subroutine resonant_subprocess_set_determine_on_shell_histories

```

Evaluate selected subprocesses. (In actual operation, the ones that have been tagged as on-shell.)

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: evaluate_subprocess &
    => resonant_subprocess_set_evaluate_subprocess

<Restricted subprocesses: procedures>+≡
  subroutine resonant_subprocess_set_evaluate_subprocess (prc_set, index_array)
    class(resonant_subprocess_set_t), intent(inout) :: prc_set
    integer, dimension(:), intent(in) :: index_array
    call prc_set%evt%evaluate_subprocess (index_array)
  end subroutine resonant_subprocess_set_evaluate_subprocess

```

Extract the matrix elements of the master process / the resonant subprocesses. After the previous routine has been executed, they should be available and stored in the corresponding process instances.

```

<Restricted subprocesses: resonant subprocess set: TBP>+≡
  procedure :: get_master_sqme &
    => resonant_subprocess_set_get_master_sqme
  procedure :: get_subprocess_sqme &
    => resonant_subprocess_set_get_subprocess_sqme

<Restricted subprocesses: procedures>+≡
  function resonant_subprocess_set_get_master_sqme (prc_set) result (sqme)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    real(default) :: sqme

```

```

    sqme = prc_set%evt%get_master_sqme ()
end function resonant_subprocess_set_get_master_sqme

subroutine resonant_subprocess_set_get_subprocess_sqme (prc_set, sqme)
    class(resonant_subprocess_set_t), intent(in) :: prc_set
    real(default), dimension(:), intent(inout) :: sqme
    integer :: i
    call prc_set%evt%get_subprocess_sqme (sqme)
end subroutine resonant_subprocess_set_get_subprocess_sqme

```

We use the calculations of resonant matrix elements to determine probabilities for all resonance configurations.

<Restricted subprocesses: resonant subprocess set: TBP>+≡

```

    procedure :: compute_probabilities &
        => resonant_subprocess_set_compute_probabilities

```

<Restricted subprocesses: procedures>+≡

```

    subroutine resonant_subprocess_set_compute_probabilities (prc_set, prob_array)
        class(resonant_subprocess_set_t), intent(inout) :: prc_set
        real(default), dimension(:), allocatable, intent(out) :: prob_array
        integer, dimension(:), allocatable :: index_array
        real(default) :: sqme, sqme_sum, sqme_bg
        real(default), dimension(:), allocatable :: sqme_res
        integer :: n
        n = size (prc_set%subprocess)
        allocate (prob_array (0:n), source = 0._default)
        call prc_set%evt%compute_probabilities ()
        call prc_set%evt%get_selector_weights (prob_array)
    end subroutine resonant_subprocess_set_compute_probabilities

```

33.8.8 Unit tests

Test module, followed by the stand-alone unit-test procedures.

<restricted_subprocesses_ut.f90>≡

<File header>

```

module restricted_subprocesses_ut
    use unit_tests
    use restricted_subprocesses_uti

```

<Standard module head>

<Restricted subprocesses: public test>

contains

<Restricted subprocesses: test driver>

```

end module restricted_subprocesses_ut

```

<restricted_subprocesses_uti.f90>≡

<File header>

```

module restricted_subprocesses_util

  <Use kinds>
  <Use strings>
  use io_units, only: free_unit
  use format_defs, only: FMT_10, FMT_12
  use lorentz, only: vector4_t, vector3_moving, vector4_moving
  use particle_specifiers, only: new_prt_spec
  use process_libraries, only: process_library_t
  use resonances, only: resonance_info_t
  use resonances, only: resonance_history_t
  use resonances, only: resonance_history_set_t
  use state_matrices, only: FM_IGNORE_HELICITY
  use particles, only: particle_set_t
  use model_data, only: model_data_t
  use models, only: syntax_model_file_init, syntax_model_file_final
  use models, only: model_t
  use rng_base_util, only: rng_test_factory_t
  use mci_base, only: mci_t
  use phs_base, only: phs_config_t
  use phs_forests, only: syntax_phs_forest_init, syntax_phs_forest_final
  use phs_wood, only: phs_wood_config_t
  use process_libraries, only: process_def_entry_t
  use process_libraries, only: process_component_def_t
  use prclib_stacks, only: prclib_entry_t
  use prc_core_def, only: prc_core_def_t
  use prc_omega, only: omega_def_t
  use process, only: process_t
  use instances, only: process_instance_t
  use process_stacks, only: process_entry_t
  use event_transforms, only: evt_trivial_t
  use resonance_insertion, only: evt_resonance_t
  use integrations, only: integrate_process
  use rt_data, only: rt_data_t

  use restricted_subprocesses

  <Standard module head>

  <Restricted subprocesses: test declarations>

  <Restricted subprocesses: test auxiliary types>

  <Restricted subprocesses: public test auxiliary>

contains

  <Restricted subprocesses: tests>

  <Restricted subprocesses: test auxiliary>

end module restricted_subprocesses_util

```

API: driver for the unit tests below.

```
<Restricted subprocesses: public test>≡
    public :: restricted_subprocesses_test

<Restricted subprocesses: test driver>≡
    subroutine restricted_subprocesses_test (u, results)
        integer, intent(in) :: u
        type(test_results_t), intent(inout) :: results
    <Restricted subprocesses: execute tests>
    end subroutine restricted_subprocesses_test
```

subprocess configuration

Initialize a `restricted_subprocess_configuration_t` object which represents a given process with a defined resonance history.

```
<Restricted subprocesses: execute tests>≡
    call test (restricted_subprocesses_1, "restricted_subprocesses_1", &
        "single subprocess", &
        u, results)

<Restricted subprocesses: test declarations>≡
    public :: restricted_subprocesses_1

<Restricted subprocesses: tests>≡
    subroutine restricted_subprocesses_1 (u)
        integer, intent(in) :: u
        type(rt_data_t) :: global
        type(resonance_info_t) :: res_info
        type(resonance_history_t) :: res_history
        type(string_t) :: prc_name
        type(string_t), dimension(2) :: prt_in
        type(string_t), dimension(3) :: prt_out
        type(restricted_process_configuration_t) :: prc_config

        write (u, "(A)")  "* Test output: restricted_subprocesses_1"
        write (u, "(A)")  "* Purpose: create subprocess list from resonances"
        write (u, "(A)")

        call syntax_model_file_init ()

        call global%global_init ()
        call global%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true.)
        call global%select_model (var_str ("SM"))

        write (u, "(A)")  "* Create resonance history"
        write (u, "(A)")

        call res_info%init (3, -24, global%model, 5)
        call res_history%add_resonance (res_info)
        call res_history%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Create process configuration"
```

```

write (u, "(A)")

prc_name = "restricted_subprocesses_1_p"
prt_in(1) = "e-"
prt_in(2) = "e+"
prt_out(1) = "d"
prt_out(2) = "u"
prt_out(3) = "W+"

call prc_config%init_resonant_process (prc_name, &
    new_prt_spec (prt_in), new_prt_spec (prt_out), &
    res_history, global%model, global%var_list)

call prc_config%write (u)

write (u, *)
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_1"

end subroutine restricted_subprocesses_1

```

Subprocess library configuration

Create a process library that represents restricted subprocesses for a given set of resonance histories

```

<Restricted subprocesses: execute tests>+≡
    call test (restricted_subprocesses_2, "restricted_subprocesses_2", &
        "subprocess library", &
        u, results)

<Restricted subprocesses: test declarations>+≡
    public :: restricted_subprocesses_2

<Restricted subprocesses: tests>+≡
    subroutine restricted_subprocesses_2 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        type(resonance_info_t) :: res_info
        type(resonance_history_t), dimension(2) :: res_history
        type(resonance_history_set_t) :: res_history_set
        type(string_t) :: libname
        type(string_t), dimension(2) :: prt_in
        type(string_t), dimension(3) :: prt_out
        type(resonant_subprocess_set_t) :: prc_set
        type(process_library_t), pointer :: lib
        logical :: exist

        write (u, "(A)")  "* Test output: restricted_subprocesses_2"
    end subroutine

```

```

write (u, "(A)")  "*" Purpose: create subprocess library from resonances"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%select_model (var_str ("SM"))

write (u, "(A)")  "*" Create resonance histories"
write (u, "(A)")

call res_info%init (3, -24, global%model, 5)
call res_history(1)%add_resonance (res_info)
call res_history(1)%write (u)

call res_info%init (7, 23, global%model, 5)
call res_history(2)%add_resonance (res_info)
call res_history(2)%write (u)

call res_history_set%init ()
call res_history_set%enter (res_history(1))
call res_history_set%enter (res_history(2))
call res_history_set%freeze ()

write (u, "(A)")
write (u, "(A)")  "*" Empty restricted subprocess set"
write (u, "(A)")

write (u, "(A,1x,L1)")  "active =", prc_set%is_active ()
write (u, "(A)")

call prc_set%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "*" Fill restricted subprocess set"
write (u, "(A)")

libname = "restricted_subprocesses_2_p_R"
prt_in(1) = "e-"
prt_in(2) = "e+"
prt_out(1) = "d"
prt_out(2) = "u"
prt_out(3) = "W+"

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set, 1)
call prc_set%create_library (libname, global, exist)
if (.not. exist) then
    call prc_set%add_to_library (1, &
        new_prt_spec (prt_in), new_prt_spec (prt_out), &
        global)
end if

```

```

call prc_set%freeze_library (global)

write (u, "(A,1x,L1)") "active =", prc_set%is_active ()
write (u, "(A)")

call prc_set%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Queries"
write (u, "(A)")

write (u, "(A,1x,I0)") "n_process =", prc_set%get_n_process ()
write (u, "(A)")
write (u, "(A,A,A)") "libname = '", char (prc_set%get_libname ()), "'"
write (u, "(A)")
write (u, "(A,A,A)") "proc_id(1) = '", char (prc_set%get_proc_id (1)), "'"
write (u, "(A,A,A)") "proc_id(2) = '", char (prc_set%get_proc_id (2)), "'"

write (u, "(A)")
write (u, "(A)")  "* Process library"
write (u, "(A)")

call prc_set%compile_library (global)

lib => global%prclib_stack%get_library_ptr (libname)
if (associated (lib)) call lib%write (u, libpath=.false.)

write (u, *)
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_2"

end subroutine restricted_subprocesses_2

```

Auxiliary: Test processes

Auxiliary subroutine that constructs the process library for the above test. This parallels a similar subroutine in `processes_uti`, but this time we want an O'MEGA process.

```

<Restricted subprocesses: public test auxiliary>≡
  public :: prepare_resonance_test_library

<Restricted subprocesses: test auxiliary>≡
  subroutine prepare_resonance_test_library &
    (lib, libname, procname, model, global, u)
    type(process_library_t), target, intent(out) :: lib
    type(string_t), intent(in) :: libname
    type(string_t), intent(in) :: procname

```

```

class(model_data_t), intent(in), pointer :: model
type(rt_data_t), intent(in), target :: global
integer, intent(in) :: u
type(string_t), dimension(:), allocatable :: prt_in, prt_out
class(prc_core_def_t), allocatable :: def
type(process_def_entry_t), pointer :: entry

call lib%init (libname)

allocate (prt_in (2), prt_out (3))
prt_in = [var_str ("e+"), var_str ("e-")]
prt_out = [var_str ("d"), var_str ("ubar"), var_str ("W+")]

allocate (omega_def_t :: def)
select type (def)
type is (omega_def_t)
    call def%init (model%get_name (), prt_in, prt_out, &
        ovm=.false., ufo=.false.)
end select
allocate (entry)
call entry%init (procname, &
    model_name = model%get_name (), &
    n_in = 2, n_components = 1, &
    requires_resonances = .true.)
call entry%import_component (1, n_out = size (prt_out), &
    prt_in = new_prt_spec (prt_in), &
    prt_out = new_prt_spec (prt_out), &
    method = var_str ("omega"), &
    variant = def)
call entry%write (u)

call lib%append (entry)

call lib%configure (global%os_data)
call lib%write_makefile (global%os_data, force = .true., verbose = .false.)
call lib%clean (global%os_data, distclean = .false.)
call lib%write_driver (force = .true.)
call lib%load (global%os_data)

end subroutine prepare_resonance_test_library

```

Kinematics and resonance selection

Prepare an actual process with resonant subprocesses. Insert kinematics and apply the resonance selector in an associated event transform.

```

(Restricted subprocesses: execute tests)+≡
    call test (restricted_subprocesses_3, "restricted_subprocesses_3", &
        "resonance kinematics and probability", &
        u, results)

(Restricted subprocesses: test declarations)+≡
    public :: restricted_subprocesses_3

```



```

<Restricted subprocesses: tests>+≡
subroutine restricted_subprocesses_3 (u)
  integer, intent(in) :: u
  type(rt_data_t), target :: global
  class(model_t), pointer :: model
  class(model_data_t), pointer :: model_data
  type(string_t) :: libname, libname_res
  type(string_t) :: procname
  type(process_component_def_t), pointer :: process_component_def
  type(prclib_entry_t), pointer :: lib_entry
  type(process_library_t), pointer :: lib
  logical :: exist
  type(process_t), pointer :: process
  type(process_instance_t), target :: process_instance
  type(resonance_history_set_t), dimension(1) :: res_history_set
  type(resonant_subprocess_set_t) :: prc_set
  type(particle_set_t) :: pset
  real(default) :: sqrts, mw, pp
  real(default), dimension(3) :: p3
  type(vector4_t), dimension(:), allocatable :: p
  real(default), dimension(:), allocatable :: m
  integer, dimension(:), allocatable :: pdg
  real(default), dimension(:), allocatable :: sqme
  logical, dimension(:), allocatable :: mask
  real(default) :: on_shell_limit
  integer, dimension(:), allocatable :: i_array
  real(default), dimension(:), allocatable :: prob_array
  type(evt_resonance_t), target :: evt_resonance
  integer :: i, u_dump

  write (u, "(A)")  "* Test output: restricted_subprocesses_3"
  write (u, "(A)")  "* Purpose: handle process and resonance kinematics"
  write (u, "(A)")

  call syntax_model_file_init ()
  call syntax_phs_forest_init ()

  call global%global_init ()
  call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
  call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
  call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
  call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
  call global%set_log (var_str ("?resonance_history"), &
    .true., is_known = .true.)

  call global%select_model (var_str ("SM"))
  allocate (model)
  call model%init_instance (global%model)
  model_data => model

```

```

libname = "restricted_subprocesses_3_lib"
libname_res = "restricted_subprocesses_3_lib_res"
procname = "restricted_subprocesses_3_p"

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
      (lib, libname, procname, model_data, global, u)

call integrate_process (procname, global, &
      local_stack = .true., init_only = .true.)

process => global%process_stack%get_process_ptr (procname)

call process_instance%init (process)
call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"
write (u, "(A)")

call process%extract_resonance_history_set &
      (res_history_set(1), include_trivial=.true., i_component=1)
call res_history_set(1)%write (u)

write (u, "(A)")
write (u, "(A)")  "* Build resonant-subprocess library"
write (u, "(A)")

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set(1), 1)

process_component_def => process%get_component_def_ptr (1)
call prc_set%create_library (libname_res, global, exist)
if (.not. exist) then
  call prc_set%add_to_library (1, &
    process_component_def%get_prt_spec_in (), &
    process_component_def%get_prt_spec_out (), &
    global)
end if
call prc_set%freeze_library (global)
call prc_set%compile_library (global)
call prc_set%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Build particle set"
write (u, "(A)")

```

```

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (pdg (5), p (5), m (5))
pdg(1) = -11
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
pdg(2) = 11
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
m(2) = 0
pdg(3) = 1
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
pdg(4) = -2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
pdg(5) = 24
p(5) = vector4_moving (sqrts/2,-pp, 1)
m(5) = mw

call pset%init_direct (0, 2, 0, 0, 3, pdg, model)
call pset%set_momentum (p, m**2)
call pset%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Fill process instance"

! workflow from event_recalculate
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1)
call process_instance%recover &
    (1, 1, update_sqme=.true., recover_phs=.false.)
call process_instance%evaluate_event_data (weight = 1._default)

write (u, "(A)")
write (u, "(A)")  "* Prepare resonant subprocesses"

call prc_set%prepare_process_objects (global)
call prc_set%prepare_process_instances (global)

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call prc_set%connect_transform (evt_resonance)
call evt_resonance%connect (process_instance, model)

call prc_set%fill_momenta ()

write (u, "(A)")
write (u, "(A)")  "* Show squared matrix element of master process,"

```

```

write (u, "(A)") " should coincide with 2nd subprocess sqme"
write (u, "(A)")

write (u, "(1x,I0,1x," // FMT_12 // ")") 0, prc_set%get_master_sqme ()

write (u, "(A)")
write (u, "(A)") "* Compute squared matrix elements &
    &of selected resonant subprocesses [1,2]"
write (u, "(A)")

call prc_set%evaluate_subprocess ([1,2])

allocate (sqme (3), source = 0._default)
call prc_set%get_subprocess_sqme (sqme)
do i = 1, size (sqme)
    write (u, "(1x,I0,1x," // FMT_12 // ")") i, sqme(i)
end do
deallocate (sqme)

write (u, "(A)")
write (u, "(A)") "* Compute squared matrix elements &
    &of all resonant subprocesses"
write (u, "(A)")

call prc_set%evaluate_subprocess ([1,2,3])

allocate (sqme (3), source = 0._default)
call prc_set%get_subprocess_sqme (sqme)
do i = 1, size (sqme)
    write (u, "(1x,I0,1x," // FMT_12 // ")") i, sqme(i)
end do
deallocate (sqme)

write (u, "(A)")
write (u, "(A)") "* Write process instances to file &
    &restricted_subprocesses_3_lib_res.dat"

u_dump = free_unit ()
open (unit = u_dump, file = "restricted_subprocesses_3_lib_res.dat", &
    action = "write", status = "replace")
call prc_set%dump_instances (u_dump)
close (u_dump)

write (u, "(A)")
write (u, "(A)") "* Determine on-shell resonant subprocesses"
write (u, "(A)")

on_shell_limit = 0
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
write (u, "(1x,A,9(1x,I0))") "resonant =", i_array

on_shell_limit = 0.1_default

```

```

write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
write (u, "(1x,A,9(1x,I0))") "resonant =", i_array

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
write (u, "(1x,A,9(1x,I0))") "resonant =", i_array

on_shell_limit = 10000._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
write (u, "(1x,A,9(1x,I0))") "resonant =", i_array

write (u, "(A)")
write (u, "(A)")  "* Compute probabilities for applicable resonances"
write (u, "(A)")  " and initialize the process selector"
write (u, "(A)")  " (The first number is the probability for background)"
write (u, "(A)")

on_shell_limit = 0
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
call prc_set%compute_probabilities (prob_array)
write (u, "(1x,A,9(1x,"// FMT_12 // ")") "resonant =", prob_array
call prc_set%write (u, testflag=.true.)
write (u, *)

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
call prc_set%compute_probabilities (prob_array)
write (u, "(1x,A,9(1x,"// FMT_12 // ")") "resonant =", prob_array
call prc_set%write (u, testflag=.true.)
write (u, *)

on_shell_limit = 10000._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call prc_set%set_on_shell_limit (on_shell_limit)
call prc_set%determine_on_shell_histories (1, i_array)
call prc_set%compute_probabilities (prob_array)
write (u, "(1x,A,9(1x,"// FMT_12 // ")") "resonant =", prob_array
write (u, *)
call prc_set%write (u, testflag=.true.)
write (u, *)

write (u, "(A)")  "* Cleanup"

call global%final ()

```

```

call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_3"

end subroutine restricted_subprocesses_3

```

Event transform

Prepare an actual process with resonant subprocesses. Prepare the resonance selector for a fixed event and apply the resonance-insertion event transform.

```

<Restricted subprocesses: execute tests>+≡
    call test (restricted_subprocesses_4, "restricted_subprocesses_4", &
               "event transform", &
               u, results)

<Restricted subprocesses: test declarations>+≡
    public :: restricted_subprocesses_4

<Restricted subprocesses: tests>+≡
    subroutine restricted_subprocesses_4 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        class(model_t), pointer :: model
        class(model_data_t), pointer :: model_data
        type(string_t) :: libname, libname_res
        type(string_t) :: procname
        type(process_component_def_t), pointer :: process_component_def
        type(prclib_entry_t), pointer :: lib_entry
        type(process_library_t), pointer :: lib
        logical :: exist
        type(process_t), pointer :: process
        type(process_instance_t), target :: process_instance
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(resonant_subprocess_set_t) :: prc_set
        type(particle_set_t) :: pset
        real(default) :: sqrts, mw, pp
        real(default), dimension(3) :: p3
        type(vector4_t), dimension(:), allocatable :: p
        real(default), dimension(:), allocatable :: m
        integer, dimension(:), allocatable :: pdg
        real(default) :: on_shell_limit
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        real(default) :: probability
        integer :: i

        write (u, "(A)")  "* Test output: restricted_subprocesses_4"
        write (u, "(A)")  "* Purpose: employ event transform"
        write (u, "(A)")

        call syntax_model_file_init ()

```

```

call syntax_phs_forest_init ()

call global%global_init ()
call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%set_log (var_str ("?resonance_history"), &
    .true., is_known = .true.)

call global%select_model (var_str ("SM"))
allocate (model)
call model%init_instance (global%model)
model_data => model

libname = "restricted_subprocesses_4_lib"
libname_res = "restricted_subprocesses_4_lib_res"
procname = "restricted_subprocesses_4_p"

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
    (lib, libname, procname, model_data, global, u)

call integrate_process (procname, global, &
    local_stack = .true., init_only = .true.)

process => global%process_stack%get_process_ptr (procname)

call process_instance%init (process)
call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"

call process%extract_resonance_history_set &
    (res_history_set(1), include_trivial=.false., i_component=1)

write (u, "(A)")
write (u, "(A)")  "* Build resonant-subprocess library"

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set(1), 1)

```

```

process_component_def => process%get_component_def_ptr (1)
call prc_set%create_library (libname_res, global, exist)
if (.not. exist) then
    call prc_set%add_to_library (1, &
        process_component_def%get_prt_spec_in (), &
        process_component_def%get_prt_spec_out (), &
        global)
end if
call prc_set%freeze_library (global)
call prc_set%compile_library (global)

write (u, "(A)")
write (u, "(A)")  "* Build particle set"
write (u, "(A)")

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default  ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (pdg (5), p (5), m (5))
pdg(1) = -11
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
pdg(2) = 11
p(2) = vector4_moving (sqrts/2, -sqrts/2, 3)
m(2) = 0
pdg(3) = 1
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
pdg(4) = -2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
pdg(5) = 24
p(5) = vector4_moving (sqrts/2, -pp, 1)
m(5) = mw

call pset%init_direct (0, 2, 0, 0, 3, pdg, model)
call pset%set_momentum (p, m**2)

write (u, "(A)")  "* Fill process instance"
write (u, "(A)")

! workflow from event_recalculate
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1)
call process_instance%recover &
    (1, 1, update_sqme=.true., recover_phs=.false.)
call process_instance%evaluate_event_data (weight = 1._default)

write (u, "(A)")  "* Prepare resonant subprocesses"

```



```

write (u, "(A)")

call prc_set%prepare_process_objects (global)
call prc_set%prepare_process_instances (global)

write (u, "(A)")  "* Fill trivial event transform (deliberately w/o color)"
write (u, "(A)")

call evt_trivial%connect (process_instance, model)
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize resonance-insertion event transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%connect (process_instance, model)
call prc_set%connect_transform (evt_resonance)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute probabilities for applicable resonances"
write (u, "(A)")  "  and initialize the process selector"
write (u, "(A)")

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") "on_shell_limit =", on_shell_limit
call evt_resonance%set_on_shell_limit (on_shell_limit)

write (u, "(A)")
write (u, "(A)")  "* Evaluate resonance-insertion event transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (1, .false.)

call evt_resonance%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: restricted_subprocesses_4"

```

```
end subroutine restricted_subprocesses_4
```

Gaussian turnoff

Identical to the previous process, except that we apply a Gaussian turnoff to the resonance kinematics, which affects the subprocess selector.

```
(Restricted subprocesses: execute tests)+≡
  call test (restricted_subprocesses_5, "restricted_subprocesses_5", &
    "event transform with gaussian turnoff", &
    u, results)

(Restricted subprocesses: test declarations)+≡
  public :: restricted_subprocesses_5

(Restricted subprocesses: tests)+≡
  subroutine restricted_subprocesses_5 (u)
    integer, intent(in) :: u
    type(rt_data_t), target :: global
    class(model_t), pointer :: model
    class(model_data_t), pointer :: model_data
    type(string_t) :: libname, libname_res
    type(string_t) :: procname
    type(process_component_def_t), pointer :: process_component_def
    type(prclib_entry_t), pointer :: lib_entry
    type(process_library_t), pointer :: lib
    logical :: exist
    type(process_t), pointer :: process
    type(process_instance_t), target :: process_instance
    type(resonance_history_set_t), dimension(1) :: res_history_set
    type(resonant_subprocess_set_t) :: prc_set
    type(particle_set_t) :: pset
    real(default) :: sqrts, mw, pp
    real(default), dimension(3) :: p3
    type(vector4_t), dimension(:), allocatable :: p
    real(default), dimension(:), allocatable :: m
    integer, dimension(:), allocatable :: pdg
    real(default) :: on_shell_limit
    real(default) :: on_shell_turnoff
    type(evt_trivial_t), target :: evt_trivial
    type(evt_resonance_t), target :: evt_resonance
    real(default) :: probability
    integer :: i

    write (u, "(A)")  "* Test output: restricted_subprocesses_5"
    write (u, "(A)")  "* Purpose: employ event transform &
      &with gaussian turnoff"
    write (u, "(A)")

    call syntax_model_file_init ()
    call syntax_phs_forest_init ()

    call global%global_init ()
    call global%append_log (&
```

```

        var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%set_log (var_str ("?resonance_history"), &
    .true., is_known = .true.)

call global%select_model (var_str ("SM"))
allocate (model)
call model%init_instance (global%model)
model_data => model

libname = "restricted_subprocesses_5_lib"
libname_res = "restricted_subprocesses_5_lib_res"
procname = "restricted_subprocesses_5_p"

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
    (lib, libname, procname, model_data, global, u)

call integrate_process (procname, global, &
    local_stack = .true., init_only = .true.)

process => global%process_stack%get_process_ptr (procname)

call process_instance%init (process)
call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"

call process%extract_resonance_history_set &
    (res_history_set(1), include_trivial=.false., i_component=1)

write (u, "(A)")
write (u, "(A)")  "* Build resonant-subprocess library"

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set(1), 1)

process_component_def => process%get_component_def_ptr (1)
call prc_set%create_library (libname_res, global, exist)
if (.not. exist) then
    call prc_set%add_to_library (1, &

```

```

        process_component_def%get_prt_spec_in (), &
        process_component_def%get_prt_spec_out (), &
        global)
end if
call prc_set%freeze_library (global)
call prc_set%compile_library (global)

write (u, "(A)")
write (u, "(A)")  "* Build particle set"
write (u, "(A)")

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default  ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (pdg (5), p (5), m (5))
pdg(1) = -11
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
pdg(2) = 11
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
m(2) = 0
pdg(3) = 1
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
pdg(4) = -2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
pdg(5) = 24
p(5) = vector4_moving (sqrts/2,-pp, 1)
m(5) = mw

call pset%init_direct (0, 2, 0, 0, 3, pdg, model)
call pset%set_momentum (p, m**2)

write (u, "(A)")  "* Fill process instance"
write (u, "(A)")

! workflow from event_recalculate
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1)
call process_instance%recover &
(1, 1, update_sqme=.true., recover_phs=.false.)
call process_instance%evaluate_event_data (weight = 1._default)

write (u, "(A)")  "* Prepare resonant subprocesses"
write (u, "(A)")

call prc_set%prepare_process_objects (global)
call prc_set%prepare_process_instances (global)

```

```

write (u, "(A)")  "* Fill trivial event transform (deliberately w/o color)"
write (u, "(A)")

call evt_trivial%connect (process_instance, model)
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize resonance-insertion event transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%connect (process_instance, model)
call prc_set%connect_transform (evt_resonance)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute probabilities for applicable resonances"
write (u, "(A)")  " and initialize the process selector"
write (u, "(A)")

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")")  "on_shell_limit  =", &
    on_shell_limit
call evt_resonance%set_on_shell_limit (on_shell_limit)

on_shell_turnoff = 1._default
write (u, "(1x,A,1x," // FMT_10 // ")")  "on_shell_turnoff =", &
    on_shell_turnoff
call evt_resonance%set_on_shell_turnoff (on_shell_turnoff)

write (u, "(A)")
write (u, "(A)")  "* Evaluate resonance-insertion event transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (1, .false.)

call evt_resonance%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

write (u, "(A)")

```

```

        write (u, "(A)")  "* Test output end: restricted_subprocesses_5"

    end subroutine restricted_subprocesses_5

```

Event transform

The same process and event again. This time, switch off the background contribution, so the selector becomes trivial.

```

<Restricted subprocesses: execute tests>+≡
    call test (restricted_subprocesses_6, "restricted_subprocesses_6", &
        "event transform with background switched off", &
        u, results)

<Restricted subprocesses: test declarations>+≡
    public :: restricted_subprocesses_6

<Restricted subprocesses: tests>+≡
    subroutine restricted_subprocesses_6 (u)
        integer, intent(in) :: u
        type(rt_data_t), target :: global
        class(model_t), pointer :: model
        class(model_data_t), pointer :: model_data
        type(string_t) :: libname, libname_res
        type(string_t) :: procname
        type(process_component_def_t), pointer :: process_component_def
        type(prclib_entry_t), pointer :: lib_entry
        type(process_library_t), pointer :: lib
        logical :: exist
        type(process_t), pointer :: process
        type(process_instance_t), target :: process_instance
        type(resonance_history_set_t), dimension(1) :: res_history_set
        type(resonant_subprocess_set_t) :: prc_set
        type(particle_set_t) :: pset
        real(default) :: sqrts, mw, pp
        real(default), dimension(3) :: p3
        type(vector4_t), dimension(:), allocatable :: p
        real(default), dimension(:), allocatable :: m
        integer, dimension(:), allocatable :: pdg
        real(default) :: on_shell_limit
        real(default) :: background_factor
        type(evt_trivial_t), target :: evt_trivial
        type(evt_resonance_t), target :: evt_resonance
        real(default) :: probability
        integer :: i

        write (u, "(A)")  "* Test output: restricted_subprocesses_6"
        write (u, "(A)")  "*   Purpose: employ event transform &
            &with background switched off"
        write (u, "(A)")

        call syntax_model_file_init ()
        call syntax_phs_forest_init ()

```

```

call global%global_init ()
call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%set_log (var_str ("?resonance_history"), &
    .true., is_known = .true.)

call global%select_model (var_str ("SM"))
allocate (model)
call model%init_instance (global%model)
model_data => model

libname = "restricted_subprocesses_6_lib"
libname_res = "restricted_subprocesses_6_lib_res"
procname = "restricted_subprocesses_6_p"

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
    (lib, libname, procname, model_data, global, u)

call integrate_process (procname, global, &
    local_stack = .true., init_only = .true.)

process => global%process_stack%get_process_ptr (procname)

call process_instance%init (process)
call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Extract resonance history set"

call process%extract_resonance_history_set &
    (res_history_set(1), include_trivial=.false., i_component=1)

write (u, "(A)")
write (u, "(A)")  "* Build resonant-subprocess library"

call prc_set%init (1)
call prc_set%fill_resonances (res_history_set(1), 1)

process_component_def => process%get_component_def_ptr (1)
call prc_set%create_library (libname_res, global, exist)

```

```

if (.not. exist) then
  call prc_set%add_to_library (1, &
    process_component_def%get_prt_spec_in (), &
    process_component_def%get_prt_spec_out (), &
    global)
end if
call prc_set%freeze_library (global)
call prc_set%compile_library (global)

write (u, "(A)")
write (u, "(A)")  "* Build particle set"
write (u, "(A)")

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default  ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (pdg (5), p (5), m (5))
pdg(1) = -11
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
pdg(2) = 11
p(2) = vector4_moving (sqrts/2,-sqrts/2, 3)
m(2) = 0
pdg(3) = 1
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
pdg(4) = -2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
pdg(5) = 24
p(5) = vector4_moving (sqrts/2,-pp, 1)
m(5) = mw

call pset%init_direct (0, 2, 0, 0, 3, pdg, model)
call pset%set_momentum (p, m**2)

write (u, "(A)")  "* Fill process instance"
write (u, "(A)")

! workflow from event_recalculate
call process_instance%choose_mci (1)
call process_instance%set_trace (pset, 1)
call process_instance%recover &
  (1, 1, update_sqme=.true., recover_phs=.false.)
call process_instance%evaluate_event_data (weight = 1._default)

write (u, "(A)")  "* Prepare resonant subprocesses"
write (u, "(A)")

```



```

call prc_set%prepare_process_objects (global)
call prc_set%prepare_process_instances (global)

write (u, "(A)")  "* Fill trivial event transform (deliberately w/o color)"
write (u, "(A)")

call evt_trivial%connect (process_instance, model)
call evt_trivial%set_particle_set (pset, 1, 1)
call evt_trivial%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize resonance-insertion event transform"
write (u, "(A)")

evt_trivial%next => evt_resonance
evt_resonance%previous => evt_trivial

call evt_resonance%set_resonance_data (res_history_set)
call evt_resonance%select_component (1)
call evt_resonance%connect (process_instance, model)
call prc_set%connect_transform (evt_resonance)
call evt_resonance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Compute probabilities for applicable resonances"
write (u, "(A)")  " and initialize the process selector"
write (u, "(A)")

on_shell_limit = 10._default
write (u, "(1x,A,1x," // FMT_10 // ")") &
    "on_shell_limit    =", on_shell_limit
call evt_resonance%set_on_shell_limit (on_shell_limit)

background_factor = 0
write (u, "(1x,A,1x," // FMT_10 // ")") &
    "background_factor =", background_factor
call evt_resonance%set_background_factor (background_factor)

write (u, "(A)")
write (u, "(A)")  "* Evaluate resonance-insertion event transform"
write (u, "(A)")

call evt_resonance%prepare_new_event (1, 1)
call evt_resonance%generate_weighted (probability)
call evt_resonance%make_particle_set (1, .false.)

call evt_resonance%write (u, testflag=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()
call syntax_phs_forest_final ()
call syntax_model_file_final ()

```

```
write (u, "(A)")  
write (u, "(A)")  "* Test output end: restricted_subprocesses_6"  
  
end subroutine restricted_subprocesses_6
```

33.9 Simulation

This module manages simulation: event generation and reading/writing of event files. The `simulation` object is intended to be used (via a pointer) outside of WHIZARD, if events are generated individually by an external driver.

```
<simulations.f90>≡  
  <File header>  
  
  module simulations  
  
    <Use kinds>  
    <Use strings>  
    <Use debug>  
    use io_units  
    use format_utils, only: write_separator  
    use format_defs, only: FMT_15, FMT_19  
    use os_interface  
    use numeric_utils  
    use string_utils, only: str  
    use diagnostics  
    use lorentz, only: vector4_t  
    use sm_qcd  
    use md5  
    use variables, only: var_list_t  
    use eval_trees  
    use model_data  
    use flavors  
    use particles  
    use state_matrices, only: FM_IGNORE_HELICITY  
    use beam_structures, only: beam_structure_t  
    use beams  
    use rng_base  
    use rng_stream, only: rng_stream_t  
    use selectors  
    use resonances, only: resonance_history_set_t  
    use process_libraries, only: process_library_t  
    use process_libraries, only: process_component_def_t  
    use prc_core  
    ! TODO: (bcn 2016-09-13) should be ideally only pcm_base  
    use pcm, only: pcm_nlo_t, pcm_nlo_workspace_t  
    ! TODO: (bcn 2016-09-13) details of process config should not be necessary here  
    use process_config, only: COMP_REAL_FIN  
    use process  
    use instances  
    use event_base  
    use event_handles, only: event_handle_t  
    use events  
    use event_transforms  
    use shower  
    use eio_data  
    use eio_base  
    use rt_data  
  
    use dispatch_beams, only: dispatch_qcd
```

```

use dispatch_rng, only: dispatch_rng_factory
use dispatch_rng, only: update_rng_seed_in_var_list
use dispatch_me_methods, only: dispatch_core_update, dispatch_core_restore
use dispatch_transforms, only: dispatch_evt_isr_epa_handler
use dispatch_transforms, only: dispatch_evt_resonance
use dispatch_transforms, only: dispatch_evt_decay
use dispatch_transforms, only: dispatch_evt_shower
use dispatch_transforms, only: dispatch_evt_hadrons
use dispatch_transforms, only: dispatch_evt_nlo

use integrations
use event_streams
use restricted_subprocesses, only: resonant_subprocess_set_t
use restricted_subprocesses, only: get_libname_res

use evt_nlo

<Use mpi f08>

<Standard module head>

<Simulations: public>

<Simulations: types>

<Simulations: interfaces>

contains

<Simulations: procedures>

end module simulations

```

33.9.1 Event counting

In this object we collect statistical information about an event sample or sub-sample.

```

<Simulations: types>≡
  type :: counter_t
    integer :: total = 0
    integer :: generated = 0
    integer :: read = 0
    integer :: positive = 0
    integer :: negative = 0
    integer :: zero = 0
    integer :: excess = 0
    integer :: dropped = 0
    real(default) :: max_excess = 0
    real(default) :: sum_excess = 0
    logical :: reproduce_xsection = .false.
    real(default) :: mean = 0
    real(default) :: varsq = 0
    integer :: nlo_weight_counter = 0

```

```

contains
  <Simulations: counter: TBP>
end type counter_t

```

Output.

```

<Simulations: counter: TBP>≡
  procedure :: write => counter_write

<Simulations: procedures>≡
  subroutine counter_write (counter, unit)
    class(counter_t), intent(in) :: counter
    integer, intent(in), optional :: unit
    integer :: u
    u = given_output_unit (unit)
1   format (3x,A,I0)
2   format (5x,A,I0)
3   format (5x,A,ES19.12)
    write (u, 1) "Events total      = ", counter%total
    write (u, 2) "generated        = ", counter%generated
    write (u, 2) "read            = ", counter%read
    write (u, 2) "positive weight = ", counter%positive
    write (u, 2) "negative weight = ", counter%negative
    write (u, 2) "zero weight     = ", counter%zero
    write (u, 2) "excess weight  = ", counter%excess
    if (counter%excess /= 0) then
      write (u, 3) "max excess      = ", counter%max_excess
      write (u, 3) "avg excess      = ", counter%sum_excess / counter%total
    end if
    write (u, 1) "Events dropped   = ", counter%dropped
  end subroutine counter_write

```

This is a screen message: if there was an excess, display statistics.

```

<Simulations: counter: TBP>+≡
  procedure :: show_excess => counter_show_excess

<Simulations: procedures>+≡
  subroutine counter_show_excess (counter)
    class(counter_t), intent(in) :: counter
    if (counter%excess > 0) then
      write (msg_buffer, "(A,1x,I0,1x,A,1x,'(,F7.3,' %)'") &
        "Encountered events with excess weight:", counter%excess, &
        "events", 100 * counter%excess / real (counter%total)
      call msg_warning ()
      write (msg_buffer, "(A,ES10.3)") &
        "Maximum excess weight =", counter%max_excess
      call msg_message ()
      write (msg_buffer, "(A,ES10.3)") &
        "Average excess weight =", counter%sum_excess / counter%total
      call msg_message ()
    end if
  end subroutine counter_show_excess

```

If events have been dropped during simulation of weighted events, issue a message here. If a fraction `n_dropped / n_total` of the events fail the cuts, we keep generating new ones until we have `n_total` events with `weight > 0`. Thus, the total sum of weights will be a fraction of `n_dropped / n_total` too large. However, we do not know how many events will pass or fail the cuts prior to generating them so we leave it to the user to correct for this factor.

<Simulations: counter: TBP>+≡

```
procedure :: show_dropped => counter_show_dropped
```

<Simulations: procedures>+≡

```
subroutine counter_show_dropped (counter)
  class(counter_t), intent(in) :: counter
  if (counter%dropped > 0) then
    write (msg_buffer, "(A,1x,I0,1x,'(',A,1x,I0,')')") &
      "Dropped events (weight zero) =", &
      counter%dropped, "total", counter%dropped + counter%total
    call msg_message ()
    write (msg_buffer, "(A,ES15.8)") &
      "All event weights must be rescaled by f =", &
      real (counter%total, default) &
      / real (counter%dropped + counter%total, default)
    call msg_warning ()
  end if
end subroutine counter_show_dropped
```

<Simulations: counter: TBP>+≡

```
procedure :: show_mean_and_variance => counter_show_mean_and_variance
```

<Simulations: procedures>+≡

```
subroutine counter_show_mean_and_variance (counter)
  class(counter_t), intent(in) :: counter
  if (counter%reproduce_xsection .and. counter%nlo_weight_counter > 1) then
    print *, "Reconstructed cross-section from event weights: "
    print *, counter%mean, '+-', sqrt (counter%varsq / (counter%nlo_weight_counter - 1))
  end if
end subroutine counter_show_mean_and_variance
```

Count an event. The weight and event source are optional; by default we assume that the event has been generated and has positive weight.

The optional integer `n_dropped` counts weighted events with weight zero that were encountered while generating the current event, but dropped (because of their zero weight). Accumulating this number allows for renormalizing event weight sums in histograms, after the generation step has been completed.

<Simulations: counter: TBP>+≡

```
procedure :: record => counter_record
```

<Simulations: procedures>+≡

```
subroutine counter_record (counter, weight, excess, n_dropped, from_file)
  class(counter_t), intent(inout) :: counter
  real(default), intent(in), optional :: weight, excess
  integer, intent(in), optional :: n_dropped
  logical, intent(in), optional :: from_file
  counter%total = counter%total + 1
```

```

if (present (from_file)) then
  if (from_file) then
    counter%read = counter%read + 1
  else
    counter%generated = counter%generated + 1
  end if
else
  counter%generated = counter%generated + 1
end if
if (present (weight)) then
  if (weight > 0) then
    counter%positive = counter%positive + 1
  else if (weight < 0) then
    counter%negative = counter%negative + 1
  else
    counter%zero = counter%zero + 1
  end if
else
  counter%positive = counter%positive + 1
end if
if (present (excess)) then
  if (excess > 0) then
    counter%excess = counter%excess + 1
    counter%max_excess = max (counter%max_excess, excess)
    counter%sum_excess = counter%sum_excess + excess
  end if
end if
if (present (n_dropped)) then
  counter%dropped = counter%dropped + n_dropped
end if
end subroutine counter_record

```

<MPI: Simulations: counter: TBP>≡

```

procedure :: allreduce_record => counter_allreduce_record

```

<MPI: Simulations: procedures>≡

```

subroutine counter_allreduce_record (counter)
  class(counter_t), intent(inout) :: counter
  integer :: read, generated
  integer :: positive, negative, zero, excess, dropped
  real(default) :: max_excess, sum_excess
  read = counter%read
  generated = counter%generated
  positive = counter%positive
  negative = counter%negative
  zero = counter%zero
  excess = counter%excess
  max_excess = counter%max_excess
  sum_excess = counter%sum_excess
  dropped = counter%dropped
  call MPI_ALLREDUCE (read, counter%read, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
  call MPI_ALLREDUCE (generated, counter%generated, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
  call MPI_ALLREDUCE (positive, counter%positive, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
  call MPI_ALLREDUCE (negative, counter%negative, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)

```

```

call MPI_ALLREDUCE (zero, counter%zero, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
call MPI_ALLREDUCE (excess, counter%excess, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
call MPI_ALLREDUCE (max_excess, counter%max_excess, 1, MPI_DOUBLE_PRECISION, MPI_MAX, MPI_COMM_WORLD)
call MPI_ALLREDUCE (sum_excess, counter%sum_excess, 1, MPI_DOUBLE_PRECISION, MPI_SUM, MPI_COMM_WORLD)
call MPI_ALLREDUCE (dropped, counter%dropped, 1, MPI_INTEGER, MPI_SUM, MPI_COMM_WORLD)
!! \todo{sbrass - Implement allreduce of mean and variance, relevant for weighted events.}
end subroutine counter_allreduce_record

```

<Simulations: counter: TBP>+≡

```

procedure :: record_mean_and_variance => &
  counter_record_mean_and_variance

```

<Simulations: procedures>+≡

```

subroutine counter_record_mean_and_variance (counter, weight, i_nlo)
  class(counter_t), intent(inout) :: counter
  real(default), intent(in) :: weight
  integer, intent(in) :: i_nlo
  real(default), save :: weight_buffer = 0._default
  integer, save :: nlo_count = 1
  if (.not. counter%reproduce_xsection) return
  if (i_nlo == 1) then
    call flush_weight_buffer (weight_buffer, nlo_count)
    weight_buffer = weight
    nlo_count = 1
  else
    weight_buffer = weight_buffer + weight
    nlo_count = nlo_count + 1
  end if
contains
  subroutine flush_weight_buffer (w, n_nlo)
    real(default), intent(in) :: w
    integer, intent(in) :: n_nlo
    integer :: n
    real(default) :: mean_new
    counter%nlo_weight_counter = counter%nlo_weight_counter + 1
    !!! Minus 1 to take into account offset from initialization
    n = counter%nlo_weight_counter - 1
    if (n > 0) then
      mean_new = counter%mean + (w / n_nlo - counter%mean) / n
      if (n > 1) &
        counter%varsq = counter%varsq - counter%varsq / (n - 1) + &
          n * (mean_new - counter%mean)**2
      counter%mean = mean_new
    end if
  end subroutine flush_weight_buffer
end subroutine counter_record_mean_and_variance

```

33.9.2 Simulation: component sets

For each set of process components that share a MCI entry in the process configuration, we keep a separate event record.

<Simulations: types>+≡


```

type :: mci_set_t
  private
  integer :: n_components = 0
  integer, dimension(:), allocatable :: i_component
  type(string_t), dimension(:), allocatable :: component_id
  logical :: has_integral = .false.
  real(default) :: integral = 0
  real(default) :: error = 0
  real(default) :: weight_mci = 0
  type(counter_t) :: counter
contains
  <Simulations: mci set: TBP>
end type mci_set_t

```

Output.

```

<Simulations: mci set: TBP>≡
  procedure :: write => mci_set_write

<Simulations: procedures>+≡
  subroutine mci_set_write (object, unit, pacified)
    class(mci_set_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: pacified
    logical :: pacify
    integer :: u, i
    u = given_output_unit (unit)
    pacify = .false.; if (present (pacified)) pacify = pacified
    write (u, "(3x,A)") "Components:"
    do i = 1, object%n_components
      write (u, "(5x,I0,A,A,A)") object%i_component(i), &
        ": ", char (object%component_id(i)), ""
    end do
    if (object%has_integral) then
      if (pacify) then
        write (u, "(3x,A," // FMT_15 // ")") "Integral = ", object%integral
        write (u, "(3x,A," // FMT_15 // ")") "Error = ", object%error
        write (u, "(3x,A,F9.6)") "Weight = ", object%weight_mci
      else
        write (u, "(3x,A," // FMT_19 // ")") "Integral = ", object%integral
        write (u, "(3x,A," // FMT_19 // ")") "Error = ", object%error
        write (u, "(3x,A,F13.10)") "Weight = ", object%weight_mci
      end if
    else
      write (u, "(3x,A)") "Integral = [undefined]"
    end if
    call object%counter%write (u)
  end subroutine mci_set_write

```

Initialize: Get the indices and names for the process components that will contribute to this set.

```

<Simulations: mci set: TBP>+≡
  procedure :: init => mci_set_init

```

<Simulations: procedures>+≡

```

subroutine mci_set_init (object, i_mci, process)
  class(mci_set_t), intent(out) :: object
  integer, intent(in) :: i_mci
  type(process_t), intent(in), target :: process
  integer :: i
  call process%get_i_component (i_mci, object%i_component)
  object%n_components = size (object%i_component)
  allocate (object%component_id (object%n_components))
  do i = 1, size (object%component_id)
    object%component_id(i) = &
      process%get_component_id (object%i_component(i))
  end do
  if (process%has_integral (i_mci)) then
    object%integral = process%get_integral (i_mci)
    object%error = process%get_error (i_mci)
    object%has_integral = .true.
  end if
end subroutine mci_set_init

```

33.9.3 Process-core Safe

This is an object that temporarily holds a process core object. We need this while rescanning a process with modified parameters. After the rescan, we want to restore the original state.

<Simulations: types>+≡

```

type :: core_safe_t
  class(prc_core_t), allocatable :: core
end type core_safe_t

```

33.9.4 Process Object

The simulation works on process objects. This subroutine makes a process object available for simulation. The process is in the process stack. `use_process` implies that the process should already exist as an object in the process stack. If integration is not yet done, do it. Any generated process object should be put on the global stack, if it is separate from the local one.

<Simulations: procedures>+≡

```

subroutine prepare_process &
  (process, process_id, use_process, integrate, local, global)
  type(process_t), pointer, intent(out) :: process
  type(string_t), intent(in) :: process_id
  logical, intent(in) :: use_process, integrate
  type(rt_data_t), intent(inout), target :: local
  type(rt_data_t), intent(inout), optional, target :: global
  type(rt_data_t), pointer :: current
  if (debug_on) call msg_debug (D_CORE, "prepare_process")
  if (debug_on) call msg_debug (D_CORE, "global present", present (global))
  if (present (global)) then
    current => global
  end if
end subroutine prepare_process

```

```

else
    current => local
end if
process => current%process_stack%get_process_ptr (process_id)
if (debug_on) call msg_debug (D_CORE, "use_process", use_process)
if (debug_on) call msg_debug (D_CORE, "associated process", associated (process))
if (use_process .and. .not. associated (process)) then
    if (integrate) then
        call msg_message ("Simulate: process '" &
            // char (process_id) // "' needs integration")
    else
        call msg_message ("Simulate: process '" &
            // char (process_id) // "' needs initialization")
    end if
    if (present (global)) then
        call integrate_process (process_id, local, global, &
            init_only = .not. integrate)
    else
        call integrate_process (process_id, local, &
            local_stack = .true., init_only = .not. integrate)
    end if
    if (signal_is_pending ()) return
    process => current%process_stack%get_process_ptr (process_id)
    if (associated (process)) then
        if (integrate) then
            call msg_message ("Simulate: integration done")
            call current%process_stack%fill_result_vars (process_id)
        else
            call msg_message ("Simulate: process initialization done")
        end if
    else
        call msg_fatal ("Simulate: process '" &
            // char (process_id) // "' could not be initialized: aborting")
    end if
else if (.not. associated (process)) then
    if (present (global)) then
        call integrate_process (process_id, local, global, &
            init_only = .true.)
    else
        call integrate_process (process_id, local, &
            local_stack = .true., init_only = .true.)
    end if
    process => current%process_stack%get_process_ptr (process_id)
    call msg_message &
        ("Simulate: process '" &
            // char (process_id) // "' : enabled for rescan only")
end if
end subroutine prepare_process

```

33.9.5 Simulation-entry object

For each process that we consider for event generation, we need a separate entry. The entry separately records the process ID and run ID. The `weight_mci` array

is used for selecting a component set (which shares an MCI record inside the process container) when generating an event for the current process.

The simulation entry is an extension of the `event_t` event record. This core object contains configuration data, pointers to the process and process instance, the expressions, flags and values that are evaluated at runtime, and the resulting particle set.

The entry explicitly allocates the `process_instance`, which becomes the process-specific workspace for the event record.

If entries with differing environments are present simultaneously, we may need to switch QCD parameters and/or the model event by event. In this case, the `qcd` and/or `model` components are present.

For the purpose of NLO events, `entry_t` contains a pointer list to other simulation-entries. This is due to the fact that we have to associate an event for each component of the fixed order simulation, i.e. one N -particle event and N_{phs} $N + 1$ -particle events. However, all entries share the same event transforms.

```

<Simulations: types>+≡
  type, extends (event_t) :: entry_t
  private
    type(string_t) :: process_id
    type(string_t) :: library
    type(string_t) :: run_id
    logical :: has_integral = .false.
    real(default) :: integral = 0
    real(default) :: error = 0
    real(default) :: process_weight = 0
    logical :: valid = .false.
    type(counter_t) :: counter
    integer :: n_in = 0
    integer :: n_mci = 0
    type(mci_set_t), dimension(:), allocatable :: mci_sets
    type(selector_t) :: mci_selector
    logical :: has_resonant_subprocess_set = .false.
    type(resonant_subprocess_set_t) :: resonant_subprocess_set
    type(core_safe_t), dimension(:), allocatable :: core_safe
    class(model_data_t), pointer :: model => null ()
    type(qcd_t) :: qcd
    type(entry_t), pointer :: first => null ()
    type(entry_t), pointer :: next => null ()
    class(evt_t), pointer :: evt_powheg => null ()
  contains
    <Simulations: entry: TBP>
  end type entry_t

```

Output. Write just the configuration, the event is written by a separate routine.

The `verbose` option is unused, it is required by the interface of the base-object method.

```

<Simulations: entry: TBP>≡
  procedure :: write_config => entry_write_config

<Simulations: procedures>+≡
  subroutine entry_write_config (object, unit, pacified)
    class(entry_t), intent(in) :: object

```

```

integer, intent(in), optional :: unit
logical, intent(in), optional :: pacified
logical :: pacify
integer :: u, i
u = given_output_unit (unit)
pacify = .false.; if (present (pacified)) pacify = pacified
write (u, "(3x,A,A,A)") "Process = ', char (object%process_id), "'
write (u, "(3x,A,A,A)") "Library = ', char (object%library), "'
write (u, "(3x,A,A,A)") "Run = ', char (object%run_id), "'
write (u, "(3x,A,L1)") "is valid = ", object%valid
if (object%has_integral) then
  if (pacify) then
    write (u, "(3x,A," // FMT_15 // ")") "Integral = ", object%integral
    write (u, "(3x,A," // FMT_15 // ")") "Error = ", object%error
    write (u, "(3x,A,F9.6)") "Weight = ", object%process_weight
  else
    write (u, "(3x,A," // FMT_19 // ")") "Integral = ", object%integral
    write (u, "(3x,A," // FMT_19 // ")") "Error = ", object%error
    write (u, "(3x,A,F13.10)") "Weight = ", object%process_weight
  end if
else
  write (u, "(3x,A)") "Integral = [undefined]"
end if
write (u, "(3x,A,I0)") "MCI sets = ", object%n_mci
call object%counter%write (u)
do i = 1, size (object%mci_sets)
  write (u, "(A)")
  write (u, "(1x,A,I0,A)") "MCI set #", i, ":"
  call object%mci_sets(i)%write (u, pacified)
end do
if (object%resonant_subprocess_set%is_active ()) then
  write (u, "(A)")
  call object%write_resonant_subprocess_data (u)
end if
if (allocated (object%core_safe)) then
  do i = 1, size (object%core_safe)
    write (u, "(1x,A,I0,A)") "Saved process-component core #", i, ":"
    call object%core_safe(i)%core%write (u)
  end do
end if
end if
end subroutine entry_write_config

```

Finalizer. The `instance` pointer component of the `event_t` base type points to a target which we did explicitly allocate in the `entry_init` procedure. Therefore, we finalize and explicitly deallocate it here. Then we call the finalizer of the base type.

```

<Simulations: entry: TBP>+≡
  procedure :: final => entry_final

<Simulations: procedures>+≡
  subroutine entry_final (object)
    class(entry_t), intent(inout) :: object
    integer :: i
    if (associated (object%instance)) then

```

```

do i = 1, object%n_mci
  call object%instance%final_simulation (i)
end do
call object%instance%final ()
deallocate (object%instance)
end if
call object%event_t%final ()
end subroutine entry_final

```

Copy the content of an entry into another one, except for the next-pointer

(Simulations: entry: TBP)+≡

```

procedure :: copy_entry => entry_copy_entry

```

(Simulations: procedures)+≡

```

subroutine entry_copy_entry (entry1, entry2)
  class(entry_t), intent(in), target :: entry1
  type(entry_t), intent(inout), target :: entry2
  call entry1%event_t%clone (entry2%event_t)
  entry2%process_id = entry1%process_id
  entry2%library = entry1%library
  entry2%run_id = entry1%run_id
  entry2%has_integral = entry1%has_integral
  entry2%integral = entry1%integral
  entry2%error = entry1%error
  entry2%process_weight = entry1%process_weight
  entry2%valid = entry1%valid
  entry2%counter = entry1%counter
  entry2%n_in = entry1%n_in
  entry2%n_mci = entry1%n_mci
  if (allocated (entry1%pci_sets)) then
    allocate (entry2%pci_sets (size (entry1%pci_sets)))
    entry2%pci_sets = entry1%pci_sets
  end if
  entry2%pci_selector = entry1%pci_selector
  if (allocated (entry1%core_safe)) then
    allocate (entry2%core_safe (size (entry1%core_safe)))
    entry2%core_safe = entry1%core_safe
  end if
  entry2%model => entry1%model
  entry2%qcd = entry1%qcd
end subroutine entry_copy_entry

```

Simulation-entry initialization

Search for a process entry and allocate a process instance as an anonymous object, temporarily accessible via the `process_instance` pointer. Assign data by looking at the process object and at the environment.

If `n_alt` is set, we prepare for additional alternate sqme and weight entries.

The `compile` flag is only false if we do not need the Whizard process at all, just its definition. In that case, we skip process initialization.

Otherwise, and if the process object is not found initially: if `integrate` is set, attempt an integration pass and try again. Otherwise, just initialize the

object.

If **generate** is set, prepare the MCI objects for generating new events. For pure rescanning, this is not necessary.

If **resonance_history** is set, we create a separate process library which contains all possible restricted subprocesses with distinct resonance histories. These processes will not be integrated, but their matrix element codes are used for determining probabilities of resonance histories. Note that this can work only if the process method is OMega, and the phase-space method is 'wood'.

When done, we assign the **instance** and **process** pointers of the base type by the **connect** method, so we can reference them later.

TODO: In case of NLO event generation, copying the configuration from the master process is rather intransparent. For instance, we override the process var list by the global var list.

```

<Simulations: entry: TBP>+≡
  procedure :: init => entry_init

<Simulations: procedures>+≡
  subroutine entry_init &
    (entry, process_id, &
     use_process, integrate, generate, update_sqme, &
     support_resonance_history, &
     local, global, n_alt)
    class(entry_t), intent(inout), target :: entry
    type(string_t), intent(in) :: process_id
    logical, intent(in) :: use_process, integrate, generate, update_sqme
    logical, intent(in) :: support_resonance_history
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    integer, intent(in), optional :: n_alt
    type(process_t), pointer :: process, master_process
    type(process_instance_t), pointer :: process_instance
    type(process_library_t), pointer :: prclib_saved
    integer :: i
    logical :: res_include_trivial
    logical :: combined_integration
    integer :: selected_mci
    selected_mci = 0
    if (debug_on) call msg_debug (D_CORE, "entry_init")
    if (debug_on) call msg_debug (D_CORE, "process_id", process_id)
    call prepare_process &
      (master_process, process_id, use_process, integrate, local, global)
    if (signal_is_pending ()) return

    if (associated (master_process)) then
      if (.not. master_process%has_matrix_element ()) then
        entry%has_integral = .true.
        entry%process_id = process_id
        entry%valid = .false.
        return
      end if
    else
      call entry%basic_init (local%var_list)
      entry%has_integral = .false.

```

```

        entry%process_id = process_id
        call entry%import_process_def_characteristics (local%prclib, process_id)
        entry%valid = .true.
        return
    end if

    call entry%basic_init (local%var_list, n_alt)

    entry%process_id = process_id
    if (generate .or. integrate) then
        entry%run_id = master_process%get_run_id ()
        process => master_process
    else
        call local%set_log (var_str ("?rebuild_phase_space"), &
            .false., is_known = .true.)
        call local%set_log (var_str ("?check_phs_file"), &
            .false., is_known = .true.)
        call local%set_log (var_str ("?rebuild_grids"), &
            .false., is_known = .true.)
        entry%run_id = &
            local%var_list%get_sval (var_str ("$_run_id"))
        if (update_sqme) then
            call prepare_local_process (process, process_id, local)
        else
            process => master_process
        end if
    end if

    call entry%import_process_characteristics (process)

    allocate (entry%mci_sets (entry%n_mci))
    do i = 1, size (entry%mci_sets)
        call entry%mci_sets(i)%init (i, master_process)
    end do

    call entry%import_process_results (master_process)
    call entry%prepare_expressions (local)

    if (process%is_nlo_calculation ()) then
        call process%init_nlo_settings (global%var_list)
    end if
    combined_integration = local%get_lval (var_str ("?combined_nlo_integration"))
    if (.not. combined_integration) &
        selected_mci = process%extract_active_component_mci ()
    call prepare_process_instance (process_instance, process, local%model, &
        local = local)

    if (generate) then
        if (selected_mci > 0) then
            call process%prepare_simulation (selected_mci)
            call process_instance%init_simulation (selected_mci, entry%config%safety_factor, &
                local%get_lval (var_str ("?keep_failed_events")))
        else
            do i = 1, entry%n_mci

```



```

        call process%prepare_simulation (i)
        call process_instance%init_simulation (i, entry%config%safety_factor, &
            local%get_lval (var_str ("?keep_failed_events")))
    end do
end if
end if

if (support_resonance_history) then
    prclib_saved => local%prclib
    call entry%setup_resonant_subprocesses (local, process)
    if (entry%has_resonant_subprocess_set) then
        if (signal_is_pending ()) return
        call entry%compile_resonant_subprocesses (local)
        if (signal_is_pending ()) return
        call entry%prepare_resonant_subprocesses (local, global)
        if (signal_is_pending ()) return
        call entry%prepare_resonant_subprocess_instances (local)
    end if
    if (signal_is_pending ()) return
    if (associated (prclib_saved)) call local%update_prclib (prclib_saved)
end if

call entry%setup_event_transforms (process, local)

call dispatch_qcd (entry%qcd, local%get_var_list_ptr (), local%os_data)

call entry%connect_qcd ()

if (present (global)) then
    call entry%connect (process_instance, local%model, global%process_stack)
else
    call entry%connect (process_instance, local%model, local%process_stack)
end if
call entry%setup_expressions ()

entry%model => process%get_model_ptr ()

entry%valid = .true.

end subroutine entry_init

```

<Simulations: entry: TBP>+≡
 procedure :: set_active_real_components => entry_set_active_real_components

<Simulations: procedures>+≡
 subroutine entry_set_active_real_components (entry)
 class(entry_t), intent(inout) :: entry
 integer :: i_active_real
 select type (pcm => entry%instance%pcm)
 class is (pcm_nlo_t)
 i_active_real = entry%instance%get_real_of_mci ()
 if (debug_on) call msg_debug2 (D_CORE, "i_active_real", i_active_real)
 if (associated (entry%evt_powheg)) then
 select type (evt => entry%evt_powheg)

```

type is (evt_shower_t)
  if (entry%process%get_component_type(i_active_real) == COMP_REAL_FIN) then
    if (debug_on) call msg_debug (D_CORE, "Disabling Powheg matching for ", i_active_real)
    call evt%disable_powheg_matching ()
  else
    if (debug_on) call msg_debug (D_CORE, "Enabling Powheg matching for ", i_active_real)
    call evt%enable_powheg_matching ()
  end if
class default
  call msg_fatal ("powheg-evt should be evt_shower_t!")
end select
end if
end select
end subroutine entry_set_active_real_components

```

Part of simulation-entry initialization: set up a process object for local use.

(Simulations: procedures)+≡

```

subroutine prepare_local_process (process, process_id, local)
  type(process_t), pointer, intent(inout) :: process
  type(string_t), intent(in) :: process_id
  type(rt_data_t), intent(inout), target :: local
  type(integration_t) :: intg
  call intg%create_process (process_id)
  call intg%init_process (local)
  call intg%setup_process (local, verbose=.false.)
  process => intg%get_process_ptr ()
end subroutine prepare_local_process

```

Part of simulation-entry initialization: set up a process instance matching the selected process object.

The model that we can provide as an extra argument can modify particle settings (polarization) in the density matrices that will be constructed. It does not affect parameters.

(Simulations: procedures)+≡

```

subroutine prepare_process_instance &
  (process_instance, process, model, local)
  type(process_instance_t), pointer, intent(inout) :: process_instance
  type(process_t), intent(inout), target :: process
  class(model_data_t), intent(in), optional :: model
  type(rt_data_t), intent(in), optional, target :: local
  allocate (process_instance)
  call process_instance%init (process)
  if (process%is_nlo_calculation ()) then
    select type (pcm_work => process_instance%pcm_work)
    type is (pcm_nlo_workspace_t)
      select type (pcm => process_instance%pcm)
      type is (pcm_nlo_t)
        if (.not. pcm%settings%combined_integration) &
          call pcm_work%set_radiation_event ()
        if (pcm%settings%fixed_order_nlo) &
          call pcm_work%set_fixed_order_event_mode ()
      end select
    end select
  end if
end subroutine prepare_process_instance

```

```

        end select
        call process%prepare_any_external_code ()
    end if
    call process_instance%setup_event_data (model)
end subroutine prepare_process_instance

```

Part of simulation-entry initialization: query the process for basic information.

```

⟨Simulations: entry: TBP⟩+≡
    procedure, private :: import_process_characteristics &
        => entry_import_process_characteristics

⟨Simulations: procedures⟩+≡
    subroutine entry_import_process_characteristics (entry, process)
        class(entry_t), intent(inout) :: entry
        type(process_t), intent(in), target :: process
        entry%library = process%get_library_name ()
        entry%n_in = process%get_n_in ()
        entry%n_mci = process%get_n_mci ()
    end subroutine entry_import_process_characteristics

```

This is the alternative form which applies if there is no process entry, but just a process definition which we take from the provided prclib definition library.

```

⟨Simulations: entry: TBP⟩+≡
    procedure, private :: import_process_def_characteristics &
        => entry_import_process_def_characteristics

⟨Simulations: procedures⟩+≡
    subroutine entry_import_process_def_characteristics (entry, prclib, id)
        class(entry_t), intent(inout) :: entry
        type(process_library_t), intent(in), target :: prclib
        type(string_t), intent(in) :: id
        entry%library = prclib%get_name ()
        entry%n_in = prclib%get_n_in (id)
    end subroutine entry_import_process_def_characteristics

```

Part of simulation-entry initialization: query the process for integration results.

```

⟨Simulations: entry: TBP⟩+≡
    procedure, private :: import_process_results &
        => entry_import_process_results

⟨Simulations: procedures⟩+≡
    subroutine entry_import_process_results (entry, process)
        class(entry_t), intent(inout) :: entry
        type(process_t), intent(in), target :: process
        if (process%has_integral ()) then
            entry%integral = process%get_integral ()
            entry%error = process%get_error ()
            call entry%set_sigma (entry%integral)
            entry%has_integral = .true.
        end if
    end subroutine entry_import_process_results

```

Part of simulation-entry initialization: create expression factory objects and store them.

```

<Simulations: entry: TBP>+≡
  procedure, private :: prepare_expressions &
    => entry_prepare_expressions

<Simulations: procedures>+≡
  subroutine entry_prepare_expressions (entry, local)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(in), target :: local
    type(eval_tree_factory_t) :: expr_factory
    call expr_factory%init (local%pn%selection_lexpr)
    call entry%set_selection (expr_factory)
    call expr_factory%init (local%pn%reweight_lexpr)
    call entry%set_reweight (expr_factory)
    call expr_factory%init (local%pn%analysis_lexpr)
    call entry%set_analysis (expr_factory)
  end subroutine entry_prepare_expressions

```

Extra (NLO) entries

Initializes the list of additional NLO entries. The routine gets the information about how many entries to associate from `region_data`.

```

<Simulations: entry: TBP>+≡
  procedure :: setup_additional_entries => entry_setup_additional_entries

<Simulations: procedures>+≡
  subroutine entry_setup_additional_entries (entry)
    class(entry_t), intent(inout), target :: entry
    type(entry_t), pointer :: current_entry
    integer :: i, n_phs
    type(evt_nlo_t), pointer :: evt
    integer :: mode
    evt => null ()
    select type (pcm => entry%instance%pcm)
    type is (pcm_nlo_t)
      n_phs = pcm%region_data%n_phs
    end select
    select type (entry)
    type is (entry_t)
      current_entry => entry
      current_entry%first => entry
      call get_nlo_evt_ptr (current_entry, evt, mode)
      if (mode > EVT_NLO_SEPARATE_BORNLIKE) then
        allocate (evt%particle_set_nlo (n_phs + 1))
        evt%event_deps%n_phs = n_phs
        evt%qcd = entry%qcd
        do i = 1, n_phs
          allocate (current_entry%next)
          current_entry%next%first => current_entry%first
          current_entry => current_entry%next
          call entry%copy_entry (current_entry)
          current_entry%i_event = i
        end do
      end if
    end select
  end subroutine entry_setup_additional_entries

```

```

        end do
    else
        allocate (evt%particle_set_nlo (1))
    end if
end select
contains
subroutine get_nlo_evt_ptr (entry, evt, mode)
    type(entry_t), intent(in), target :: entry
    type(evt_nlo_t), intent(out), pointer :: evt
    integer, intent(out) :: mode
    class(evt_t), pointer :: current_evt
    evt => null ()
    current_evt => entry%transform_first
    do
        select type (current_evt)
        type is (evt_nlo_t)
            evt => current_evt
            mode = evt%mode
            exit
        end select
        if (associated (current_evt%next)) then
            current_evt => current_evt%next
        else
            call msg_fatal ("evt_nlo not in list of event transforms")
        end if
    end do
end subroutine get_nlo_evt_ptr
end subroutine entry_setup_additional_entries

```

<Simulations: entry: TBP>+≡

```

procedure :: get_first => entry_get_first

```

<Simulations: procedures>+≡

```

function entry_get_first (entry) result (entry_out)
    class(entry_t), intent(in), target :: entry
    type(entry_t), pointer :: entry_out
    entry_out => null ()
    select type (entry)
    type is (entry_t)
        if (entry%is_nlo ()) then
            entry_out => entry%first
        else
            entry_out => entry
        end if
    end select
end function entry_get_first

```

<Simulations: entry: TBP>+≡

```

procedure :: get_next => entry_get_next

```

<Simulations: procedures>+≡

```

function entry_get_next (entry) result (next_entry)
    class(entry_t), intent(in) :: entry
    type(entry_t), pointer :: next_entry

```

```

next_entry => null ()
if (associated (entry%next)) then
    next_entry => entry%next
else
    call msg_fatal ("Get next entry: No next entry")
end if
end function entry_get_next

```

<Simulations: entry: TBP>+≡
 procedure :: count_nlo_entries => entry_count_nlo_entries

<Simulations: procedures>+≡
 function entry_count_nlo_entries (entry) result (n)
 class(entry_t), intent(in), target :: entry
 integer :: n
 type(entry_t), pointer :: current_entry
 n = 1
 if (.not. associated (entry%next)) then
 return
 else
 current_entry => entry%next
 do
 n = n + 1
 if (.not. associated (current_entry%next)) exit
 current_entry => current_entry%next
 end do
 end if
end function entry_count_nlo_entries

<Simulations: entry: TBP>+≡
 procedure :: reset_nlo_counter => entry_reset_nlo_counter

<Simulations: procedures>+≡
 subroutine entry_reset_nlo_counter (entry)
 class(entry_t), intent(inout) :: entry
 class(evt_t), pointer :: evt
 evt => entry%transform_first
 do
 select type (evt)
 type is (evt_nlo_t)
 evt%i_evaluation = 0
 exit
 end select
 if (associated (evt%next)) evt => evt%next
 end do
end subroutine entry_reset_nlo_counter

<Simulations: entry: TBP>+≡
 procedure :: determine_if_powheg_matching => entry_determine_if_powheg_matching

<Simulations: procedures>+≡
 subroutine entry_determine_if_powheg_matching (entry)
 class(entry_t), intent(inout) :: entry
 class(evt_t), pointer :: current_transform

```

    if (associated (entry%transform_first)) then
      current_transform => entry%transform_first
    do
      select type (current_transform)
      type is (evt_shower_t)
        if (current_transform%contains_powheg_matching ()) &
          entry%evt_powheg => current_transform
        exit
      end select
      if (associated (current_transform%next)) then
        current_transform => current_transform%next
      else
        exit
      end if
    end do
  end if
end subroutine entry_determine_if_powheg_matching

```

Event-transform initialization

Part of simulation-entry initialization: dispatch event transforms (decay, shower) as requested. If a transform is not applicable or switched off via some variable, it will be skipped.

Regarding resonances/decays: these two transforms are currently mutually exclusive. Resonance insertion will not be applied if there is an unstable particle in the game.

The initial particle set is the output of the trivial transform; this has already been applied when the transforms listed here are encountered. Each transform takes a particle set and produces a new one, with one exception: the decay module takes its input from the process object, ignoring the trivial transform. (Reason: spin correlations.) Therefore, the decay module must be first in line.

Settings that we don't or can't support (yet) are rejected by the embedded call to `event_transforms_check`.

```

<Simulations: entry: TBP>+≡
  procedure, private :: setup_event_transforms &
    => entry_setup_event_transforms

<Simulations: procedures>+≡
  subroutine entry_setup_event_transforms (entry, process, local)
    class(entry_t), intent(inout) :: entry
    type(process_t), intent(inout), target :: process
    type(rt_data_t), intent(in), target :: local
    class(evt_t), pointer :: evt
    type(var_list_t), pointer :: var_list
    logical :: enable_isr_handler
    logical :: enable_epa_handler
    logical :: enable_fixed_order
    logical :: enable_shower
    character(len=7) :: sample_normalization

    call event_transforms_check (entry, process, local)
    var_list => local%get_var_list_ptr ()
  end subroutine

```

```

if (process%contains_unstable (local%model)) then
  call dispatch_evt_decay (evt, local%var_list)
  if (associated (evt)) call entry%import_transform (evt)
end if

if (entry%resonant_subprocess_set%is_active ()) then
  call dispatch_evt_resonance (evt, local%var_list, &
    entry%resonant_subprocess_set%get_resonance_history_set (), &
    entry%resonant_subprocess_set%get_libname ())
  if (associated (evt)) then
    call entry%resonant_subprocess_set%connect_transform (evt)
    call entry%resonant_subprocess_set%set_on_shell_limit &
      (local%get_rval (var_str ("resonance_on_shell_limit")))
    call entry%resonant_subprocess_set%set_on_shell_turnoff &
      (local%get_rval (var_str ("resonance_on_shell_turnoff")))
    call entry%resonant_subprocess_set%set_background_factor &
      (local%get_rval (var_str ("resonance_background_factor")))
    call entry%import_transform (evt)
  end if
end if

enable_fixed_order = local%get_lval (var_str ("?fixed_order_nlo_events"))
if (enable_fixed_order) then
  call dispatch_evt_nlo &
    (evt, local%get_lval (var_str ("?keep_failed_events")))
  call entry%import_transform (evt)
end if

enable_isr_handler = local%get_lval (var_str ("?isr_handler"))
enable_epa_handler = local%get_lval (var_str ("?epa_handler"))
if (enable_isr_handler .or. enable_epa_handler) then
  call dispatch_evt_isr_epa_handler (evt, local%var_list)
  if (associated (evt)) call entry%import_transform (evt)
end if

enable_shower = local%get_lval (var_str ("?allow_shower")) .and. &
  (local%get_lval (var_str ("?ps_isr_active")) &
  .or. local%get_lval (var_str ("?ps_fsr_active")) &
  .or. local%get_lval (var_str ("?muli_active")) &
  .or. local%get_lval (var_str ("?mlm_matching")) &
  .or. local%get_lval (var_str ("?ckkw_matching")) &
  .or. local%get_lval (var_str ("?powheg_matching")))
if (enable_shower) then
  call dispatch_evt_shower (evt, var_list, local%model, &
    local%fallback_model, local%os_data, local%beam_structure, &
    process)
  call entry%import_transform (evt)
end if

if (local%get_lval (var_str ("?hadronization_active"))) then
  call dispatch_evt_hadrons (evt, var_list, local%fallback_model)
  call entry%import_transform (evt)
end if

```



```
end subroutine entry_setup_event_transforms
```

This routine rejects all event-transform settings which we don't support at present.

(Simulations: procedures)+≡

```
subroutine event_transforms_check (entry, process, local)
  class(entry_t), intent(in) :: entry
  type(process_t), intent(in), target :: process
  type(rt_data_t), intent(in), target :: local

  if (local%get_lval (var_str ("?fixed_order_nlo_events"))) then
    if (local%get_lval (var_str ("?unweighted"))) then
      call msg_fatal ("NLO fixed-order events have to be generated with &
        &?unweighted = false")
    end if
    select case (char (local%get_sval (var_str ("sample_normalization"))))
    case ("sigma", "auto")
    case default
      call msg_fatal ("NLO fixed-order events: only &
        &sample_normalization = 'sigma' is supported.")
    end select
    if (process%contains_unstable (local%model)) then
      call msg_fatal ("NLO fixed-order events: unstable final-state &
        &particles not supported yet")
    end if
    if (entry%resonant_subprocess_set%is_active ()) then
      call msg_fatal ("NLO fixed-order events: resonant subprocess &
        &insertion not supported")
    end if
    if (local%get_lval (var_str ("?isr_handler")) &
      .or. local%get_lval (var_str ("?epa_handler"))) then
      call msg_fatal ("NLO fixed-order events: ISR handler for &
        &photon-pT generation not supported yet")
    end if
  end if

  if (process%contains_unstable (local%model) &
    .and. entry%resonant_subprocess_set%is_active ()) then
    call msg_fatal ("Simulation: resonant subprocess insertion with &
      &unstable final-state particles not supported")
  end if

end subroutine event_transforms_check
```

Process/MCI selector

Compute weights. The integral in the argument is the sum of integrals for all processes in the sample. After computing the process weights, we repeat the normalization procedure for the process components.

(Simulations: entry: TBP)+≡

```
procedure :: init_mci_selector => entry_init_mci_selector
```

<Simulations: procedures>+≡

```

subroutine entry_init_mci_selector (entry, negative_weights)
  class(entry_t), intent(inout), target :: entry
  logical, intent(in), optional :: negative_weights
  type(entry_t), pointer :: current_entry
  integer :: i, j, k
  if (debug_on) call msg_debug (D_CORE, "entry_init_mci_selector")
  if (entry%has_integral) then
    select type (entry)
    type is (entry_t)
      current_entry => entry
      do j = 1, current_entry%count_nlo_entries ()
        if (j > 1) current_entry => current_entry%get_next ()
        do k = 1, size(current_entry%mci_sets%integral)
          if (debug_on) call msg_debug (D_CORE, "current_entry%mci_sets(k)%integral", &
            current_entry%mci_sets(k)%integral)
        end do
        call current_entry%mci_selector%init &
          (current_entry%mci_sets%integral, negative_weights)
        do i = 1, current_entry%n_mci
          current_entry%mci_sets(i)%weight_mci = &
            current_entry%mci_selector%get_weight (i)
        end do
      end do
    end select
  end if
end subroutine entry_init_mci_selector

```

Select a MCI entry, using the embedded random-number generator.

<Simulations: entry: TBP>+≡

```

procedure :: select_mci => entry_select_mci

```

<Simulations: procedures>+≡

```

function entry_select_mci (entry) result (i_mci)
  class(entry_t), intent(inout) :: entry
  integer :: i_mci
  if (debug_on) call msg_debug2 (D_CORE, "entry_select_mci")
  i_mci = entry%process%extract_active_component_mci ()
  if (i_mci == 0) call entry%mci_selector%generate (entry%rng, i_mci)
  if (debug_on) call msg_debug2 (D_CORE, "i_mci", i_mci)
end function entry_select_mci

```

Entries: event-wise updates

Record an event for this entry, i.e., increment the appropriate counters.

<Simulations: entry: TBP>+≡

```

procedure :: record => entry_record

```

<Simulations: procedures>+≡

```

subroutine entry_record (entry, i_mci, from_file)
  class(entry_t), intent(inout) :: entry
  integer, intent(in) :: i_mci
  logical, intent(in), optional :: from_file

```

```

real(default) :: weight, excess
integer :: n_dropped
weight = entry%get_weight_prc ()
excess = entry%get_excess_prc ()
n_dropped = entry%get_n_dropped ()
call entry%counter%record (weight, excess, n_dropped, from_file)
if (i_mci > 0) then
  call entry%mci_sets(i_mci)%counter%record (weight, excess)
end if
end subroutine entry_record

```

Update and restore the process core that this entry accesses, when parameters change. If explicit arguments `model`, `qcd`, or `helicity_selection` are provided, use those. Otherwise use the parameters stored in the process object.

These two procedures come with a caching mechanism which guarantees that the current core object is saved when calling `update_process`, and restored by calling `restore_process`. If the flag `saved` is unset, saving is skipped, and the `restore` procedure should not be called.

(Simulations: entry: TBP)+≡

```

procedure :: update_process => entry_update_process
procedure :: restore_process => entry_restore_process

```

(Simulations: procedures)+≡

```

subroutine entry_update_process &
  (entry, model, qcd, helicity_selection, saved)
  class(entry_t), intent(inout) :: entry
  class(model_data_t), intent(in), optional, target :: model
  type(qcd_t), intent(in), optional :: qcd
  type(helicity_selection_t), intent(in), optional :: helicity_selection
  logical, intent(in), optional :: saved
  type(process_t), pointer :: process
  class(prc_core_t), allocatable :: core
  integer :: i, n_terms
  class(model_data_t), pointer :: model_local
  type(qcd_t) :: qcd_local
  logical :: use_saved
  if (present (model)) then
    model_local => model
  else
    model_local => entry%model
  end if
  if (present (qcd)) then
    qcd_local = qcd
  else
    qcd_local = entry%qcd
  end if
  use_saved = .true.; if (present (saved)) use_saved = saved
  process => entry%get_process_ptr ()
  n_terms = process%get_n_terms ()
  if (use_saved) allocate (entry%core_safe (n_terms))
  do i = 1, n_terms
    if (process%has_matrix_element (i, is_term_index = .true.)) then
      call process%extract_core (i, core)
    end if
  end do
end subroutine entry_update_process

```

```

        if (use_saved) then
            call dispatch_core_update (core, &
                model_local, helicity_selection, qcd_local, &
                entry%core_safe(i)%core)
        else
            call dispatch_core_update (core, &
                model_local, helicity_selection, qcd_local)
        end if
        call process%restore_core (i, core)
    end if
end do
end subroutine entry_update_process

subroutine entry_restore_process (entry)
    class(entry_t), intent(inout) :: entry
    type(process_t), pointer :: process
    class(prc_core_t), allocatable :: core
    integer :: i, n_terms
    process => entry%get_process_ptr ()
    n_terms = process%get_n_terms ()
    do i = 1, n_terms
        if (process%has_matrix_element (i, is_term_index = .true.)) then
            call process%extract_core (i, core)
            call dispatch_core_restore (core, entry%core_safe(i)%core)
            call process%restore_core (i, core)
        end if
    end do
    deallocate (entry%core_safe)
end subroutine entry_restore_process

```

<Simulations: entry: TBP>+≡

```

    procedure :: connect_qcd => entry_connect_qcd

```

<Simulations: procedures>+≡

```

subroutine entry_connect_qcd (entry)
    class(entry_t), intent(inout), target :: entry
    class(evt_t), pointer :: evt
    evt => entry%transform_first
    do while (associated (evt))
        select type (evt)
            type is (evt_shower_t)
                evt%qcd = entry%qcd
                if (allocated (evt%matching)) then
                    evt%matching%qcd = entry%qcd
                end if
            end select
            evt => evt%next
        end do
    end subroutine entry_connect_qcd

```

33.9.6 Handling resonant subprocesses

Resonant subprocesses are required if we want to determine resonance histories when generating events. The feature is optional, to be switched on by the user.

This procedure initializes a new, separate process library that contains copies of the current process, restricted to the relevant resonance histories. (If this library exists already, it is just kept.) The histories can be extracted from the process object.

The code has to match the assignments in `create_resonant_subprocess_library`. The library may already exist – in that case, here it will be recovered without recompilation.

```

⟨Simulations: entry: TBP⟩+=
  procedure :: setup_resonant_subprocesses &
    => entry_setup_resonant_subprocesses

⟨Simulations: procedures⟩+=
  subroutine entry_setup_resonant_subprocesses (entry, global, process)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(inout), target :: global
    type(process_t), intent(in), target :: process
    type(string_t) :: libname
    type(resonance_history_set_t) :: res_history_set
    type(process_library_t), pointer :: lib
    type(process_component_def_t), pointer :: process_component_def
    logical :: req_resonant, library_exist
    integer :: i_component
    libname = process%get_library_name ()
    lib => global%prclib_stack%get_library_ptr (libname)
    entry%has_resonant_subprocess_set = lib%req_resonant (process%get_id ())
    if (entry%has_resonant_subprocess_set) then
      libname = get_libname_res (process%get_id ())
      call entry%resonant_subprocess_set%init (process%get_n_components ())
      call entry%resonant_subprocess_set%create_library &
        (libname, global, library_exist)
      do i_component = 1, process%get_n_components ()
        call process%extract_resonance_history_set &
          (res_history_set, i_component = i_component)
        call entry%resonant_subprocess_set%fill_resonances &
          (res_history_set, i_component)
        if (.not. library_exist) then
          process_component_def &
            => process%get_component_def_ptr (i_component)
          call entry%resonant_subprocess_set%add_to_library &
            (i_component, &
              process_component_def%get_prt_spec_in (), &
              process_component_def%get_prt_spec_out (), &
              global)
        end if
      end do
      call entry%resonant_subprocess_set%freeze_library (global)
    end if
  end subroutine entry_setup_resonant_subprocesses

```

Compile the resonant-subprocesses library. The library is assumed to be the current library in the `global` object. This is a simple wrapper.

```

<Simulations: entry: TBP>+≡
  procedure :: compile_resonant_subprocesses &
    => entry_compile_resonant_subprocesses

<Simulations: procedures>+≡
  subroutine entry_compile_resonant_subprocesses (entry, global)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(inout), target :: global
    call entry%resonant_subprocess_set%compile_library (global)
  end subroutine entry_compile_resonant_subprocesses

```

Prepare process objects for the resonant-subprocesses library. The process objects are appended to the global process stack. We initialize the processes, such that we can evaluate matrix elements, but we do not need to integrate them.

```

<Simulations: entry: TBP>+≡
  procedure :: prepare_resonant_subprocesses &
    => entry_prepare_resonant_subprocesses

<Simulations: procedures>+≡
  subroutine entry_prepare_resonant_subprocesses (entry, local, global)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    call entry%resonant_subprocess_set%prepare_process_objects (local, global)
  end subroutine entry_prepare_resonant_subprocesses

```

Prepare process instances. They are linked to their corresponding process objects. Both, process and instance objects, are allocated as anonymous targets inside the `resonant_subprocess_set` component.

NOTE: those anonymous object are likely forgotten during finalization of the parent `event_t` (extended as `entry_t`) object. This should be checked! The memory leak is probably harmless as long as the event object is created once per run, not once per event.

```

<Simulations: entry: TBP>+≡
  procedure :: prepare_resonant_subprocess_instances &
    => entry_prepare_resonant_subprocess_instances

<Simulations: procedures>+≡
  subroutine entry_prepare_resonant_subprocess_instances (entry, global)
    class(entry_t), intent(inout) :: entry
    type(rt_data_t), intent(in), target :: global
    call entry%resonant_subprocess_set%prepare_process_instances (global)
  end subroutine entry_prepare_resonant_subprocess_instances

```

Display the resonant subprocesses. This includes, upon request, the resonance set that defines those subprocess, and a short or long account of the process objects themselves.

```

<Simulations: entry: TBP>+≡
  procedure :: write_resonant_subprocess_data &
    => entry_write_resonant_subprocess_data

```

<Simulations: procedures>+≡

```

subroutine entry_write_resonant_subprocess_data (entry, unit)
  class(entry_t), intent(in) :: entry
  integer, intent(in), optional :: unit
  integer :: u, i
  u = given_output_unit (unit)
  call entry%resonant_subprocess_set%write (unit)
  write (u, "(1x,A,I0)") "Resonant subprocesses refer to &
    &process component #", 1
end subroutine entry_write_resonant_subprocess_data

```

Display of the master process for the current event, for diagnostics.

<Simulations: entry: TBP>+≡

```

procedure :: write_process_data => entry_write_process_data

```

<Simulations: procedures>+≡

```

subroutine entry_write_process_data &
  (entry, unit, show_process, show_instance, verbose)
  class(entry_t), intent(in) :: entry
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: show_process
  logical, intent(in), optional :: show_instance
  logical, intent(in), optional :: verbose
  integer :: u, i
  logical :: s_proc, s_inst, verb
  type(process_t), pointer :: process
  type(process_instance_t), pointer :: instance
  u = given_output_unit (unit)
  s_proc = .false.; if (present (show_process)) s_proc = show_process
  s_inst = .false.; if (present (show_instance)) s_inst = show_instance
  verb = .false.; if (present (verbose)) verb = verbose
  if (s_proc .or. s_inst) then
    write (u, "(1x,A,':')") "Process data"
    if (s_proc) then
      process => entry%process
      if (associated (process)) then
        if (verb) then
          call write_separator (u, 2)
          call process%write (.false., u)
        else
          call process%show (u, verbose=.false.)
        end if
      else
        write (u, "(3x,A)") "[not associated]"
      end if
    end if
    if (s_inst) then
      instance => entry%instance
      if (associated (instance)) then
        if (verb) then
          call instance%write (u)
        else
          call instance%write_header (u)
        end if
      end if
    end if
  end if

```

```

        else
            write (u, "(3x,A)") "Process instance: [not associated]"
        end if
    end if
end if
end if
end subroutine entry_write_process_data

```

33.9.7 Entries for alternative environment

Entries for alternate environments. [No additional components anymore, so somewhat redundant.]

```

⟨Simulations: types⟩+≡
    type, extends (entry_t) :: alt_entry_t
    contains
        ⟨Simulations: alt entry: TBP⟩
    end type alt_entry_t

```

The alternative entries are there to re-evaluate the event, given momenta, in a different context.

Therefore, we allocate a local process object and use this as the reference for the local process instance, when initializing the entry. We temporarily import the `process` object into an `integration_t` wrapper, to take advantage of the associated methods. The local process object is built in the context of the current environment, here called `global`. Then, we initialize the process instance.

The `master_process` object contains the integration results to which we refer when recalculating an event. Therefore, we use this object instead of the locally built `process` when we extract the integration results.

The locally built `process` object should be finalized when done. It remains accessible via the `event_t` base object of `entry`, which contains pointers to the process and instance.

```

⟨Simulations: alt entry: TBP⟩≡
    procedure :: init_alt => alt_entry_init

⟨Simulations: procedures⟩+≡
    subroutine alt_entry_init (entry, process_id, master_process, local)
        class(alt_entry_t), intent(inout), target :: entry
        type(string_t), intent(in) :: process_id
        type(process_t), intent(in), target :: master_process
        type(rt_data_t), intent(inout), target :: local
        type(process_t), pointer :: process
        type(process_instance_t), pointer :: process_instance
        type(string_t) :: run_id
        integer :: i

        call msg_message ("Simulate: initializing alternate process setup ...")

        run_id = &
            local%var_list%get_sval (var_str ("run_id"))
        call local%set_log (var_str ("?rebuild_phase_space"), &
            .false., is_known = .true.)
    end subroutine alt_entry_init

```



```

call local%set_log (var_str ("?check_phs_file"), &
    .false., is_known = .true.)
call local%set_log (var_str ("?rebuild_grids"), &
    .false., is_known = .true.)

call entry%basic_init (local%var_list)

call prepare_local_process (process, process_id, local)
entry%process_id = process_id
entry%run_id = run_id

call entry%import_process_characteristics (process)

allocate (entry%mci_sets (entry%n_mci))
do i = 1, size (entry%mci_sets)
    call entry%mci_sets(i)%init (i, master_process)
end do

call entry%import_process_results (master_process)
call entry%prepare_expressions (local)

call prepare_process_instance (process_instance, process, local%model)
call entry%setup_event_transforms (process, local)

call entry%connect (process_instance, local%model, local%process_stack)
call entry%setup_expressions ()

entry%model => process%get_model_ptr ()

call msg_message ("... alternate process setup complete.")

end subroutine alt_entry_init

```

Copy the particle set from the master entry to the alternate entry. This is the particle set of the hard process.

```

<Simulations: alt entry: TBP>+≡
    procedure :: fill_particle_set => entry_fill_particle_set

<Simulations: procedures>+≡
    subroutine entry_fill_particle_set (alt_entry, entry)
        class(alt_entry_t), intent(inout) :: alt_entry
        class(entry_t), intent(in), target :: entry
        type(particle_set_t) :: pset
        call entry%get_hard_particle_set (pset)
        call alt_entry%set_hard_particle_set (pset)
        call pset%final ()
    end subroutine entry_fill_particle_set

```

33.9.8 The simulation object

Each simulation object corresponds to an event sample, identified by the `sample_id`.

The simulation may cover several processes simultaneously. All process-specific data, including the event records, are stored in the **entry** subobjects. The **current** index indicates which record was selected last. **version** is foreseen to contain a tag on the WHIZARD event file version. It can be

```

<Simulations: public>≡
    public :: simulation_t

<Simulations: types>+≡
    type :: simulation_t
        private
        type(rt_data_t), pointer :: local => null ()
        type(string_t) :: sample_id
        logical :: unweighted = .true.
        logical :: negative_weights = .false.
        logical :: support_resonance_history = .false.
        logical :: respect_selection = .true.
        integer :: norm_mode = NORM_UNDEFINED
        logical :: update_sqme = .false.
        logical :: update_weight = .false.
        logical :: update_event = .false.
        logical :: recover_beams = .false.
        logical :: pacify = .false.
        integer :: n_max_tries = 10000
        integer :: n_prc = 0
        integer :: n_alt = 0
        logical :: has_integral = .false.
        logical :: valid = .false.
        real(default) :: integral = 0
        real(default) :: error = 0
        integer :: version = 1
        character(32) :: md5sum_prc = ""
        character(32) :: md5sum_cfg = ""
        character(32), dimension(:), allocatable :: md5sum_alt
        type(entry_t), dimension(:), allocatable :: entry
        type(alt_entry_t), dimension(:,:), allocatable :: alt_entry
        type(selector_t) :: process_selector
        integer :: n_evt_requested = 0
        integer :: event_index_offset = 0
        logical :: event_index_set = .false.
        integer :: event_index = 0
        integer :: split_n_evt = 0
        integer :: split_n_kbytes = 0
        integer :: split_index = 0
        type(counter_t) :: counter
        class(rng_t), allocatable :: rng
        integer :: i_prc = 0
        integer :: i_mci = 0
        real(default) :: weight = 0
        real(default) :: excess = 0
        integer :: n_dropped = 0
    contains
        <Simulations: simulation: TBP>
end type simulation_t

```

Output of the simulation data

`write_config` writes just the configuration. `write` as a method of the base type `event_t` writes the current event and process instance, depending on options.

(Simulations: simulation: TBP)≡

```
procedure :: write => simulation_write
```

(Simulations: procedures)+≡

```
subroutine simulation_write (object, unit, testflag)
  class(simulation_t), intent(in) :: object
  integer, intent(in), optional :: unit
  logical, intent(in), optional :: testflag
  logical :: pacified
  integer :: u, i
  u = given_output_unit (unit)
  pacified = object%pacify; if (present (testflag)) pacified = testflag
  call write_separator (u, 2)
  write (u, "(1x,A,A,A)") "Event sample: '", char (object%sample_id), "'
  write (u, "(3x,A,I0)") "Processes      = ", object%n_prc
  if (object%n_alt > 0) then
    write (u, "(3x,A,I0)") "Alt.wgts      = ", object%n_alt
  end if
  write (u, "(3x,A,L1)") "Unweighted   = ", object%unweighted
  write (u, "(3x,A,A)") "Event norm   = ", &
    char (event_normalization_string (object%norm_mode))
  write (u, "(3x,A,L1)") "Neg. weights = ", object%negative_weights
  write (u, "(3x,A,L1)") "Res. history = ", object%support_resonance_history
  write (u, "(3x,A,L1)") "Respect sel. = ", object%respect_selection
  write (u, "(3x,A,L1)") "Update sqme  = ", object%update_sqme
  write (u, "(3x,A,L1)") "Update wgt   = ", object%update_weight
  write (u, "(3x,A,L1)") "Update event = ", object%update_event
  write (u, "(3x,A,L1)") "Recov. beams = ", object%recover_beams
  write (u, "(3x,A,L1)") "Pacify       = ", object%pacify
  write (u, "(3x,A,I0)") "Max. tries   = ", object%n_max_tries
  if (object%has_integral) then
    if (pacified) then
      write (u, "(3x,A," // FMT_15 // ")") &
        "Integral      = ", object%integral
      write (u, "(3x,A," // FMT_15 // ")") &
        "Error          = ", object%error
    else
      write (u, "(3x,A," // FMT_19 // ")") &
        "Integral      = ", object%integral
      write (u, "(3x,A," // FMT_19 // ")") &
        "Error          = ", object%error
    end if
  else
    write (u, "(3x,A)") "Integral      = [undefined]"
  end if
  write (u, "(3x,A,L1)") "Sim. valid   = ", object%valid
  write (u, "(3x,A,I0)") "Ev.file ver. = ", object%version
  if (object%md5sum_prc /= "") then
    write (u, "(3x,A,A,A)") "MD5 sum (proc) = '", object%md5sum_prc, "'"
  end if
  if (object%md5sum_cfg /= "") then
```

```

        write (u, "(3x,A,A,A)") "MD5 sum (config) = ', object%md5sum_cfg, '"
    end if
    write (u, "(3x,A,I0)") "Events requested = ", object%n_evt_requested
    if (object%event_index_offset /= 0) then
        write (u, "(3x,A,I0)") "Event index offset= ", object%event_index_offset
    end if
    if (object%event_index_set) then
        write (u, "(3x,A,I0)") "Event index      = ", object%event_index
    end if
    if (object%split_n_evt > 0 .or. object%split_n_kbytes > 0) then
        write (u, "(3x,A,I0)") "Events per file   = ", object%split_n_evt
        write (u, "(3x,A,I0)") "KBytes per file   = ", object%split_n_kbytes
        write (u, "(3x,A,I0)") "First file index = ", object%split_index
    end if
    call object%counter%write (u)
    call write_separator (u)
    if (object%i_prc /= 0) then
        write (u, "(1x,A)") "Current event:"
        write (u, "(3x,A,I0,A,A)") "Process #", &
            object%i_prc, ": ", &
            char (object%entry(object%i_prc)%process_id)
        write (u, "(3x,A,I0)") "MCI set #", object%i_mci
        write (u, "(3x,A," // FMT_19 // ")") "Weight      = ", object%weight
        if (.not. vanishes (object%excess)) &
            write (u, "(3x,A," // FMT_19 // ")") "Excess      = ", object%excess
        write (u, "(3x,A,I0)") "Zero-weight events dropped = ", object%n_dropped
    else
        write (u, "(1x,A,I0,A,A)") "Current event: [undefined]"
    end if
    call write_separator (u)
    if (allocated (object%rng)) then
        call object%rng%write (u)
    else
        write (u, "(3x,A)") "Random-number generator: [undefined]"
    end if
    if (allocated (object%entry)) then
        do i = 1, size (object%entry)
            if (i == 1) then
                call write_separator (u, 2)
            else
                call write_separator (u)
            end if
            write (u, "(1x,A,I0,A)") "Process #", i, ":"
            call object%entry(i)%write_config (u, pacified)
        end do
    end if
    call write_separator (u, 2)
end subroutine simulation_write

```

Write the current event record. If an explicit index is given, write that event record.

We implement writing to `unit` (event contents / debugging format) and writing to an `eio` event stream (storage). We include a `testflag` in order to

suppress numerical noise in the testsuite.

```
<Simulations: simulation: TBP>+≡
  generic :: write_event => write_event_unit
  procedure :: write_event_unit => simulation_write_event_unit

<Simulations: procedures>+≡
  subroutine simulation_write_event_unit &
    (object, unit, i_prc, verbose, testflag)
    class(simulation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    logical, intent(in), optional :: verbose
    integer, intent(in), optional :: i_prc
    logical, intent(in), optional :: testflag
    logical :: pacified
    integer :: current
    pacified = .false.; if (present(testflag)) pacified = testflag
    pacified = pacified .or. object%pacify
    if (present (i_prc)) then
      current = i_prc
    else
      current = object%i_prc
    end if
    if (current > 0) then
      call object%entry(current)%write (unit, verbose = verbose, &
        testflag = pacified)
    else
      call msg_fatal ("Simulation: write event: no process selected")
    end if
  end subroutine simulation_write_event_unit
```

This writes one of the alternate events, if allocated.

```
<Simulations: simulation: TBP>+≡
  procedure :: write_alt_event => simulation_write_alt_event

<Simulations: procedures>+≡
  subroutine simulation_write_alt_event (object, unit, j_alt, i_prc, &
    verbose, testflag)
    class(simulation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: j_alt
    integer, intent(in), optional :: i_prc
    logical, intent(in), optional :: verbose
    logical, intent(in), optional :: testflag
    integer :: i, j
    if (present (j_alt)) then
      j = j_alt
    else
      j = 1
    end if
    if (present (i_prc)) then
      i = i_prc
    else
      i = object%i_prc
    end if
```

```

if (i > 0) then
  if (j > 0 .and. j <= object%n_alt) then
    call object%alt_entry(i,j)%write (unit, verbose = verbose, &
      testflag = testflag)
  else
    call msg_fatal ("Simulation: write alternate event: out of range")
  end if
else
  call msg_fatal ("Simulation: write alternate event: no process selected")
end if
end subroutine simulation_write_alt_event

```

This writes the contents of the resonant subprocess set in the current event record.

```

<Simulations: simulation: TBP>+≡
  procedure :: write_resonant_subprocess_data &
    => simulation_write_resonant_subprocess_data

<Simulations: procedures>+≡
  subroutine simulation_write_resonant_subprocess_data (object, unit, i_prc)
    class(simulation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: i_prc
    integer :: i
    if (present (i_prc)) then
      i = i_prc
    else
      i = object%i_prc
    end if
    call object%entry(i)%write_resonant_subprocess_data (unit)
  end subroutine simulation_write_resonant_subprocess_data

```

The same for the master process, as an additional debugging aid.

```

<Simulations: simulation: TBP>+≡
  procedure :: write_process_data &
    => simulation_write_process_data

<Simulations: procedures>+≡
  subroutine simulation_write_process_data &
    (object, unit, i_prc, &
      show_process, show_instance, verbose)
    class(simulation_t), intent(in) :: object
    integer, intent(in), optional :: unit
    integer, intent(in), optional :: i_prc
    logical, intent(in), optional :: show_process
    logical, intent(in), optional :: show_instance
    logical, intent(in), optional :: verbose
    integer :: i
    if (present (i_prc)) then
      i = i_prc
    else
      i = object%i_prc
    end if
    call object%entry(i)%write_process_data &

```

```

        (unit, show_process, show_instance, verbose)
    end subroutine simulation_write_process_data

```

Write the actual efficiency of the simulation run. We get the total number of events stored in the simulation counter and compare this with the total number of calls stored in the event entries.

In order not to miscount samples that are partly read from file, use the **generated** counter, not the **total** counter.

```

<Simulations: simulation: TBP>+≡
    procedure :: show_efficiency => simulation_show_efficiency

<Simulations: procedures>+≡
    subroutine simulation_show_efficiency (simulation)
        class(simulation_t), intent(inout) :: simulation
        integer :: n_events, n_calls
        real(default) :: eff
        n_events = simulation%counter%generated
        n_calls = sum (simulation%entry%get_actual_calls_total ())
        if (n_calls > 0) then
            eff = real (n_events, kind=default) / n_calls
            write (msg_buffer, "(A,1x,F6.2,1x,A)") &
                "Events: actual unweighting efficiency =", 100 * eff, "%"
            call msg_message ()
        end if
    end subroutine simulation_show_efficiency

```

Compute the checksum of the process set. We retrieve the MD5 sums of all processes. This depends only on the process definitions, while parameters are not considered. The configuration checksum is retrieved from the MCI records in the process objects and furthermore includes beams, parameters, integration results, etc., so matching the latter should guarantee identical physics.

```

<Simulations: simulation: TBP>+≡
    procedure :: compute_md5sum => simulation_compute_md5sum

<Simulations: procedures>+≡
    subroutine simulation_compute_md5sum (simulation)
        class(simulation_t), intent(inout) :: simulation
        type(process_t), pointer :: process
        type(string_t) :: buffer
        integer :: j, i, n_mci, i_mci, n_component, i_component
        if (simulation%md5sum_prc == "") then
            buffer = ""
            do i = 1, simulation%n_prc
                if (.not. simulation%entry(i)%valid) cycle
                process => simulation%entry(i)%get_process_ptr ()
                if (associated (process)) then
                    n_component = process%get_n_components ()
                    do i_component = 1, n_component
                        if (process%has_matrix_element (i_component)) then
                            buffer = buffer // process%get_md5sum_prc (i_component)
                        end if
                    end do
                end if
            end do
        end if
    end subroutine simulation_compute_md5sum

```

```

        end do
        simulation%md5sum_prc = md5sum (char (buffer))
    end if
    if (simulation%md5sum_cfg == "") then
        buffer = ""
        do i = 1, simulation%n_prc
            if (.not. simulation%entry(i)%valid) cycle
            process => simulation%entry(i)%get_process_ptr ()
            if (associated (process)) then
                n_mci = process%get_n_mci ()
                do i_mci = 1, n_mci
                    buffer = buffer // process%get_md5sum_mci (i_mci)
                end do
            end if
        end do
        simulation%md5sum_cfg = md5sum (char (buffer))
    end if
    do j = 1, simulation%n_alt
        if (simulation%md5sum_alt(j) == "") then
            buffer = ""
            do i = 1, simulation%n_prc
                process => simulation%alt_entry(i,j)%get_process_ptr ()
                if (associated (process)) then
                    buffer = buffer // process%get_md5sum_cfg ()
                end if
            end do
            simulation%md5sum_alt(j) = md5sum (char (buffer))
        end if
    end do
end subroutine simulation_compute_md5sum

```

Simulation-object finalizer

```

<Simulations: simulation: TBP>+≡
    procedure :: final => simulation_final

<Simulations: procedures>+≡
    subroutine simulation_final (object)
        class(simulation_t), intent(inout) :: object
        integer :: i, j
        if (allocated (object%entry)) then
            do i = 1, size (object%entry)
                call object%entry(i)%final ()
            end do
        end if
        if (allocated (object%alt_entry)) then
            do j = 1, size (object%alt_entry, 2)
                do i = 1, size (object%alt_entry, 1)
                    call object%alt_entry(i,j)%final ()
                end do
            end do
        end if
        if (allocated (object%rng)) call object%rng%final ()
    end subroutine simulation_final

```



```
end subroutine simulation_final
```

Simulation-object initialization

We can deduce all data from the given list of process IDs and the global data set. The process objects are taken from the stack. Once the individual integrals are known, we add them (and the errors), to get the sample integral.

If there are alternative environments, we suspend initialization for setting up alternative process objects, then restore the master process and its parameters. The generator or rescanner can then switch rapidly between processes.

If **integrate** is set, we make sure that all affected processes are integrated before simulation. This is necessary if we want to actually generate events. If **integrate** is unset, we do not need the integral because we just rescan existing events. In that case, we just need compiled matrix elements.

If **generate** is set, we prepare for actually generating events. Otherwise, we may only read and rescan events.

```
<Simulations: simulation: TBP>+≡
  procedure :: init => simulation_init

<Simulations: procedures>+≡
  subroutine simulation_init (simulation, &
    process_id, integrate, generate, local, global, alt_env)
    class(simulation_t), intent(out), target :: simulation
    type(string_t), dimension(:), intent(in) :: process_id
    logical, intent(in) :: integrate, generate
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), optional, target :: global
    type(rt_data_t), dimension(:), intent(inout), optional, target :: alt_env
    class(rng_factory_t), allocatable :: rng_factory
    integer :: next_rng_seed
    type(string_t) :: norm_string, version_string
    logical :: use_process
    integer :: i, j
    type(string_t) :: sample_suffix
  <Simulations: simulation init: extra variables>
    sample_suffix = ""
  <Simulations: simulation init: extra init>
    simulation%local => local
    simulation%sample_id = &
      local%get_sval (var_str ("sample"))
    simulation%unweighted = &
      local%get_lval (var_str ("unweighted"))
    simulation%negative_weights = &
      local%get_lval (var_str ("negative_weights"))
    simulation%support_resonance_history = &
      local%get_lval (var_str ("resonance_history"))
    simulation%respect_selection = &
      local%get_lval (var_str ("sample_select"))
    version_string = &
      local%get_sval (var_str ("event_file_version"))
    norm_string = &
      local%get_sval (var_str ("sample_normalization"))
```

```

simulation%norm_mode = &
    event_normalization_mode (norm_string, simulation%unweighted)
simulation%pacify = &
    local%get_lval (var_str ("?sample_pacify"))
simulation%event_index_offset = &
    local%get_ival (var_str ("event_index_offset"))
simulation%n_max_tries = &
    local%get_ival (var_str ("sample_max_tries"))
simulation%split_n_evt = &
    local%get_ival (var_str ("sample_split_n_evt"))
simulation%split_n_kbytes = &
    local%get_ival (var_str ("sample_split_n_kbytes"))
simulation%split_index = &
    local%get_ival (var_str ("sample_split_index"))
simulation%update_sqme = &
    local%get_lval (var_str ("?update_sqme"))
simulation%update_weight = &
    local%get_lval (var_str ("?update_weight"))
simulation%update_event = &
    local%get_lval (var_str ("?update_event"))
simulation%recover_beams = &
    local%get_lval (var_str ("?recover_beams"))
simulation%counter%reproduce_xsection = &
    local%get_lval (var_str ("?check_event_weights_against_xsection"))
use_process = &
    integrate .or. generate &
    .or. simulation%update_sqme &
    .or. simulation%update_weight &
    .or. simulation%update_event &
    .or. present (alt_env)
select case (size (process_id))
case (0)
    call msg_error ("Simulation: no process selected")
case (1)
    write (msg_buffer, "(A,A,A)") &
        "Starting simulation for process '", &
        char (process_id(1)), "'"
    call msg_message ()
case default
    write (msg_buffer, "(A,A,A)") &
        "Starting simulation for processes '", &
        char (process_id(1)), "' etc."
    call msg_message ()
end select
select case (char (version_string))
case ("", "2.2.4")
    simulation%version = 2
case ("2.2")
    simulation%version = 1
case default
    simulation%version = 0
end select
if (simulation%version == 0) then
    call msg_fatal ("Event file format '" &

```

```

        // char (version_string) &
        // '' is not compatible with this version.")
end if
simulation%n_prc = size (process_id)
allocate (simulation%entry (simulation%n_prc))
if (present (alt_env)) then
    simulation%n_alt = size (alt_env)
    do i = 1, simulation%n_prc
        call simulation%entry(i)%init (process_id(i), &
            use_process, integrate, generate, &
            simulation%update_sqme, &
            simulation%support_resonance_history, &
            local, global, simulation%n_alt)
        if (signal_is_pending ()) return
    end do
    simulation%valid = any (simulation%entry%valid)
    if (.not. simulation%valid) then
        call msg_error ("Simulate: no process has a valid matrix element.")
        return
    end if
    call simulation%update_processes ()
    allocate (simulation%alt_entry (simulation%n_prc, simulation%n_alt))
    allocate (simulation%md5sum_alt (simulation%n_alt))
    simulation%md5sum_alt = ""
    do j = 1, simulation%n_alt
        do i = 1, simulation%n_prc
            call simulation%alt_entry(i,j)%init_alt (process_id(i), &
                simulation%entry(i)%get_process_ptr (), alt_env(j))
            if (signal_is_pending ()) return
        end do
    end do
    call simulation%restore_processes ()
else
    do i = 1, simulation%n_prc
        call simulation%entry(i)%init &
            (process_id(i), &
            use_process, integrate, generate, &
            simulation%update_sqme, &
            simulation%support_resonance_history, &
            local, global)
        call simulation%entry(i)%determine_if_powheg_matching ()
        if (signal_is_pending ()) return
        if (simulation%entry(i)%is_nlo ()) &
            call simulation%entry(i)%setup_additional_entries ()
    end do
    simulation%valid = any (simulation%entry%valid)
    if (.not. simulation%valid) then
        call msg_error ("Simulate: " &
            // "no process has a valid matrix element.")
        return
    end if
end if
!!! if this becomes conditional, some ref files will need update (seed change)
!   if (generate) then

```

```

        call dispatch_rng_factory (rng_factory, local%var_list, next_rng_seed)
        call update_rng_seed_in_var_list (local%var_list, next_rng_seed)
        call rng_factory%make (simulation%rng)
        <Simulations: simulation init: extra RNG init>
!    end if
    if (all (simulation%entry%has_integral)) then
        simulation%integral = sum (simulation%entry%integral)
        simulation%error = sqrt (sum (simulation%entry%error ** 2))
        simulation%has_integral = .true.
        if (integrate .and. generate) then
            do i = 1, simulation%n_prc
                if (simulation%entry(i)%integral < 0 .and. .not. &
                    simulation%negative_weights) then
                    call msg_fatal ("Integral of process '" // &
                        char (process_id (i)) // "'is negative.")
                end if
            end do
        end if
    else
        if (integrate .and. generate) &
            call msg_error ("Simulation contains undefined integrals.")
    end if
    if (simulation%integral > 0 .or. &
        (simulation%integral < 0 .and. simulation%negative_weights)) then
        simulation%valid = .true.
    else if (generate) then
        call msg_error ("Simulate: " &
            // "sum of process integrals must be positive; skipping.")
        simulation%valid = .false.
    else
        simulation%valid = .true.
    end if
    if (simulation%sample_id == "") then
        simulation%sample_id = simulation%get_default_sample_name ()
    end if
    simulation%sample_id = simulation%sample_id // sample_suffix
    if (simulation%valid) call simulation%compute_md5sum ()
end subroutine simulation_init

```

The RNG initialization depends on serial/MPI mode.

<Simulations: simulation init: extra variables>≡

<MPI: Simulations: simulation init: extra variables>≡

```
integer :: rank, n_size
```

<Simulations: simulation init: extra init>≡

<MPI: Simulations: simulation init: extra init>≡

```
call mpi_get_comm_id (n_size, rank)
if (n_size > 1) then
    sample_suffix = var_str ("-") // str (rank)
end if

```

<Simulations: simulation init: extra RNG init>≡

```

<MPI: Simulations: simulation init: extra RNG init>≡
do i = 2, rank + 1
  select type (rng => simulation%rng)
  type is (rng_stream_t)
    call rng%next_substream ()
    if (i == rank) &
      call msg_message ("Simulate: Advance RNG for parallel event generation")
  class default
    call rng%write ()
    call msg_bug ("Parallel event generation: random-number generator &
      &must be 'rng_stream'.")
  end select
end do

```

The number of events that we want to simulate is determined by the settings of `n_events`, `luminosity`, and `?unweighted`. For weighted events, we take `n_events` at face value as the number of matrix element calls. For unweighted events, if the process is a decay, `n_events` is the number of unweighted events. In these cases, the luminosity setting is ignored.

For unweighted events with a scattering process, we calculate the event number that corresponds to the luminosity, given the current value of the integral. We then compare this with `n_events` and choose the larger number.

```

<Simulations: simulation: TBP>+≡
  procedure :: compute_n_events => simulation_compute_n_events

<Simulations: procedures>+≡
  subroutine simulation_compute_n_events (simulation, n_events)
    class(simulation_t), intent(in) :: simulation
    integer, intent(out) :: n_events
    real(default) :: lumi, x_events_lumi
    integer :: n_events_lumi
    logical :: is_scattering
    n_events = &
      simulation%local%get_ival (var_str ("n_events"))
    lumi = &
      simulation%local%get_rval (var_str ("luminosity"))
    if (simulation%unweighted) then
      is_scattering = simulation%entry(1)%n_in == 2
      if (is_scattering) then
        x_events_lumi = abs (simulation%integral * lumi)
        if (x_events_lumi < huge (n_events)) then
          n_events_lumi = nint (x_events_lumi)
        else
          call msg_message ("Simulation: luminosity too large, &
            &limiting number of events")
          n_events_lumi = huge (n_events)
        end if
      if (n_events_lumi > n_events) then
        call msg_message ("Simulation: using n_events as computed from &
          &luminosity value")
        n_events = n_events_lumi
      else
        write (msg_buffer, "(A,1x,I0)") &
          "Simulation: requested number of events =", n_events
      end if
    end if
  end subroutine

```

```

        call msg_message ()
        if (.not. vanishes (simulation%integral)) then
            write (msg_buffer, "(A,1x,ES11.4)" &
                "          corr. to luminosity [fb-1] = ", &
                n_events / simulation%integral
            )
            call msg_message ()
        end if
    end if
end if
end if
end if
end subroutine simulation_compute_n_events

```

Configuration of the OpenMP parameters, in case OpenMP is active. We use the settings accessible via the local environment.

```

<Simulations: simulation: TBP>+≡
    procedure :: setup_openmp => simulation_setup_openmp

<Simulations: procedures>+≡
    subroutine simulation_setup_openmp (simulation)
        class(simulation_t), intent(inout) :: simulation

        call openmp_set_num_threads_verbose &
            (simulation%local%get_ival (var_str ("openmp_num_threads")), &
            simulation%local%get_lval (var_str ("?openmp_logging")))

    end subroutine simulation_setup_openmp

```

Configuration of the event-stream array – i.e., the setup of output file formats.

```

<Simulations: simulation: TBP>+≡
    procedure :: prepare_event_streams => simulation_prepare_event_streams

<Simulations: procedures>+≡
    subroutine simulation_prepare_event_streams (sim, es_array)
        class(simulation_t), intent(inout) :: sim
        type(event_stream_array_t), intent(out) :: es_array

        integer :: n_events
        logical :: rebuild_events, read_raw, write_raw
        integer :: checkpoint, callback
        integer :: n_fmt
        type(event_sample_data_t) :: data
        type(string_t), dimension(:), allocatable :: sample_fmt

        n_events = &
            sim%n_evt_requested
        rebuild_events = &
            sim%local%get_lval (var_str ("?rebuild_events"))
        read_raw = &
            sim%local%get_lval (var_str ("?read_raw")) .and. .not. rebuild_events
        write_raw = &
            sim%local%get_lval (var_str ("?write_raw"))
        checkpoint = &
            sim%local%get_ival (var_str ("checkpoint"))
        callback = &

```

```

        sim%local%get_ival (var_str ("event_callback_interval"))
if (read_raw) then
    inquire (file = char (sim%sample_id) // ".evx", exist = read_raw)
end if
if (allocated (sim%local%sample_fmt)) then
    n_fmt = size (sim%local%sample_fmt)
else
    n_fmt = 0
end if
data = sim%get_data ()
data%n_evt = n_events
data%nlo_multiplier = sim%get_n_nlo_entries (1)
if (read_raw) then
    allocate (sample_fmt (n_fmt))
    if (n_fmt > 0) sample_fmt = sim%local%sample_fmt
    call es_array%init (sim%sample_id, &
        sample_fmt, sim%local, &
        data = data, &
        input = var_str ("raw"), &
        allow_switch = write_raw, &
        checkpoint = checkpoint, &
        callback = callback)
else if (write_raw) then
    allocate (sample_fmt (n_fmt + 1))
    if (n_fmt > 0) sample_fmt(:n_fmt) = sim%local%sample_fmt
    sample_fmt(n_fmt+1) = var_str ("raw")
    call es_array%init (sim%sample_id, &
        sample_fmt, sim%local, &
        data = data, &
        checkpoint = checkpoint, &
        callback = callback)
else if (allocated (sim%local%sample_fmt) &
    .or. checkpoint > 0 &
    .or. callback > 0) then
    allocate (sample_fmt (n_fmt))
    if (n_fmt > 0) sample_fmt = sim%local%sample_fmt
    call es_array%init (sim%sample_id, &
        sample_fmt, sim%local, &
        data = data, &
        checkpoint = checkpoint, &
        callback = callback)
end if
end subroutine simulation_prepare_event_streams

```

<Simulations: simulation: TBP>+≡

```

    procedure :: get_n_nlo_entries => simulation_get_n_nlo_entries

```

<Simulations: procedures>+≡

```

function simulation_get_n_nlo_entries (simulation, i_prc) result (n_extra)
    class(simulation_t), intent(in) :: simulation
    integer, intent(in) :: i_prc
    integer :: n_extra
    n_extra = simulation%entry(i_prc)%count_nlo_entries ()
end function simulation_get_n_nlo_entries

```

Initialize the process selector, using the entry integrals as process weights.

```

<Simulations: simulation: TBP>+=
  procedure :: init_process_selector => simulation_init_process_selector

<Simulations: procedures>+=
  subroutine simulation_init_process_selector (simulation)
    class(simulation_t), intent(inout) :: simulation
    integer :: i
    if (simulation%has_integral) then
      call simulation%process_selector%init (simulation%entry%integral, &
        negative_weights = simulation%negative_weights)
      do i = 1, simulation%n_prc
        associate (entry => simulation%entry(i))
          if (.not. entry%valid) then
            call msg_warning ("Process '" // char (entry%process_id) // &
              "' : matrix element vanishes, no events can be generated.")
            cycle
          end if
          call entry%init_mci_selector (simulation%negative_weights)
          entry%process_weight = simulation%process_selector%get_weight (i)
        end associate
      end do
    end if
  end subroutine simulation_init_process_selector

```

Select a process, using the random-number generator.

```

<Simulations: simulation: TBP>+=
  procedure :: select_prc => simulation_select_prc

<Simulations: procedures>+=
  function simulation_select_prc (simulation) result (i_prc)
    class(simulation_t), intent(inout) :: simulation
    integer :: i_prc
    call simulation%process_selector%generate (simulation%rng, i_prc)
  end function simulation_select_prc

```

Select a MCI set for the selected process.

```

<Simulations: simulation: TBP>+=
  procedure :: select_mci => simulation_select_mci

<Simulations: procedures>+=
  function simulation_select_mci (simulation) result (i_mci)
    class(simulation_t), intent(inout) :: simulation
    integer :: i_mci
    i_mci = 0
    if (simulation%i_prc /= 0) then
      i_mci = simulation%entry(simulation%i_prc)%select_mci ()
    end if
  end function simulation_select_mci

```


Generate-event loop

The requested number of events should be set by this, in time for the event-array initializers that may use this number.

```
<Simulations: simulation: TBP>+≡
  procedure :: set_n_events_requested => simulation_set_n_events_requested
  procedure :: get_n_events_requested => simulation_get_n_events_requested

<Simulations: procedures>+≡
  subroutine simulation_set_n_events_requested (simulation, n)
    class(simulation_t), intent(inout) :: simulation
    integer, intent(in) :: n

    simulation%n_evt_requested = n

  end subroutine simulation_set_n_events_requested

  function simulation_get_n_events_requested (simulation) result (n)
    class(simulation_t), intent(in) :: simulation
    integer :: n

    n = simulation%n_evt_requested

  end function simulation_get_n_events_requested
```

Generate the number of events that has been set by `simulation_set_n_events_requested`. First select a process and a component set, then generate an event for that process and factorize the quantum state. The pair of random numbers can be used for factorization.

When generating events, we drop all configurations where the event is marked as incomplete. This happens if the event fails cuts. In fact, such events are dropped already by the sampler if unweighting is in effect, so this can happen only for weighted events. By setting a limit given by `sample_max_tries` (user parameter), we can avoid an endless loop.

The `begin_it` and `end_it` limits are equal to 1 and the number of events, respectively, in serial mode, but differ for MPI mode.

TODO: When reading from file, event transforms cannot be applied because the process instance will not be complete. (?)

```
<Simulations: simulation: TBP>+≡
  procedure :: generate => simulation_generate

<Simulations: procedures>+≡
  subroutine simulation_generate (simulation, es_array)
    class(simulation_t), intent(inout), target :: simulation
    type(event_stream_array_t), intent(inout), optional :: es_array

    integer :: begin_it, end_it
    integer :: i, j, k

    call simulation%before_first_event (begin_it, end_it, es_array)
    do i = begin_it, end_it
      call simulation%next_event (es_array)
    end do
```

```

        call simulation%after_last_event (begin_it, end_it)

    end subroutine simulation_generate

```

The header of the event loop: with all necessary information present in the `simulation` and `es_array` objects, and given a number of events `n` to generate, we prepare for actually generating/reading/writing events.

The procedure returns the real iteration bounds `begin_it` and `end_it` for the event loop. This is nontrivial only for MPI; in serial mode those are equal to 1 and to `n_events`, respectively.

```

<Simulations: simulation: TBP>+=
    procedure :: before_first_event => simulation_before_first_event

<Simulations: procedures>+=
    subroutine simulation_before_first_event (simulation, begin_it, end_it, &
        es_array)
        class(simulation_t), intent(inout), target :: simulation
        integer, intent(out) :: begin_it
        integer, intent(out) :: end_it
        type(event_stream_array_t), intent(inout), optional :: es_array

        integer :: n_evt_requested
        logical :: has_input
        integer :: n_events_print
        logical :: is_leading_order
        logical :: is_weighted
        logical :: is_polarized

        n_evt_requested = simulation%n_evt_requested
        n_events_print = n_evt_requested * simulation%get_n_nlo_entries (1)
        is_leading_order = (n_events_print == n_evt_requested)

        has_input = .false.
        if (present (es_array)) has_input = es_array%has_input ()

        is_weighted = .not. simulation%entry(1)%config%unweighted
        is_polarized = simulation%entry(1)%config%factorization_mode &
            /= FM_IGNORE_HELICITY

        call simulation%startup_message_generate ( &
            has_input = has_input, &
            is_weighted = is_weighted, &
            is_polarized = is_polarized, &
            is_leading_order = is_leading_order, &
            n_events = n_events_print)

        call simulation%entry%set_n (n_evt_requested)
        if (simulation%n_alt > 0) call simulation%alt_entry%set_n (n_evt_requested)
        call simulation%init_event_index ()

        begin_it = 1
        end_it = n_evt_requested
    <Simulations: simulation generate: extra init>

```

```
end subroutine simulation_before_first_event
```

Keep the user informed:

```
<Simulations: simulation: TBP>+≡
```

```
  procedure, private :: startup_message_generate &  
    => simulation_startup_message_generate
```

```
<Simulations: procedures>+≡
```

```
  subroutine simulation_startup_message_generate (simulation, &  
    has_input, is_weighted, is_polarized, is_leading_order, n_events)  
    class(simulation_t), intent(in) :: simulation  
    logical, intent(in) :: has_input  
    logical, intent(in) :: is_weighted  
    logical, intent(in) :: is_polarized  
    logical, intent(in) :: is_leading_order  
    integer, intent(in) :: n_events  
  
    type(string_t) :: str1, str2, str3, str4  
  
    if (has_input) then  
        str1 = "Events: reading"  
    else  
        str1 = "Events: generating"  
    end if  
    if (is_weighted) then  
        str2 = "weighted"  
    else  
        str2 = "unweighted"  
    end if  
    if (is_polarized) then  
        str3 = ", polarized"  
    else  
        str3 = ", unpolarized"  
    end if  
    str4 = ""  
    if (.not. is_leading_order) str4 = " NLO"  
  
    write (msg_buffer, "(A,1X,I0,1X,A,1X,A)") char (str1), n_events, &  
        char (str2) // char(str3) // char(str4), "events ..."  
    call msg_message ()  
  
    write (msg_buffer, "(A,1x,A)") "Events: event normalization mode", &  
        char (event_normalization_string (simulation%norm_mode))  
    call msg_message ()  
  
end subroutine simulation_startup_message_generate
```

The body of the event loop: generate and process a single event.

Optionally transfer the current event to one of the provided event handles, for in and/or output streams. This works for any stream for which the I/O stream type matches the event-handle type.

```
<Simulations: simulation: TBP>+≡
```

```
  procedure :: next_event => simulation_next_event
```

<Simulations: procedures>+≡

```

subroutine simulation_next_event &
  (simulation, es_array, event_handle_out, event_handle_in)
  class(simulation_t), intent(inout) :: simulation
  type(event_stream_array_t), intent(inout), optional :: es_array
  class(event_handle_t), intent(inout), optional :: event_handle_out
  class(event_handle_t), intent(inout), optional :: event_handle_in

  type(entry_t), pointer :: current_entry
  logical :: generate_new
  logical :: passed
  integer :: j, k

  call simulation%increment_event_index ()

  if (present (es_array)) then
    call simulation%read_event &
      (es_array, .true., generate_new, event_handle_in)
  else
    generate_new = .true.
  end if

  if (generate_new) then
    simulation%i_prc = simulation%select_prc ()
    simulation%i_mci = simulation%select_mci ()

    associate (entry => simulation%entry(simulation%i_prc))

      entry%instance%i_mci = simulation%i_mci
      call entry%set_active_real_components ()
      current_entry => entry%get_first ()

      do k = 1, current_entry%count_nlo_entries ()
        if (k > 1) then
          current_entry => current_entry%get_next ()
          current_entry%particle_set => current_entry%first%particle_set
          current_entry%particle_set_is_valid &
            = current_entry%first%particle_set_is_valid
        end if
        do j = 1, simulation%n_max_tries
          if (.not. current_entry%valid) call msg_warning &
            ("Process '" // char (current_entry%process_id) // "': " // &
            "matrix element vanishes, no events can be generated.")
          call current_entry%generate (simulation%i_mci, i_nlo = k)
          if (signal_is_pending ()) return
          call simulation%counter%record_mean_and_variance &
            (current_entry%weight_prc, k)
          if (current_entry%has_valid_particle_set ()) exit
        end do
      end do
      if (entry%is_nlo ()) call entry%reset_nlo_counter ()

      if (.not. entry%has_valid_particle_set ()) then
        write (msg_buffer, "(A,I0,A)") "Simulation: failed to &

```

```

        &generate valid event after ", &
        simulation%n_max_tries, " tries (sample_max_tries)"
    call msg_fatal ()
end if

current_entry => entry%get_first ()
do k = 1, current_entry%count_nlo_entries ()
    if (k > 1) current_entry => current_entry%get_next ()
    call current_entry%set_index (simulation%get_event_index ())
    call current_entry%evaluate_expressions ()
end do
if (signal_is_pending ()) return

simulation%n_dropped = entry%get_n_dropped ()
if (entry%passed_selection ()) then
    simulation%weight = entry%get_weight_ref ()
    simulation%excess = entry%get_excess_prc ()
end if
call simulation%counter%record &
    (simulation%weight, simulation%excess, simulation%n_dropped)
call entry%record (simulation%i_mci)

end associate

else

    associate (entry => simulation%entry(simulation%i_prc))

        call simulation%set_event_index (entry%get_index ())
        call entry%accept_sqme_ref ()
        call entry%accept_weight_ref ()
        call entry%check ()
        call entry%evaluate_expressions ()
        if (signal_is_pending ()) return

        simulation%n_dropped = entry%get_n_dropped ()
        if (entry%passed_selection ()) then
            simulation%weight = entry%get_weight_ref ()
            simulation%excess = entry%get_excess_prc ()
        end if
        call simulation%counter%record &
            (simulation%weight, simulation%excess, simulation%n_dropped, &
            from_file=.true.)
        call entry%record (simulation%i_mci, from_file=.true.)

    end associate

end if

call simulation%calculate_alt_entries ()
if (simulation%pacify) call pacify (simulation)
if (signal_is_pending ()) return

if (simulation%respect_selection) then

```

```

        passed = simulation%entry(simulation%i_prc)%passed_selection ()
    else
        passed = .true.
    end if
    if (present (es_array)) then
        call simulation%write_event (es_array, passed, event_handle_out)
    end if

end subroutine simulation_next_event

```

Cleanup after last event: compute and show summary information.

```

<Simulations: simulation: TBP>+≡
    procedure :: after_last_event => simulation_after_last_event

<Simulations: procedures>+≡
    subroutine simulation_after_last_event (simulation, begin_it, end_it)
        class(simulation_t), intent(inout) :: simulation
        integer, intent(in) :: begin_it, end_it

        call msg_message ("          ... event sample complete.")
    <Simulations: simulation generate: extra finalize>

        if (simulation%unweighted) call simulation%show_efficiency ()
        call simulation%counter%show_excess ()
        call simulation%counter%show_dropped ()
        call simulation%counter%show_mean_and_variance ()

    end subroutine simulation_after_last_event

```

MPI additions

Below, we define code chunks that differ between the serial and MPI versions.

Extra logging for MPI only.

```

<Simulations: simulation: TBP>+≡
    procedure :: activate_extra_logging => simulation_activate_extra_logging

<Simulations: procedures>+≡
    subroutine simulation_activate_extra_logging (simulation)
        class(simulation_t), intent(in) :: simulation
    <Simulations: activate extra logging>
    end subroutine simulation_activate_extra_logging

<Simulations: activate extra logging>≡
<MPI: Simulations: activate extra logging>≡
    logical :: mpi_logging
    integer :: rank, n_size
    call mpi_get_comm_id (n_size, rank)
    mpi_logging = &
        (simulation%local%get_sval (var_str ("integration_method")) == "vamp2" &
        .and. n_size > 1) &
        .or. simulation%local%get_lval (var_str ("?mpi_logging"))
    call mpi_set_logging (mpi_logging)

```

Extra subroutine to be called before the first event:

```
<Simulations: simulation generate: extra init>≡
```

```
<MPI: Simulations: simulation generate: extra init>≡
```

```
call simulation%init_event_loop_mpi (n_evt_requested, begin_it, end_it)
```

Extra subroutine to be called after the last event:

```
<Simulations: simulation generate: extra finalize>≡
```

```
<MPI: Simulations: simulation generate: extra finalize>≡
```

```
call simulation%final_event_loop_mpi (begin_it, end_it)
```

For MPI event generation, the event-loop interval (1...n) is split up into intervals of `n_workers`.

```
<MPI: Simulations: simulation: TBP>≡
```

```
procedure, private :: init_event_loop_mpi => simulation_init_event_loop_mpi
```

```
<MPI: Simulations: procedures>+≡
```

```
subroutine simulation_init_event_loop_mpi &  
    (simulation, n_events, begin_it, end_it)  
class(simulation_t), intent(inout) :: simulation  
integer, intent(in) :: n_events  
integer, intent(out) :: begin_it, end_it
```

```
integer :: rank, n_workers
```

```
call MPI_COMM_SIZE (MPI_COMM_WORLD, n_workers)
```

```
if (n_workers < 2) then
```

```
    begin_it = 1; end_it = n_events
```

```
    return
```

```
end if
```

```
call MPI_COMM_RANK (MPI_COMM_WORLD, rank)
```

```
if (rank == 0) then
```

```
    call compute_and_scatter_intervals (n_events, begin_it, end_it)
```

```
else
```

```
    call retrieve_intervals (begin_it, end_it)
```

```
end if
```

```
!! Event index starts by 0 (before incrementing when the first event gets generated/read in).
```

```
!! Proof: event_index_offset in [0, N], start_it in [1, N].
```

```
simulation%event_index_offset = simulation%event_index_offset + (begin_it - 1)
```

```
call simulation%init_event_index ()
```

```
write (msg_buffer, "(A,IO,A,IO,A)") &
```

```
    & "MPI: generate events [", begin_it, ":", end_it, "]"
```

```
call msg_message ()
```

contains

```
subroutine compute_and_scatter_intervals (n_events, begin_it, end_it)
```

```
integer, intent(in) :: n_events
```

```
integer, intent(out) :: begin_it, end_it
```

```
integer, dimension(:), allocatable :: all_begin_it, all_end_it
```

```
integer :: rank, n_workers, n_events_per_worker
```

```
call MPI_COMM_RANK (MPI_COMM_WORLD, rank)
```

```

    call MPI_COMM_SIZE (MPI_COMM_WORLD, n_workers)
    allocate (all_begin_it (n_workers), source = 1)
    allocate (all_end_it (n_workers), source = n_events)
    n_events_per_worker = floor (real (n_events, default) / n_workers)
    all_begin_it = [(1 + rank * n_events_per_worker, rank = 0, n_workers - 1)]
    all_end_it = [(rank * n_events_per_worker, rank = 1, n_workers)]
    all_end_it(n_workers) = n_events
    call MPI_SCATTER (all_begin_it, 1, MPI_INTEGER, begin_it, 1, MPI_INTEGER, 0, MPI_COMM_WORLD)
    call MPI_SCATTER (all_end_it, 1, MPI_INTEGER, end_it, 1, MPI_INTEGER, 0, MPI_COMM_WORLD)

end subroutine compute_and_scatter_intervals

subroutine retrieve_intervals (begin_it, end_it)
    integer, intent(out) :: begin_it, end_it

    integer :: local_begin_it, local_end_it

    call MPI_SCATTER (local_begin_it, 1, MPI_INTEGER, begin_it, 1, MPI_INTEGER, 0, MPI_COMM_WORLD)
    call MPI_SCATTER (local_end_it, 1, MPI_INTEGER, end_it, 1, MPI_INTEGER, 0, MPI_COMM_WORLD)

end subroutine retrieve_intervals

end subroutine simulation_init_event_loop_mpi

```

Synchronize, reduce and collect stuff after the event loop has completed.

(MPI: Simulations: simulation: TBP)+≡

```

    procedure, private :: final_event_loop_mpi => simulation_final_event_loop_mpi

```

(MPI: Simulations: procedures)+≡

```

subroutine simulation_final_event_loop_mpi (simulation, begin_it, end_it)
    class(simulation_t), intent(inout) :: simulation
    integer, intent(in) :: begin_it, end_it

    integer :: n_workers, n_events_local, n_events_global

    call MPI_Barrier (MPI_COMM_WORLD)
    call MPI_COMM_SIZE (MPI_COMM_WORLD, n_workers)
    if (n_workers < 2) return
    n_events_local = end_it - begin_it + 1
    call MPI_ALLREDUCE (n_events_local, n_events_global, 1, MPI_INTEGER, MPI_SUM, &
        & MPI_COMM_WORLD)
    write (msg_buffer, "(2(A,1X,I0))") &
        "MPI: Number of generated events locally", n_events_local, " and in world", n_events_global
    call msg_message ()
    call simulation%counter%allreduce_record ()

end subroutine simulation_final_event_loop_mpi

```

Alternate environments

Compute the event matrix element and weight for all alternative environments, given the current event and selected process. We first copy the particle set,

then temporarily update the process core with local parameters, recalculate everything, and restore the process core.

The event weight is obtained by rescaling the original event weight with the ratio of the new and old `sqme` values. (In particular, if the old value was zero, the weight will stay zero.)

Note: this may turn out to be inefficient because we always replace all parameters and recalculate everything, once for each event and environment. However, a more fine-grained control requires more code. In any case, while we may keep multiple process cores (which stay constant for a simulation run), we still have to update the external matrix element parameters event by event. The matrix element “object” is present only once.

```

<Simulations: simulation: TBP>+≡
  procedure :: calculate_alt_entries => simulation_calculate_alt_entries

<Simulations: procedures>+≡
  subroutine simulation_calculate_alt_entries (simulation)
    class(simulation_t), intent(inout) :: simulation
    real(default) :: sqme_prc, weight_prc, factor
    real(default), dimension(:), allocatable :: sqme_alt, weight_alt
    integer :: n_alt, i, j
    i = simulation%i_prc
    n_alt = simulation%n_alt
    if (n_alt == 0) return
    allocate (sqme_alt (n_alt), weight_alt (n_alt))
    associate (entry => simulation%entry(i))
      do j = 1, n_alt
        if (signal_is_pending ()) return
        if (simulation%update_weight) then
          factor = entry%get_kinematical_weight ()
        else
          sqme_prc = entry%get_sqme_prc ()
          weight_prc = entry%get_weight_prc ()
          if (sqme_prc /= 0) then
            factor = weight_prc / sqme_prc
          else
            factor = 0
          end if
        end if
      end do
    end if
    associate (alt_entry => simulation%alt_entry(i,j))
      call alt_entry%update_process (saved=.false.)
      call alt_entry%select &
        (entry%get_i_mci (), entry%get_i_term (), entry%get_channel ())
      call alt_entry%fill_particle_set (entry)
      call alt_entry%recalculate &
        (update_sqme = .true., &
         recover_beams = simulation%recover_beams, &
         weight_factor = factor)
      if (signal_is_pending ()) return
      call alt_entry%accept_sqme_prc ()
      call alt_entry%update_normalization ()
      call alt_entry%accept_weight_prc ()
      call alt_entry%check ()
      call alt_entry%set_index (simulation%get_event_index ())
      call alt_entry%evaluate_expressions ()
    end associate
  end subroutine

```

```

        if (signal_is_pending ()) return
        sqme_alt(j) = alt_entry%get_sqme_ref ()
        if (alt_entry%passed_selection ()) then
            weight_alt(j) = alt_entry%get_weight_ref ()
        end if
    end associate
end do
call entry%update_process (saved=.false.)
call entry%set (sqme_alt = sqme_alt, weight_alt = weight_alt)
call entry%check ()
call entry%store_alt_values ()
end associate
end subroutine simulation_calculate_alt_entries

```

These routines take care of temporary parameter redefinitions that we want to take effect while recalculating the matrix elements. We extract the core(s) of the processes that we are simulating, apply the changes, and make sure that the changes are actually used. This is the duty of `dispatch_core_update`. When done, we restore the original versions using `dispatch_core_restore`.

(Simulations: simulation: TBP)+≡

```

procedure :: update_processes => simulation_update_processes
procedure :: restore_processes => simulation_restore_processes

```

(Simulations: procedures)+≡

```

subroutine simulation_update_processes (simulation, &
    model, qcd, helicity_selection)
    class(simulation_t), intent(inout) :: simulation
    class(model_data_t), intent(in), optional, target :: model
    type(qcd_t), intent(in), optional :: qcd
    type(helicity_selection_t), intent(in), optional :: helicity_selection
    integer :: i
    do i = 1, simulation%n_prc
        call simulation%entry(i)%update_process &
            (model, qcd, helicity_selection)
    end do
end subroutine simulation_update_processes

subroutine simulation_restore_processes (simulation)
    class(simulation_t), intent(inout) :: simulation
    integer :: i
    do i = 1, simulation%n_prc
        call simulation%entry(i)%restore_process ()
    end do
end subroutine simulation_restore_processes

```

Rescan-Events Loop

Rescan an undefined number of events.

If `update_event` or `update_sqme` is set, we have to recalculate the event, starting from the particle set. If the latter is set, this includes the squared matrix element (i.e., the amplitude is evaluated). Otherwise, only kinematics and observables derived from it are recovered.

If any of the update flags is set, we will come up with separate `sqme_prc` and `weight_prc` values. (The latter is only distinct if `update_weight` is set.) Otherwise, we accept the reference values.

```

(Simulations: simulation: TBP)+≡
  procedure :: rescan => simulation_rescan

(Simulations: procedures)+≡
  subroutine simulation_rescan (simulation, n, es_array, global)
    class(simulation_t), intent(inout) :: simulation
    integer, intent(in) :: n
    type(event_stream_array_t), intent(inout) :: es_array
    type(rt_data_t), intent(inout) :: global
    type(qcd_t) :: qcd
    type(string_t) :: str1, str2, str3
    logical :: complete, check_match
    str1 = "Rescanning"
    if (simulation%entry(1)%config%unweighted) then
      str2 = "unweighted"
    else
      str2 = "weighted"
    end if
    simulation%n_evt_requested = n
    call simulation%entry%set_n (n)
    if (simulation%update_sqme .or. simulation%update_weight) then
      call dispatch_qcd (qcd, global%get_var_list_ptr (), global%os_data)
      call simulation%update_processes &
        (global%model, qcd, global%get_helicity_selection ())
      str3 = "(process parameters updated) "
    else
      str3 = ""
    end if
    write (msg_buffer, "(A,1x,A,1x,A,A,A)") char (str1), char (str2), &
      "events ", char (str3), "..."
    call msg_message ()
    call simulation%init_event_index ()
    check_match = .not. global%var_list%get_lval (var_str ("?rescan_force"))
    do
      call simulation%increment_event_index ()
      call simulation%read_event (es_array, .false., complete)
      if (complete) exit
      if (simulation%update_event &
        .or. simulation%update_sqme &
        .or. simulation%update_weight) then
        call simulation%recalculate (check_match = check_match)
        if (signal_is_pending ()) return
        associate (entry => simulation%entry(simulation%i_prc))
          call entry%update_normalization ()
          if (simulation%update_event) then
            call entry%evaluate_transforms ()
          end if
          call entry%check ()
          call entry%evaluate_expressions ()
          if (signal_is_pending ()) return
          simulation%n_dropped = entry%get_n_dropped ()
        end associate
      end if
    end do
  end subroutine

```

```

simulation%weight = entry%get_weight_prc ()
call simulation%counter%record &
    (simulation%weight, n_dropped=simulation%n_dropped, from_file=.true.)
call entry%record (simulation%i_mci, from_file=.true.)
end associate
else
associate (entry => simulation%entry(simulation%i_prc))
call entry%accept_sqme_ref ()
call entry%accept_weight_ref ()
call entry%check ()
call entry%evaluate_expressions ()
if (signal_is_pending ()) return
simulation%n_dropped = entry%get_n_dropped ()
simulation%weight = entry%get_weight_ref ()
call simulation%counter%record &
    (simulation%weight, n_dropped=simulation%n_dropped, from_file=.true.)
call entry%record (simulation%i_mci, from_file=.true.)
end associate
end if
call simulation%calculate_alt_entries ()
if (signal_is_pending ()) return
call simulation%write_event (es_array)
end do
call simulation%counter%show_dropped ()
if (simulation%update_sqme .or. simulation%update_weight) then
call simulation%restore_processes ()
end if
end if
end subroutine simulation_rescan

```

Event index

Here we handle the event index that is kept in the simulation record. The event index is valid for the current sample. When generating or reading events, we initialize the index with the offset that the user provides (if any) and increment it for each event that is generated or read from file. The event index is stored in the event-entry that is current for the event. If an event on file comes with its own index, that index overwrites the predefined one and also resets the index within the simulation record.

The event index is not connected to the `counter` object. The counter is supposed to collect statistical information. The event index is a user-level object that is visible in event records and analysis expressions.

(Simulations: simulation: TBP)+≡

```

procedure :: init_event_index => simulation_init_event_index
procedure :: increment_event_index => simulation_increment_event_index
procedure :: set_event_index => simulation_set_event_index
procedure :: get_event_index => simulation_get_event_index

```

(Simulations: procedures)+≡

```

subroutine simulation_init_event_index (simulation)
class(simulation_t), intent(inout) :: simulation
call simulation%set_event_index (simulation%event_index_offset)
end subroutine simulation_init_event_index

```

```

subroutine simulation_increment_event_index (simulation)
  class(simulation_t), intent(inout) :: simulation
  if (simulation%event_index_set) then
    simulation%event_index = simulation%event_index + 1
  end if
end subroutine simulation_increment_event_index

subroutine simulation_set_event_index (simulation, i)
  class(simulation_t), intent(inout) :: simulation
  integer, intent(in) :: i
  simulation%event_index = i
  simulation%event_index_set = .true.
end subroutine simulation_set_event_index

function simulation_get_event_index (simulation) result (i)
  class(simulation_t), intent(in) :: simulation
  integer :: i
  if (simulation%event_index_set) then
    i = simulation%event_index
  else
    i = 0
  end if
end function simulation_get_event_index

```

33.9.9 Direct event access

If we want to retrieve event information, we should expose the currently selected event `entry` within the simulation object. We recall that this is an extension of the (generic) `event` type. Assuming that we will restrict this to read access, we return a pointer.

```

<Simulations: simulation: TBP>+≡
  procedure :: get_process_index => simulation_get_process_index
  procedure :: get_event_ptr => simulation_get_event_ptr

<Simulations: procedures>+≡
  function simulation_get_process_index (simulation) result (i_prc)
    class(simulation_t), intent(in), target :: simulation
    integer :: i_prc

    i_prc = simulation%i_prc

  end function simulation_get_process_index

  function simulation_get_event_ptr (simulation) result (event)
    class(simulation_t), intent(in), target :: simulation
    class(event_t), pointer :: event

    event => simulation%entry(simulation%i_prc)

  end function simulation_get_event_ptr

```

33.9.10 Event Stream I/O

Write an event to a generic `eio` event stream. The process index must be selected, or the current index must be available.

```

<Simulations: simulation: TBP>+≡
    generic :: write_event => write_event_eio
    procedure :: write_event_eio => simulation_write_event_eio

<Simulations: procedures>+≡
    subroutine simulation_write_event_eio (object, eio, i_prc)
        class(simulation_t), intent(in) :: object
        class(eio_t), intent(inout) :: eio
        integer, intent(in), optional :: i_prc
        logical :: increased
        integer :: current
        if (present (i_prc)) then
            current = i_prc
        else
            current = object%i_prc
        end if
        if (current > 0) then
            if (object%split_n_evt > 0 .and. object%counter%total > 1) then
                if (mod (object%counter%total, object%split_n_evt) == 1) then
                    call eio%split_out ()
                end if
            else if (object%split_n_kbytes > 0) then
                call eio%update_split_count (increased)
                if (increased) call eio%split_out ()
            end if
            call eio%output (object%entry(current)%event_t, current, pacify = object%pacify)
        else
            call msg_fatal ("Simulation: write event: no process selected")
        end if
    end subroutine simulation_write_event_eio

```

Read an event from a generic `eio` event stream. The event stream element must specify the process within the sample (`i_prc`), the MC group for this process (`i_mci`), the selected term (`i_term`), the selected MC integration `channel`, and the particle set of the event.

We may encounter EOF, which we indicate by storing 0 for the process index `i_prc`. An I/O error will be reported, and we also abort reading.

```

<Simulations: simulation: TBP>+≡
    generic :: read_event => read_event_eio
    procedure :: read_event_eio => simulation_read_event_eio

<Simulations: procedures>+≡
    subroutine simulation_read_event_eio (object, eio)
        class(simulation_t), intent(inout) :: object
        class(eio_t), intent(inout) :: eio
        integer :: iostat, current
        call eio%input_i_prc (current, iostat)
        select case (iostat)
        case (0)
            object%i_prc = current

```

```

        call eio%input_event (object%entry(current)%event_t, iostat)
    end select
    select case (iostat)
    case (:-1)
        object%i_prc = 0
        object%i_mci = 0
    case (1:)
        call msg_error ("Reading events: I/O error, aborting read")
        object%i_prc = 0
        object%i_mci = 0
    case default
        object%i_mci = object%entry(current)%get_i_mci ()
    end select
end subroutine simulation_read_event_eio

```

33.9.11 Event Stream Array

Write an event using an array of event I/O streams. The process index must be selected, or the current index must be available.

```

<Simulations: simulation: TBP>+≡
generic :: write_event => write_event_es_array
procedure :: write_event_es_array => simulation_write_event_es_array

<Simulations: procedures>+≡
subroutine simulation_write_event_es_array &
    (object, es_array, passed, event_handle)
    class(simulation_t), intent(in), target :: object
    class(event_stream_array_t), intent(inout) :: es_array
    logical, intent(in), optional :: passed
    class(event_handle_t), intent(inout), optional :: event_handle
    integer :: i_prc, event_index
    integer :: i
    type(entry_t), pointer :: current_entry
    i_prc = object%i_prc
    if (i_prc > 0) then
        event_index = object%counter%total
        current_entry => object%entry(i_prc)%get_first ()
        do i = 1, current_entry%count_nlo_entries ()
            if (i > 1) current_entry => current_entry%get_next ()
            call es_array%output (current_entry%event_t, i_prc, &
                event_index, &
                passed = passed, &
                pacify = object%pacify, &
                event_handle = event_handle)
        end do
    else
        call msg_fatal ("Simulation: write event: no process selected")
    end if
end subroutine simulation_write_event_es_array

```

Read an event using an array of event I/O streams. Reading is successful if there is an input stream within the array, and if a valid event can be read from

that stream. If there is a stream, but EOF is passed when reading the first item, we switch the channel to output and return failure but no error message, such that new events can be appended to that stream.

```

<Simulations: simulation: TBP>+=
  generic :: read_event => read_event_es_array
  procedure :: read_event_es_array => simulation_read_event_es_array

<Simulations: procedures>+=
  subroutine simulation_read_event_es_array &
    (object, es_array, enable_switch, fail, event_handle)
    class(simulation_t), intent(inout), target :: object
    class(event_stream_array_t), intent(inout), target :: es_array
    logical, intent(in) :: enable_switch
    logical, intent(out) :: fail
    class(event_handle_t), intent(inout), optional :: event_handle
    integer :: iostat, i_prc
    type(entry_t), pointer :: current_entry => null ()
    integer :: i
    if (es_array%has_input ()) then
      fail = .false.
      call es_array%input_i_prc (i_prc, iostat)
      select case (iostat)
      case (0)
        object%i_prc = i_prc
        current_entry => object%entry(i_prc)
        do i = 1, current_entry%count_nlo_entries ()
          if (i > 1) then
            call es_array%skip_eio_entry (iostat)
            current_entry => current_entry%get_next ()
          end if
          call current_entry%set_index (object%get_event_index ())
          call es_array%input_event &
            (current_entry%event_t, iostat, event_handle)
        end do
      case (:-1)
        write (msg_buffer, "(A,1x,I0,1x,A)") &
          "... event file terminates after", &
          object%counter%read, "events."
        call msg_message ()
        if (enable_switch) then
          call es_array%switch_inout ()
          write (msg_buffer, "(A,1x,I0,1x,A)") &
            "Generating remaining ", &
            object%n_evt_requested - object%counter%read, "events ..."
          call msg_message ()
        end if
        fail = .true.
        return
      end select
    end select
    select case (iostat)
    case (0)
      object%i_mci = object%entry(i_prc)%get_i_mci ()
    case default
      write (msg_buffer, "(A,1x,I0,1x,A)") &

```



```

        "Reading events: I/O error, aborting read after", &
        object%counter%read, "events."
    call msg_error ()
    object%i_prc = 0
    object%i_mci = 0
    fail = .true.
end select
else
    fail = .true.
end if
end subroutine simulation_read_event_es_array

```

33.9.12 Recover event

Recalculate the process instance contents, given an event with known particle set. The indices for MC, term, and channel must be already set. The `recalculate` method of the selected entry will import the result into `sqme_prc` and `weight_prc`.

If `recover_phs` is set (and false), do not attempt any phase-space calculation. Useful if we need only matrix elements (esp. testing); this flag is not stored in the simulation record.

```

<Simulations: simulation: TBP>+≡
    procedure :: recalculate => simulation_recalculate

<Simulations: procedures>+≡
    subroutine simulation_recalculate (simulation, recover_phs, check_match)
        class(simulation_t), intent(inout) :: simulation
        logical, intent(in), optional :: recover_phs
        logical, intent(in), optional :: check_match
        integer :: i_prc, i_comp, i_term, k
        integer :: i_mci, i_mci0, i_mci1
        integer, dimension(:), allocatable :: i_terms
        logical :: success
        i_prc = simulation%i_prc
        associate (entry => simulation%entry(i_prc))
            if (entry%selected_i_mci /= 0) then
                i_mci0 = entry%selected_i_mci
                i_mci1 = i_mci0
            else
                i_mci0 = 1
                i_mci1 = entry%process%get_n_mci ()
            end if
            SCAN_COMP: do i_mci = i_mci0, i_mci1
                i_comp = entry%process%get_master_component (i_mci)
                call entry%process%reset_selected_cores ()
                call entry%process%select_components ([i_comp])
                i_terms = entry%process%get_component_i_terms (i_comp)
                SCAN_TERM: do k = 1, size (i_terms)
                    i_term = i_terms(k)
                    call entry%select (i_mci, i_term, entry%selected_channel)
                    if (entry%selected_i_term /= 0 &
                        .and. entry%selected_i_term /= i_term) cycle SCAN_TERM

```

```

call entry%select (i_mci, i_term, entry%selected_channel)
if (simulation%update_weight) then
  call entry%recalculate &
    (update_sqme = simulation%update_sqme, &
    recover_beams = simulation%recover_beams, &
    recover_phs = recover_phs, &
    weight_factor = entry%get_kinematical_weight (), &
    check_match = check_match, &
    success = success)
else
  call entry%recalculate &
    (update_sqme = simulation%update_sqme, &
    recover_beams = simulation%recover_beams, &
    recover_phs = recover_phs, &
    check_match = check_match, &
    success = success)
end if
if (success) exit SCAN_COMP
end do SCAN_TERM
deallocate (i_terms)
end do SCAN_COMP
if (.not. success) then
  call entry%write ()
  call msg_fatal ("Simulation/recalculate: &
    &event could not be matched to the specified process")
end if
end associate
end subroutine simulation_recalculate

```

33.9.13 Extract contents of the simulation object

Return the MD5 sum that summarizes configuration and integration (but not the event file). Used for initializing the event streams.

```

<Simulations: simulation: TBP>+≡
  procedure :: get_md5sum_prc => simulation_get_md5sum_prc
  procedure :: get_md5sum_cfg => simulation_get_md5sum_cfg
  procedure :: get_md5sum_alt => simulation_get_md5sum_alt

<Simulations: procedures>+≡
  function simulation_get_md5sum_prc (simulation) result (md5sum)
    class(simulation_t), intent(in) :: simulation
    character(32) :: md5sum
    md5sum = simulation%md5sum_prc
  end function simulation_get_md5sum_prc

  function simulation_get_md5sum_cfg (simulation) result (md5sum)
    class(simulation_t), intent(in) :: simulation
    character(32) :: md5sum
    md5sum = simulation%md5sum_cfg
  end function simulation_get_md5sum_cfg

  function simulation_get_md5sum_alt (simulation, i) result (md5sum)
    class(simulation_t), intent(in) :: simulation

```

```

integer, intent(in) :: i
character(32) :: md5sum
md5sum = simulation%md5sum_alt(i)
end function simulation_get_md5sum_alt

```

Return data that may be useful for writing event files.

Usually we can refer to a previously integrated process, for which we can fetch a process pointer. Occasionally, we do not have this because we are just rescanning an externally generated file without calculation. For that situation, we generate our local beam data object using the current environment, or, in simple cases, just fetch the necessary data from the process definition and environment.

```

<Simulations: simulation: TBP>+=
  procedure :: get_data => simulation_get_data

<Simulations: procedures>+=
  function simulation_get_data (simulation, alt) result (sdata)
    class(simulation_t), intent(in) :: simulation
    logical, intent(in), optional :: alt
    type(event_sample_data_t) :: sdata
    type(process_t), pointer :: process
    type(beam_data_t), pointer :: beam_data
    type(beam_structure_t), pointer :: beam_structure
    type(flavor_t), dimension(:), allocatable :: flv
    integer :: n, i
    logical :: enable_alt, construct_beam_data
    real(default) :: sqrts
    class(model_data_t), pointer :: model
    logical :: decay_rest_frame
    type(string_t) :: process_id
    enable_alt = .true.; if (present (alt)) enable_alt = alt
    if (debug_on) call msg_debug (D_CORE, "simulation_get_data")
    if (debug_on) call msg_debug (D_CORE, "alternative setup", enable_alt)
    if (enable_alt) then
      call sdata%init (simulation%n_prc, simulation%n_alt)
      do i = 1, simulation%n_alt
        sdata%md5sum_alt(i) = simulation%get_md5sum_alt (i)
      end do
    else
      call sdata%init(simulation%n_prc)
    end if
    sdata%unweighted = simulation%unweighted
    sdata%negative_weights = simulation%negative_weights
    sdata%norm_mode = simulation%norm_mode
    process => simulation%entry(1)%get_process_ptr ()
    if (associated (process)) then
      beam_data => process%get_beam_data_ptr ()
      construct_beam_data = .false.
    else
      n = simulation%entry(1)%n_in
      sqrts = simulation%local%get_sqrts ()
      beam_structure => simulation%local%beam_structure
      call beam_structure%check_against_n_in (n, construct_beam_data)
    end if
  end function simulation_get_data

```

```

        if (construct_beam_data) then
            allocate (beam_data)
            model => simulation%local%model
            decay_rest_frame = &
                simulation%local%get_lval (var_str ("?decay_rest_frame"))
            call beam_data%init_structure (beam_structure, &
                sqrts, model, decay_rest_frame)
        else
            beam_data => null ()
        end if
    end if
    if (associated (beam_data)) then
        n = beam_data%get_n_in ()
        sdata%n_beam = n
        allocate (flv (n))
        flv = beam_data%get_flavor ()
        sdata%pdg_beam(:n) = flv%get_pdg ()
        sdata%energy_beam(:n) = beam_data%get_energy ()
        if (construct_beam_data) deallocate (beam_data)
    else
        n = simulation%entry(1)%n_in
        sdata%n_beam = n
        process_id = simulation%entry(1)%process_id
        call simulation%local%prclib%get_pdg_in_1 &
            (process_id, sdata%pdg_beam(:n))
        sdata%energy_beam(:n) = sqrts / n
    end if
    do i = 1, simulation%n_prc
        if (.not. simulation%entry(i)%valid) cycle
        process => simulation%entry(i)%get_process_ptr ()
        if (associated (process)) then
            sdata%proc_num_id(i) = process%get_num_id ()
        else
            process_id = simulation%entry(i)%process_id
            sdata%proc_num_id(i) = simulation%local%prclib%get_num_id (process_id)
        end if
        if (sdata%proc_num_id(i) == 0) sdata%proc_num_id(i) = i
        if (simulation%entry(i)%has_integral) then
            sdata%cross_section(i) = simulation%entry(i)%integral
            sdata%error(i) = simulation%entry(i)%error
        end if
    end do
    sdata%total_cross_section = sum (sdata%cross_section)
    sdata%md5sum_prc = simulation%get_md5sum_prc ()
    sdata%md5sum_cfg = simulation%get_md5sum_cfg ()
    if (simulation%split_n_evt > 0 .or. simulation%split_n_kbytes > 0) then
        sdata%split_n_evt = simulation%split_n_evt
        sdata%split_n_kbytes = simulation%split_n_kbytes
        sdata%split_index = simulation%split_index
    end if
end function simulation_get_data

```

Return a default name for the current event sample. This is the process ID of the first process.

```

<Simulations: simulation: TBP>+≡
  procedure :: get_default_sample_name => simulation_get_default_sample_name

```

```

<Simulations: procedures>+≡
  function simulation_get_default_sample_name (simulation) result (sample)
    class(simulation_t), intent(in) :: simulation
    type(string_t) :: sample
    type(process_t), pointer :: process
    sample = "whizard"
    if (simulation%n_prc > 0) then
      process => simulation%entry(1)%get_process_ptr ()
      if (associated (process)) then
        sample = process%get_id ()
      end if
    end if
  end function simulation_get_default_sample_name

```

```

<Simulations: simulation: TBP>+≡
  procedure :: is_valid => simulation_is_valid

```

```

<Simulations: procedures>+≡
  function simulation_is_valid (simulation) result (valid)
    class(simulation_t), intent(inout) :: simulation
    logical :: valid
    valid = simulation%valid
  end function simulation_is_valid

```

Return the hard-interaction particle set for event entry i_prc.

```

<Simulations: simulation: TBP>+≡
  procedure :: get_hard_particle_set => simulation_get_hard_particle_set

<Simulations: procedures>+≡
  function simulation_get_hard_particle_set (simulation, i_prc) result (pset)
    class(simulation_t), intent(in) :: simulation
    integer, intent(in) :: i_prc
    type(particle_set_t) :: pset
    call simulation%entry(i_prc)%get_hard_particle_set (pset)
  end function simulation_get_hard_particle_set

```

33.9.14 Auxiliary

Call pacify: eliminate numerical noise.

```

<Simulations: public>+≡
  public :: pacify

<Simulations: interfaces>≡
  interface pacify
    module procedure pacify_simulation
  end interface

```

```

<Simulations: procedures>+≡
  subroutine pacify_simulation (simulation)
    class(simulation_t), intent(inout) :: simulation
    integer :: i, j
    i = simulation%i_prc
    if (i > 0) then
      call pacify (simulation%entry(i))
      do j = 1, simulation%n_alt
        call pacify (simulation%alt_entry(i,j))
      end do
    end if
  end subroutine pacify_simulation

```

Manually evaluate expressions for the currently selected process. This is used only in the unit tests.

```

<Simulations: simulation: TBP>+≡
  procedure :: evaluate_expressions => simulation_evaluate_expressions

<Simulations: procedures>+≡
  subroutine simulation_evaluate_expressions (simulation)
    class(simulation_t), intent(inout) :: simulation
    call simulation%entry(simulation%i_prc)%evaluate_expressions ()
  end subroutine simulation_evaluate_expressions

```

Manually evaluate event transforms for the currently selected process. This is used only in the unit tests.

```

<Simulations: simulation: TBP>+≡
  procedure :: evaluate_transforms => simulation_evaluate_transforms

<Simulations: procedures>+≡
  subroutine simulation_evaluate_transforms (simulation)
    class(simulation_t), intent(inout) :: simulation
    associate (entry => simulation%entry(simulation%i_prc))
      call entry%evaluate_transforms ()
    end associate
  end subroutine simulation_evaluate_transforms

```

33.9.15 Unit tests

Test module, followed by the stand-alone unit-test procedures.

```

<simulations_ut.f90>≡
  <File header>

  module simulations_ut
    use unit_tests
    use simulations_ut1

    <Standard module head>

    <Simulations: public test>

    contains

```

```

    <Simulations: test driver>

    end module simulations_ut

    <simulations_uti.f90>≡
    <File header>

    module simulations_uti

        <Use kinds>
        use kinds, only: i64
        <Use strings>
        use io_units
        use format_defs, only: FMT_10, FMT_12
        use ifiles
        use lexers
        use parser
        use lorentz
        use flavors
        use interactions, only: reset_interaction_counter
        use process_libraries, only: process_library_t
        use prclib_stacks
        use phs_forests
        use event_base, only: generic_event_t
        use event_base, only: event_callback_t
        use particles, only: particle_set_t
        use eio_data
        use eio_base
        use eio_direct, only: eio_direct_t
        use eio_raw
        use eio_ascii
        use eio_dump
        use eio_callback
        use eval_trees
        use model_data, only: model_data_t
        use models
        use rt_data
        use event_streams
        use decays_ut, only: prepare_testbed
        use process, only: process_t
        use process_stacks, only: process_entry_t
        use process_configurations_ut, only: prepare_test_library
        use compilations, only: compile_library
        use integrations, only: integrate_process

        use simulations

        use restricted_subprocesses_uti, only: prepare_resonance_test_library

    <Standard module head>

    <Simulations: test declarations>

    <Simulations: test auxiliary types>

```

```
contains

<Simulations: tests>

<Simulations: test auxiliary>

end module simulations_util
```

API: driver for the unit tests below.

```
<Simulations: public test>≡
  public :: simulations_test

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

Initialization

Initialize a `simulation_t` object, including the embedded event records.

```
<Simulations: execute tests>≡
  call test (simulations_1, "simulations_1", &
    "initialization", &
    u, results)

<Simulations: test declarations>≡
  public :: simulations_1

<Simulations: tests>≡
  subroutine simulations_1 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1, procname2
    type(rt_data_t), target :: global
    type(simulation_t), target :: simulation

    write (u, "(A)")  "* Test output: simulations_1"
    write (u, "(A)")  "* Purpose: initialize simulation"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize processes"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
      0, is_known = .true.)

    libname = "simulation_1a"
```



```

procname1 = "simulation_1p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("simulations1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

procname2 = "sim_extra"

call prepare_test_library (global, libname, 1, [procname2])
call compile_library (libname, global)
call global%set_string (var_str ("$run_id"), &
    var_str ("simulations2"), is_known = .true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_string (var_str ("$sample"), &
    var_str ("sim1"), is_known = .true.)
call integrate_process (procname2, global, local_stack=.true.)

call simulation%init ([procname1, procname2], .false., .true., global)
call simulation%init_process_selector ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the first process"
write (u, "(A)")

call simulation%write_event (u, i_prc = 1)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "** Test output end: simulations_1"

end subroutine simulations_1

```

Weighted events

Generate events for a single process.

```

<Simulations: execute tests>+≡
call test (simulations_2, "simulations_2", &
    "weighted events", &
    u, results)

<Simulations: test declarations>+≡
public :: simulations_2

<Simulations: tests>+≡
subroutine simulations_2 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1
    type(rt_data_t), target :: global
    type(simulation_t), target :: simulation
    type(event_sample_data_t) :: data

    write (u, "(A)")  "** Test output: simulations_2"
    write (u, "(A)")  "** Purpose: generate events for a single process"
    write (u, "(A)")

    write (u, "(A)")  "** Initialize processes"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
        .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
        0, is_known = .true.)

    libname = "simulation_2a"
    procname1 = "simulation_2p"

    call prepare_test_library (global, libname, 1, [procname1])
    call compile_library (libname, global)

    call global%append_log (&
        var_str ("?rebuild_events"), .true., intrinsic = .true.)

    call global%set_string (var_str ("$method"), &
        var_str ("unit_test"), is_known = .true.)

```

```

call global%set_string (var_str ("phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("run_id"), &
    var_str ("simulations1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data = simulation%get_data ()
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate three events"
write (u, "(A)")

call simulation%set_n_events_requested (3)
call simulation%generate ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the last event"
write (u, "(A)")

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_2"

```

```
end subroutine simulations_2
```

Unweighted events

Generate events for a single process.

```
<Simulations: execute tests>+≡
  call test (simulations_3, "simulations_3", &
    "unweighted events", &
    u, results)

<Simulations: test declarations>+≡
  public :: simulations_3

<Simulations: tests>+≡
  subroutine simulations_3 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1
    type(rt_data_t), target :: global
    type(simulation_t), target :: simulation
    type(event_sample_data_t) :: data

    write (u, "(A)")  "* Test output: simulations_3"
    write (u, "(A)")  "* Purpose: generate unweighted events &
      &for a single process"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize processes"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
      0, is_known = .true.)

    libname = "simulation_3a"
    procname1 = "simulation_3p"

    call prepare_test_library (global, libname, 1, [procname1])
    call compile_library (libname, global)

    call global%append_log (&
      var_str ("?rebuild_events"), .true., intrinsic = .true.)

    call global%set_string (var_str ("$method"), &
      var_str ("unit_test"), is_known = .true.)
    call global%set_string (var_str ("$phs_method"), &
      var_str ("single"), is_known = .true.)
    call global%set_string (var_str ("$integration_method"), &
      var_str ("midpoint"), is_known = .true.)
    call global%set_log (var_str ("?vis_history"), &
      .false., is_known = .true.)
```

```

call global%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"),&
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("simulations1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data = simulation%get_data ()
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate three events"
write (u, "(A)")

call simulation%set_n_events_requested (3)
call simulation%generate ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the last event"
write (u, "(A)")

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_3"

end subroutine simulations_3

```

Simulating process with structure functions

Generate events for a single process.

<Simulations: execute tests>+≡

```

call test (simulations_4, "simulations_4", &
          "process with structure functions", &
          u, results)

<Simulations: test declarations>+≡
public :: simulations_4

<Simulations: tests>+≡
subroutine simulations_4 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname1
  type(rt_data_t), target :: global
  type(flavor_t) :: flv
  type(string_t) :: name
  type(simulation_t), target :: simulation
  type(event_sample_data_t) :: data

  write (u, "(A)")  "* Test output: simulations_4"
  write (u, "(A)")  "* Purpose: generate events for a single process &
                    &with structure functions"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize processes"
  write (u, "(A)")

  call syntax_model_file_init ()
  call syntax_phs_forest_init ()

  call global%global_init ()
  call global%set_log (var_str ("?omega_openmp"), &
                     .false., is_known = .true.)
  call global%set_int (var_str ("seed"), &
                     0, is_known = .true.)

  libname = "simulation_4a"
  procname1 = "simulation_4p"

  call prepare_test_library (global, libname, 1, [procname1])
  call compile_library (libname, global)

  call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
  call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
  call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

  call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
  call global%set_string (var_str ("$_method"), &
    var_str ("unit_test"), is_known = .true.)
  call global%set_string (var_str ("$_phs_method"), &
    var_str ("wood"), is_known = .true.)
  call global%set_string (var_str ("$_integration_method"), &
    var_str ("vamp"), is_known = .true.)

```

```

call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call reset_interaction_counter ()

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

write (u, "(A)")  "* Integrate"
write (u, "(A)")

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
call global%set_string (var_str ("$_sample"), &
    var_str ("simulations4"), is_known = .true.)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data = simulation%get_data ()
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate three events"
write (u, "(A)")

call simulation%set_n_events_requested (3)
call simulation%generate ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the last event"
write (u, "(A)")

```

```

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_4"

end subroutine simulations_4

```

Event I/O

Generate event for a test process, write to file and reread.

```

<Simulations: execute tests>+≡
  call test (simulations_5, "simulations_5", &
    "raw event I/O", &
    u, results)

<Simulations: test declarations>+≡
  public :: simulations_5

<Simulations: tests>+≡
  subroutine simulations_5 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1, sample
    type(rt_data_t), target :: global
    class(eio_t), allocatable :: eio
    type(simulation_t), allocatable, target :: simulation

    write (u, "(A)")  "* Test output: simulations_5"
    write (u, "(A)")  "*   Purpose: generate events for a single process"
    write (u, "(A)")  "*               write to file and reread"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize processes"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
      0, is_known = .true.)

    libname = "simulation_5a"
    procname1 = "simulation_5p"

    call prepare_test_library (global, libname, 1, [procname1])
    call compile_library (libname, global)

```



```

call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("simulations5"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations5"
call global%set_string (var_str ("sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

allocate (eio_raw_t :: eio)
call eio%init_out (sample)

write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate ()
call simulation%write_event (u)
call simulation%write_event (eio)

call eio%final ()
deallocate (eio)

```

```

call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event from file"
write (u, "(A)")

call global%set_log (var_str ("?update_sqme"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_weight"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()
allocate (eio_raw_t :: eio)
call eio%init_in (sample)

call simulation%read_event (eio)
call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Recalculate process instance"
write (u, "(A)")

call simulation%recalculate ()
call simulation%evaluate_expressions ()
call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_5"

end subroutine simulations_5

```

Event I/O

Generate event for a real process with structure functions, write to file and reread.

```

<Simulations: execute tests>+≡
call test (simulations_6, "simulations_6", &
    "raw event I/O with structure functions", &
    u, results)

```

```

<Simulations: test declarations>+=
  public :: simulations_6

<Simulations: tests>+=
  subroutine simulations_6 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1, sample
    type(rt_data_t), target :: global
    class(eio_t), allocatable :: eio
    type(simulation_t), allocatable, target :: simulation
    type(flavor_t) :: flv
    type(string_t) :: name

    write (u, "(A)")  "* Test output: simulations_6"
    write (u, "(A)")  "*   Purpose: generate events for a single process"
    write (u, "(A)")  "*               write to file and reread"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process and integrate"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
      0, is_known = .true.)

    libname = "simulation_6"
    procname1 = "simulation_6p"

    call prepare_test_library (global, libname, 1, [procname1])
    call compile_library (libname, global)

    call global%append_log (&
      var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
    call global%append_log (&
      var_str ("?rebuild_grids"), .true., intrinsic = .true.)
    call global%append_log (&
      var_str ("?rebuild_events"), .true., intrinsic = .true.)

    call global%set_string (var_str ("$method"), &
      var_str ("unit_test"), is_known = .true.)
    call global%set_string (var_str ("$phs_method"), &
      var_str ("wood"), is_known = .true.)
    call global%set_string (var_str ("$integration_method"), &
      var_str ("vamp"), is_known = .true.)
    call global%set_log (var_str ("?use_vamp_equivalences"), &
      .true., is_known = .true.)
    call global%set_log (var_str ("?vis_history"), &
      .false., is_known = .true.)
    call global%set_log (var_str ("?integration_timer"), &
      .false., is_known = .true.)
    call global%set_log (var_str ("?recover_beams"), &

```

```

        .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations6"
call global%set_string (var_str ("$_sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

allocate (eio_raw_t :: eio)
call eio%init_out (sample)

write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate ()
call pacify (simulation)
call simulation%write_event (u, verbose = .true., testflag = .true.)
call simulation%write_event (eio)

call eio%final ()
deallocate (eio)
call simulation%final ()
deallocate (simulation)

write (u, "(A)")

```

```

write (u, "(A)")  "* Re-read the event from file"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?update_sqme"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_weight"), &
    .true., is_known = .true.)

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()
allocate (eio_raw_t :: eio)
call eio%init_in (sample)

call simulation%read_event (eio)
call simulation%write_event (u, verbose = .true., testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Recalculate process instance"
write (u, "(A)")

call simulation%recalculate ()
call simulation%evaluate_expressions ()
call simulation%write_event (u, verbose = .true., testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call eio%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_6"

end subroutine simulations_6

```

Automatic Event I/O

Generate events with raw-format event file as cache: generate, reread, append.

```

<Simulations: execute tests>+≡
    call test (simulations_7, "simulations_7", &
        "automatic raw event I/O", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_7

<Simulations: tests>+≡
    subroutine simulations_7 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname1, sample

```

```

type(rt_data_t), target :: global
type(string_t), dimension(0) :: empty_string_array
type(event_sample_data_t) :: data
type(event_stream_array_t) :: es_array
type(simulation_t), allocatable, target :: simulation
type(flavor_t) :: flv
type(string_t) :: name

write (u, "(A)")  "* Test output: simulations_7"
write (u, "(A)")  "* Purpose: generate events for a single process"
write (u, "(A)")  "*           write to file and reread"
write (u, "(A)")

write (u, "(A)")  "* Initialize process and integrate"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

libname = "simulation_7"
procname1 = "simulation_7p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

```

```

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations7"
call global%set_string (var_str ("$_sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
call es_array%init (sample, [var_str ("raw")], global, data)

write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate (es_array)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")  "* Re-read the event from file and generate another one"
write (u, "(A)")

call global%set_log (&
    var_str ("?rebuild_events"), .false., is_known = .true.)

```

```

call reset_interaction_counter ()

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"))

call simulation%set_n_events_requested (2)
call simulation%generate (es_array)

call pacify (simulation)
call simulation%write_event (u, verbose = .true.)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read both events from file"
write (u, "(A)")

call reset_interaction_counter ()

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"))

call simulation%set_n_events_requested (2)
call simulation%generate (es_array)

call pacify (simulation)
call simulation%write_event (u, verbose = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call es_array%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_7"

```



```
end subroutine simulations_7
```

Rescanning Events

Generate events and rescan the resulting raw event file.

```
<Simulations: execute tests>+≡
  call test (simulations_8, "simulations_8", &
    "rescan raw event file", &
    u, results)

<Simulations: test declarations>+≡
  public :: simulations_8

<Simulations: tests>+≡
  subroutine simulations_8 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, procname1, sample
    type(rt_data_t), target :: global
    type(string_t), dimension(0) :: empty_string_array
    type(event_sample_data_t) :: data
    type(event_stream_array_t) :: es_array
    type(simulation_t), allocatable, target :: simulation
    type(flavor_t) :: flv
    type(string_t) :: name

    write (u, "(A)")  "* Test output: simulations_8"
    write (u, "(A)")  "*   Purpose: generate events for a single process"
    write (u, "(A)")  "*               write to file and rescan"
    write (u, "(A)")

    write (u, "(A)")  "* Initialize process and integrate"
    write (u, "(A)")

    call syntax_model_file_init ()

    call global%global_init ()
    call global%init_fallback_model &
      (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

    call global%set_log (var_str ("?omega_openmp"), &
      .false., is_known = .true.)
    call global%set_int (var_str ("seed"), &
      0, is_known = .true.)

    libname = "simulation_8"
    procname1 = "simulation_8p"

    call prepare_test_library (global, libname, 1, [procname1])
    call compile_library (libname, global)

    call global%append_log (&
      var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
    call global%append_log (&
      var_str ("?rebuild_grids"), .true., intrinsic = .true.)
```

```

call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &
    0._default)

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations8"
call global%set_string (var_str ("$sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()

```

```

write (u, "(1x,A,A,A)") "MD5 sum (proc) = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)") "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, [var_str ("raw")], global, &
    data)

write (u, "(A)")
write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate (es_array)

call pacify (simulation)
call simulation%write_event (u, verbose = .true., testflag = .true.)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read the event from file"
write (u, "(A)")

call reset_interaction_counter ()

allocate (simulation)
call simulation%init ([procname1], .false., .false., global)
call simulation%init_process_selector ()

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = ""
write (u, "(1x,A,A,A)") "MD5 sum (proc) = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)") "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"), input_sample = sample, allow_switch = .false.)

call simulation%rescan (1, es_array, global = global)

write (u, "(A)")

call pacify (simulation)
call simulation%write_event (u, verbose = .true., testflag = .true.)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Re-read again and recalculate"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?update_sqme"), &

```

```

        .true., is_known = .true.)
call global%set_log (var_str ("?update_event"), &
        .true., is_known = .true.)

allocate (simulation)
call simulation%init ([procname1], .false., .false., global)
call simulation%init_process_selector ()

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = ""
write (u, "(1x,A,A,A)") "MD5 sum (proc)   = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)") "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, empty_string_array, global, data, &
        input = var_str ("raw"), input_sample = sample, allow_switch = .false.)

call simulation%rescan (1, es_array, global = global)

write (u, "(A)")

call pacify (simulation)
call simulation%write_event (u, verbose = .true., testflag = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call es_array%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_8"

end subroutine simulations_8

```

Rescanning Check

Generate events and rescan with process mismatch.

```

<Simulations: execute tests>+≡
    call test (simulations_9, "simulations_9", &
        "rescan mismatch", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_9

<Simulations: tests>+≡
    subroutine simulations_9 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname1, sample
        type(rt_data_t), target :: global
        type(string_t), dimension(0) :: empty_string_array
        type(event_sample_data_t) :: data
        type(event_stream_array_t) :: es_array
        type(simulation_t), allocatable, target :: simulation

```

```

type(flavor_t) :: flv
type(string_t) :: name
logical :: error

write (u, "(A)")  "*" Test output: simulations_9"
write (u, "(A)")  "*" Purpose: generate events for a single process"
write (u, "(A)")  "*"           write to file and rescan"
write (u, "(A)")

write (u, "(A)")  "*" Initialize process and integrate"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

libname = "simulation_9"
procname1 = "simulation_9p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("wood"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("vamp"), is_known = .true.)
call global%set_log (var_str ("?use_vamp_equivalences"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%model_set_real (var_str ("ms"), &

```

```

0._default)

call flv%init (25, global%model)
name = flv%get_name ()

call global%beam_structure%init_sf ([name, name], [1])
call global%beam_structure%set_sf (1, 1, var_str ("sf_test_1"))

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call reset_interaction_counter ()

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations9"
call global%set_string (var_str ("$_sample"), &
    sample, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize raw event file"
write (u, "(A)")

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = simulation%get_md5sum_cfg ()
write (u, "(1x,A,A,A)")  "MD5 sum (proc) = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)")  "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, [var_str ("raw")], global, &
    data)

write (u, "(A)")
write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate (es_array)

call es_array%final ()
call simulation%final ()
deallocate (simulation)

write (u, "(A)")  "* Initialize event generation for different parameters"
write (u, "(A)")

```

```

call reset_interaction_counter ()

allocate (simulation)
call simulation%init ([procname1, procname1], .false., .false., global)
call simulation%init_process_selector ()

call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Attempt to re-read the events (should fail)"
write (u, "(A)")

data%md5sum_prc = simulation%get_md5sum_prc ()
data%md5sum_cfg = ""
write (u, "(1x,A,A,A)")  "MD5 sum (proc)   = '", data%md5sum_prc, "'"
write (u, "(1x,A,A,A)")  "MD5 sum (config) = '", data%md5sum_cfg, "'"
call es_array%init (sample, empty_string_array, global, data, &
    input = var_str ("raw"), input_sample = sample, &
    allow_switch = .false., error = error)

write (u, "(1x,A,L1)")  "error = ", error

call simulation%rescan (1, es_array, global = global)

call es_array%final ()
call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_9"

end subroutine simulations_9

```

Alternative weights

Generate an event for a single process and reweight it in a simultaneous calculation.

```

<Simulations: execute tests>+≡
    call test (simulations_10, "simulations_10", &
        "alternative weight", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_10

<Simulations: tests>+≡
    subroutine simulations_10 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, procname1, expr_text
        type(rt_data_t), target :: global
        type(rt_data_t), dimension(1), target :: alt_env
        type(ifile_t) :: ifile

```

```

type(stream_t) :: stream
type(parse_tree_t) :: pt_weight
type(simulation_t), target :: simulation
type(event_sample_data_t) :: data

write (u, "(A)")  "* Test output: simulations_10"
write (u, "(A)")  "* Purpose: reweight event"
write (u, "(A)")

write (u, "(A)")  "* Initialize processes"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_pexpr_init ()

call global%global_init ()
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

libname = "simulation_10a"
procname1 = "simulation_10p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$run_id"), &
    var_str ("simulations1"), is_known = .true.)

```



```

call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize alternative environment with custom weight"
write (u, "(A)")

call alt_env(1)%local_init (global)
call alt_env(1)%activate ()

expr_text = "2"
write (u, "(A,A)")  "weight = ", char (expr_text)
write (u, *)

call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_weight, stream, .true.)
call stream_final (stream)
alt_env(1)%pn%weight_expr => pt_weight%get_root_ptr ()
call alt_env(1)%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
call simulation%init ([procname1], .true., .true., global, alt_env=alt_env)
call simulation%init_process_selector ()

data = simulation%get_data ()
call data%write (u)

write (u, "(A)")
write (u, "(A)")  "* Generate an event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate ()
call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the last event"
write (u, "(A)")

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Write the event record for the alternative setup"
write (u, "(A)")

call simulation%write_alt_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

```

```

call simulation%final ()
call global%final ()

call syntax_model_file_final ()
call syntax_pexpr_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_10"

end subroutine simulations_10

```

Decays

Generate an event with subsequent partonic decays.

```

<Simulations: execute tests>+≡
call test (simulations_11, "simulations_11", &
    "decay", &
    u, results)

<Simulations: test declarations>+≡
public :: simulations_11

<Simulations: tests>+≡
subroutine simulations_11 (u)
integer, intent(in) :: u
type(rt_data_t), target :: global
type(prclib_entry_t), pointer :: lib
type(string_t) :: prefix, procname1, procname2
type(simulation_t), target :: simulation

write (u, "(A)")  "* Test output: simulations_11"
write (u, "(A)")  "* Purpose: apply decay"
write (u, "(A)")

write (u, "(A)")  "* Initialize processes"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
allocate (lib)
call global%add_prclib (lib)

call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

prefix = "simulation_11"
procname1 = prefix // "_p"
procname2 = prefix // "_d"
call prepare_testbed &
    (global%prclib, global%process_stack, &

```

```

        prefix, global%os_data, &
        scattering=.true., decay=.true.)

call global%select_model (var_str ("Test"))
call global%model%set_par (var_str ("ff"), 0.4_default)
call global%model%set_par (var_str ("mf"), &
    global%model%get_real (var_str ("ff")) &
    * global%model%get_real (var_str ("ms")))
call global%model%set_unstable (25, [procname2])

write (u, "(A)")  "* Initialize simulation object"
write (u, "(A)")

call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Generate event"
write (u, "(A)")

call simulation%set_n_events_requested (1)
call simulation%generate ()
call simulation%write (u)

write (u, *)

call simulation%write_event (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"
write (u, "(A)")

call simulation%final ()
call global%final ()

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_11"

end subroutine simulations_11

```

Split Event Files

Generate event for a real process with structure functions and write to file, accepting a limit for the number of events per file.

```

<Simulations: execute tests>+≡
    call test (simulations_12, "simulations_12", &
        "split event files", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_12

```

<Simulations: tests>+≡

```

subroutine simulations_12 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname1, sample
  type(rt_data_t), target :: global
  class(eio_t), allocatable :: eio
  type(simulation_t), allocatable, target :: simulation
  type(flavor_t) :: flv
  integer :: i_evt

  write (u, "(A)")  "* Test output: simulations_12"
  write (u, "(A)")  "*   Purpose: generate events for a single process"
  write (u, "(A)")  "*               and write to split event files"
  write (u, "(A)")

  write (u, "(A)")  "* Initialize process and integrate"
  write (u, "(A)")

  call syntax_model_file_init ()

  call global%global_init ()
  call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
  call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

  libname = "simulation_12"
  procname1 = "simulation_12p"

  call prepare_test_library (global, libname, 1, [procname1])
  call compile_library (libname, global)

  call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
  call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
  call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

  call global%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known = .true.)
  call global%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known = .true.)
  call global%set_string (var_str ("$integration_method"), &
    var_str ("midpoint"), is_known = .true.)
  call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
  call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
  call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

  call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

```

```

call global%model_set_real (var_str ("ms"), &
    0._default)

call flv%init (25, global%model)

call global%it_list%init ([1], [1000])

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations_12"
call global%set_string (var_str ("$_sample"), &
    sample, is_known = .true.)
call global%set_int (var_str ("sample_split_n_evt"), &
    2, is_known = .true.)
call global%set_int (var_str ("sample_split_index"), &
    42, is_known = .true.)
allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

call simulation%write (u)

write (u, "(A)")
write (u, "(A)")  "* Initialize ASCII event file"
write (u, "(A)")

allocate (eio_ascii_short_t :: eio)
select type (eio)
class is (eio_ascii_t); call eio%set_parameters ()
end select
call eio%init_out (sample, data = simulation%get_data ())

write (u, "(A)")  "* Generate 5 events, distributed among three files"

do i_evt = 1, 5
    call simulation%set_n_events_requested (1)
    call simulation%generate ()
    call simulation%write_event (eio)
end do

call eio%final ()
deallocate (eio)
call simulation%final ()
deallocate (simulation)

write (u, *)
call display_file ("simulations_12.42.short.evt", u)

```

```

write (u, *)
call display_file ("simulations_12.43.short.evt", u)
write (u, *)
call display_file ("simulations_12.44.short.evt", u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_12"

end subroutine simulations_12

```

Auxiliary: display file contents.

<Simulations: public test auxiliary>≡

```
public :: display_file
```

<Simulations: test auxiliary>≡

```

subroutine display_file (file, u)
  use io_units, only: free_unit
  character(*), intent(in) :: file
  integer, intent(in) :: u
  character(256) :: buffer
  integer :: u_file
  write (u, "(3A)")  "* Contents of file '", file, "':"
  write (u, *)
  u_file = free_unit ()
  open (u_file, file = file, action = "read", status = "old")
  do
    read (u_file, "(A)", end = 1) buffer
    write (u, "(A)") trim (buffer)
  end do
1  continue
end subroutine display_file

```

Callback

Generate events and execute a callback in place of event I/O.

<Simulations: execute tests>+≡

```

call test (simulations_13, "simulations_13", &
  "callback", &
  u, results)

```

<Simulations: test declarations>+≡

```
public :: simulations_13
```

<Simulations: tests>+≡

```

subroutine simulations_13 (u)
  integer, intent(in) :: u
  type(string_t) :: libname, procname1, sample
  type(rt_data_t), target :: global

```

```

class(eio_t), allocatable :: eio
type(simulation_t), allocatable, target :: simulation
type(flavor_t) :: flv
integer :: i_evt
type(simulations_13_callback_t) :: event_callback

write (u, "(A)")  "* Test output: simulations_13"
write (u, "(A)")  "* Purpose: generate events for a single process"
write (u, "(A)")  "*           and execute callback"
write (u, "(A)")

write (u, "(A)")  "* Initialize process and integrate"
write (u, "(A)")

call syntax_model_file_init ()

call global%global_init ()
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)

libname = "simulation_13"
procname1 = "simulation_13p"

call prepare_test_library (global, libname, 1, [procname1])
call compile_library (libname, global)

call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)

call global%set_string (var_str ("method"), &
    var_str ("unit_test"), is_known = .true.)
call global%set_string (var_str ("phs_method"), &
    var_str ("single"), is_known = .true.)
call global%set_string (var_str ("integration_method"), &
    var_str ("midpoint"), is_known = .true.)
call global%set_log (var_str ("?vis_history"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?integration_timer"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)

call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)

call flv%init (25, global%model)

call global%it_list%init ([1], [1000])

```

```

call global%set_string (var_str ("$_run_id"), &
    var_str ("r1"), is_known = .true.)
call integrate_process (procname1, global, local_stack=.true.)

write (u, "(A)")  "* Initialize event generation"
write (u, "(A)")

call global%set_log (var_str ("?unweighted"), &
    .false., is_known = .true.)
sample = "simulations_13"
call global%set_string (var_str ("$_sample"), &
    sample, is_known = .true.)

allocate (simulation)
call simulation%init ([procname1], .true., .true., global)
call simulation%init_process_selector ()

write (u, "(A)")  "* Prepare callback object"
write (u, "(A)")

event_callback%u = u
call global%set_event_callback (event_callback)

write (u, "(A)")  "* Initialize callback I/O object"
write (u, "(A)")

allocate (eio_callback_t :: eio)
select type (eio)
class is (eio_callback_t)
    call eio%set_parameters (callback = event_callback, &
        count_interval = 3)
end select
call eio%init_out (sample, data = simulation%get_data ())

write (u, "(A)")  "* Generate 7 events, with callback every 3 events"
write (u, "(A)")

do i_evt = 1, 7
    call simulation%set_n_events_requested (1)
    call simulation%generate ()
    call simulation%write_event (eio)
end do

call eio%final ()
deallocate (eio)
call simulation%final ()
deallocate (simulation)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call global%final ()

```



```

        write (u, "(A)")
        write (u, "(A)")  "* Test output end: simulations_13"

    end subroutine simulations_13

```

The callback object and procedure. In the type extension, we can store the output channel `u` so we know where to write into.

```

<Simulations: test auxiliary types>≡
    type, extends (event_callback_t) :: simulations_13_callback_t
        integer :: u
    contains
        procedure :: write => simulations_13_callback_write
        procedure :: proc => simulations_13_callback
    end type simulations_13_callback_t

<Simulations: test auxiliary>+≡
    subroutine simulations_13_callback_write (event_callback, unit)
        class(simulations_13_callback_t), intent(in) :: event_callback
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Hello"
    end subroutine simulations_13_callback_write

    subroutine simulations_13_callback (event_callback, i, event)
        class(simulations_13_callback_t), intent(in) :: event_callback
        integer(i64), intent(in) :: i
        class(generic_event_t), intent(in) :: event
        write (event_callback%u, "(A,I0)") "hello event #", i
    end subroutine simulations_13_callback

```

Resonant subprocess setup

Prepare a process with resonances and enter resonant subprocesses in the simulation object. Select a kinematics configuration and compute probabilities for resonant subprocesses.

The process and its initialization is taken from `processes_18`, but we need a complete `O'MEGA` matrix element here.

```

<Simulations: execute tests>+≡
    call test (simulations_14, "simulations_14", &
        "resonant subprocesses evaluation", &
        u, results)

<Simulations: test declarations>+≡
    public :: simulations_14

<Simulations: tests>+≡
    subroutine simulations_14 (u)
        integer, intent(in) :: u
        type(string_t) :: libname, libname_generated
        type(string_t) :: procname
        type(string_t) :: model_name

```

```

type(rt_data_t), target :: global
type(prclib_entry_t), pointer :: lib_entry
type(process_library_t), pointer :: lib
class(model_t), pointer :: model
class(model_data_t), pointer :: model_data
type(simulation_t), target :: simulation
type(particle_set_t) :: pset
type(eio_direct_t) :: eio_in
type(eio_dump_t) :: eio_out
real(default) :: sqrts, mw, pp
real(default), dimension(3) :: p3
type(vector4_t), dimension(:), allocatable :: p
real(default), dimension(:), allocatable :: m
integer :: u_verbose, i
real(default) :: sqme_proc
real(default), dimension(:), allocatable :: sqme
real(default) :: on_shell_limit
integer, dimension(:), allocatable :: i_array
real(default), dimension(:), allocatable :: prob_array

write (u, "(A)")  "* Test output: simulations_14"
write (u, "(A)")  "* Purpose: construct resonant subprocesses &
                  &in the simulation object"
write (u, "(A)")

write (u, "(A)")  "* Build and load a test library with one process"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_phs_forest_init ()

libname = "simulations_14_lib"
procname = "simulations_14_p"

call global%global_init ()
call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?update_sqme"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_weight"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_event"), &

```

```

        .true., is_known = .true.)

model_name = "SM"
call global%select_model (model_name)
allocate (model)
call model%init_instance (global%model)
model_data => model

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

call prepare_resonance_test_library &
      (lib, libname, procname, model_data, global, u)

write (u, "(A)")
write (u, "(A)")  "* Initialize simulation object &
                  &with resonant subprocesses"
write (u, "(A)")

call global%set_log (var_str ("?resonance_history"), &
                    .true., is_known = .true.)
call global%set_real (var_str ("resonance_on_shell_limit"), &
                     10._default, is_known = .true.)

call simulation%init ([procname], &
                     integrate=.false., generate=.false., local=global)

call simulation%write_resonant_subprocess_data (u, 1)

write (u, "(A)")
write (u, "(A)")  "* Resonant subprocesses: generated library"
write (u, "(A)")

libname_generated = procname // "_R"
lib => global%prclib_stack%get_library_ptr (libname_generated)
if (associated (lib)) call lib%write (u, libpath=.false.)

write (u, "(A)")
write (u, "(A)")  "* Generated process stack"
write (u, "(A)")

call global%process_stack%show (u)

write (u, "(A)")
write (u, "(A)")  "* Particle set"
write (u, "(A)")

pset = simulation%get_hard_particle_set (1)
call pset%write (u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Initialize object for direct access"
write (u, "(A)")

call eio_in%init_direct &
      (n_beam = 0, n_in = 2, n_rem = 0, n_vir = 0, n_out = 3, &
       pdg = [-11, 11, 1, -2, 24], model=global%model)
call eio_in%set_selection_indices (1, 1, 1, 1)

sqrts = global%get_rval (var_str ("sqrts"))
mw = 80._default  ! deliberately slightly different from true mw
pp = sqrt (sqrts**2 - 4 * mw**2) / 2

allocate (p (5), m (5))
p(1) = vector4_moving (sqrts/2, sqrts/2, 3)
m(1) = 0
p(2) = vector4_moving (sqrts/2, -sqrts/2, 3)
m(2) = 0
p3(1) = pp/2
p3(2) = mw/2
p3(3) = 0
p(3) = vector4_moving (sqrts/4, vector3_moving (p3))
m(3) = 0
p3(2) = -mw/2
p(4) = vector4_moving (sqrts/4, vector3_moving (p3))
m(4) = 0
p(5) = vector4_moving (sqrts/2, -pp, 1)
m(5) = mw
call eio_in%set_momentum (p, m**2)

call eio_in%write (u)

write (u, "(A)")
write (u, "(A)")  "* Transfer and show particle set"
write (u, "(A)")

call simulation%read_event (eio_in)
pset = simulation%get_hard_particle_set (1)
call pset%write (u)

write (u, "(A)")
write (u, "(A)")  "* (Re)calculate matrix element"
write (u, "(A)")

call simulation%recalculate (recover_phs = .false.)
call simulation%evaluate_transforms ()

write (u, "(A)")  "* Show event with sqme"
write (u, "(A)")

call eio_out%set_parameters (unit = u, &
                             weights = .true., pacify = .true., compressed = .true.)
call eio_out%init_out (var_str (""))

```

```

call simulation%write_event (eio_out)

write (u, "(A)")
write (u, "(A)")  "* Write event to separate file &
                  &'simulations_14_event_verbose.log'"

u_verbose = free_unit ()
open (unit = u_verbose, file = "simulations_14_event_verbose.log", &
      status = "replace", action = "write")
call simulation%write (u_verbose)
write (u_verbose, *)
call simulation%write_event (u_verbose, verbose = .true., testflag = .true.)
close (u_verbose)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_14"

end subroutine simulations_14

```

Resonant subprocess simulation

Prepare a process with resonances and enter resonant subprocesses in the simulation object. Simulate events with selection of resonance histories.

The process and its initialization is taken from `processes_18`, but we need a complete O'MEGA matrix element here.

```

<Simulations: execute tests>+≡
  call test (simulations_15, "simulations_15", &
            "resonant subprocesses in simulation", &
            u, results)

<Simulations: test declarations>+≡
  public :: simulations_15

<Simulations: tests>+≡
  subroutine simulations_15 (u)
    integer, intent(in) :: u
    type(string_t) :: libname, libname_generated
    type(string_t) :: procname
    type(string_t) :: model_name
    type(rt_data_t), target :: global
    type(prclib_entry_t), pointer :: lib_entry
    type(process_library_t), pointer :: lib
    class(model_t), pointer :: model
    class(model_data_t), pointer :: model_data
    type(simulation_t), target :: simulation
    real(default) :: sqrts
    type(eio_dump_t) :: eio_out

```

```

integer :: u_verbose

write (u, "(A)")  "* Test output: simulations_15"
write (u, "(A)")  "*   Purpose: generate event with resonant subprocess"
write (u, "(A)")

write (u, "(A)")  "* Build and load a test library with one process"
write (u, "(A)")

call syntax_model_file_init ()
call syntax_phs_forest_init ()

libname = "simulations_15_lib"
procname = "simulations_15_p"

call global%global_init ()
call global%append_log (&
    var_str ("?rebuild_phase_space"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_grids"), .true., intrinsic = .true.)
call global%append_log (&
    var_str ("?rebuild_events"), .true., intrinsic = .true.)
call global%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
call global%set_int (var_str ("seed"), &
    0, is_known = .true.)
call global%set_real (var_str ("sqrts"), &
    1000._default, is_known = .true.)
call global%set_log (var_str ("?recover_beams"), &
    .false., is_known = .true.)
call global%set_log (var_str ("?update_sqme"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_weight"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?update_event"), &
    .true., is_known = .true.)
call global%set_log (var_str ("?resonance_history"), &
    .true., is_known = .true.)
call global%set_real (var_str ("resonance_on_shell_limit"), &
    10._default, is_known = .true.)

model_name = "SM"
call global%select_model (model_name)
allocate (model)
call model%init_instance (global%model)
model_data => model

write (u, "(A)")  "* Initialize process library and process"
write (u, "(A)")

allocate (lib_entry)
call lib_entry%init (libname)
lib => lib_entry%process_library_t
call global%add_prclib (lib_entry)

```

```

call prepare_resonance_test_library &
    (lib, libname, procname, model_data, global, u)

write (u, "(A)")
write (u, "(A)")  "* Initialize simulation object &
    &with resonant subprocesses"
write (u, "(A)")

call global%it_list%init ([1], [1000])
call simulation%init ([procname], &
    integrate=.true., generate=.true., local=global)

call simulation%write_resonant_subprocess_data (u, 1)

write (u, "(A)")
write (u, "(A)")  "* Generate event"
write (u, "(A)")

call simulation%init_process_selector ()
call simulation%set_n_events_requested (1)
call simulation%generate ()

call eio_out%set_parameters (unit = u, &
    weights = .true., pacify = .true., compressed = .true.)
call eio_out%init_out (var_str (""))
call simulation%write_event (eio_out)

write (u, "(A)")
write (u, "(A)")  "* Write event to separate file &
    &'simulations_15_event_verbose.log'"

u_verbose = free_unit ()
open (unit = u_verbose, file = "simulations_15_event_verbose.log", &
    status = "replace", action = "write")
call simulation%write (u_verbose)
write (u_verbose, *)
call simulation%write_event (u_verbose, verbose = .true., testflag = .true.)
close (u_verbose)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call simulation%final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: simulations_15"

end subroutine simulations_15

```

Chapter 34

More Unit Tests

This chapter collects some procedures for testing that can't be provided at the point where the corresponding modules are defined, because they use other modules of a different level.

(We should move them back, collecting the high-level functionality in init/final hooks that we can set at runtime.)

34.1 Expression Testing

Expression objects are part of process and event objects, but the process and event object modules should not depend on the implementation of expressions. Here, we collect unit tests that depend on expression implementation.

```
(expr_tests_ut.f90)≡  
  <File header>  
  module expr_tests_ut  
  
    use unit_tests  
    use expr_tests_uti  
  
    <Standard module head>  
  
    <Expr tests: public test>  
  
    contains  
  
    <Expr tests: test driver>  
  
  end module expr_tests_ut  
(expr_tests_uti.f90)≡  
  <File header>  
  
  module expr_tests_uti  
  
    <Use kinds>  
    <Use strings>  
    use format_defs, only: FMT_12  
    use format_utils, only: write_separator
```



```

    use os_interface
    use sm_qcd
    use lorentz
    use ifiles
    use lexers
    use parser
    use model_data
    use interactions, only: reset_interaction_counter
    use process_libraries
    use subevents
    use subvt_expr
    use rng_base
    use mci_base
    use phs_base
    use variables, only: var_list_t
    use eval_trees
    use models
    use prc_core
    use prc_test
    use process, only: process_t
    use instances, only: process_instance_t
    use events

    use rng_base_ut, only: rng_test_factory_t
    use phs_base_ut, only: phs_test_config_t

    <Standard module head>

    <Expr tests: test declarations>

contains

    <Expr tests: tests>

    <Expr tests: test auxiliary>

end module expr_tests_util

```

34.1.1 Test

This is the master for calling self-test procedures.

```

    <Expr tests: public test>≡
        public :: subvt_expr_test

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

```

Parton-event expressions

```
<Expr tests: execute tests>≡
  call test (subevt_expr_1, "subevt_expr_1", &
    "parton-event expressions", &
    u, results)

<Expr tests: test declarations>≡
  public :: subevt_expr_1

<Expr tests: tests>≡
  subroutine subevt_expr_1 (u)
    integer, intent(in) :: u
    type(string_t) :: expr_text
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(parse_tree_t) :: pt_cuts, pt_scale, pt_fac_scale, pt_ren_scale
    type(parse_tree_t) :: pt_weight
    type(parse_node_t), pointer :: pn_cuts, pn_scale, pn_fac_scale, pn_ren_scale
    type(parse_node_t), pointer :: pn_weight
    type(eval_tree_factory_t) :: expr_factory
    type(os_data_t) :: os_data
    type(model_t), target :: model
    type(parton_expr_t), target :: expr
    real(default) :: E, Ex, m
    type(vector4_t), dimension(6) :: p
    integer :: i, pdg
    logical :: passed
    real(default) :: scale, fac_scale, ren_scale, weight

    write (u, "(A)")  "* Test output: subevt_expr_1"
    write (u, "(A)")  "* Purpose: Set up a subevt and associated &
      &process-specific expressions"
    write (u, "(A)")

    call syntax_pexpr_init ()

    call syntax_model_file_init ()
    call os_data%init ()
    call model%read (var_str ("Test.mdl"), os_data)

    write (u, "(A)")  "* Expression texts"
    write (u, "(A)")

    expr_text = "all Pt > 100 [s]"
    write (u, "(A,A)") "cuts = ", char (expr_text)
    call ifile_clear (ifile)
    call ifile_append (ifile, expr_text)
    call stream_init (stream, ifile)
    call parse_tree_init_lexpr (pt_cuts, stream, .true.)
    call stream_final (stream)
    pn_cuts => pt_cuts%get_root_ptr ()

    expr_text = "sqrts"
    write (u, "(A,A)") "scale = ", char (expr_text)
```

```

call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_scale, stream, .true.)
call stream_final (stream)
pn_scale => pt_scale%get_root_ptr ()

expr_text = "sqrts_hat"
write (u, "(A,A)") "fac_scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_fac_scale, stream, .true.)
call stream_final (stream)
pn_fac_scale => pt_fac_scale%get_root_ptr ()

expr_text = "100"
write (u, "(A,A)") "ren_scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_ren_scale, stream, .true.)
call stream_final (stream)
pn_ren_scale => pt_ren_scale%get_root_ptr ()

expr_text = "n_tot - n_in - n_out"
write (u, "(A,A)") "weight = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_weight, stream, .true.)
call stream_final (stream)
pn_weight => pt_weight%get_root_ptr ()

call ifile_final (ifile)

write (u, "(A)")
write (u, "(A)")  "* Initialize process expr"
write (u, "(A)")

call expr%setup_vars (1000._default)
call expr%var_list%append_real (var_str ("tolerance"), 0._default)
call expr%link_var_list (model%get_var_list_ptr ())

call expr_factory%init (pn_cuts)
call expr%setup_selection (expr_factory)
call expr_factory%init (pn_scale)
call expr%setup_scale (expr_factory)
call expr_factory%init (pn_fac_scale)
call expr%setup_fac_scale (expr_factory)
call expr_factory%init (pn_ren_scale)
call expr%setup_ren_scale (expr_factory)
call expr_factory%init (pn_weight)
call expr%setup_weight (expr_factory)

```

```

call write_separator (u)
call expr%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Fill subevt and evaluate expressions"
write (u, "(A)")

call subevt_init (expr%subevt_t, 6)
E = 500._default
Ex = 400._default
m = 125._default
pdg = 25
p(1) = vector4_moving (E, sqrt (E**2 - m**2), 3)
p(2) = vector4_moving (E, -sqrt (E**2 - m**2), 3)
p(3) = vector4_moving (Ex, sqrt (Ex**2 - m**2), 3)
p(4) = vector4_moving (Ex, -sqrt (Ex**2 - m**2), 3)
p(5) = vector4_moving (Ex, sqrt (Ex**2 - m**2), 1)
p(6) = vector4_moving (Ex, -sqrt (Ex**2 - m**2), 1)

call expr%reset_contents ()
do i = 1, 2
    call subevt_set_beam (expr%subevt_t, i, pdg, p(i), m**2)
end do
do i = 3, 4
    call subevt_set_incoming (expr%subevt_t, i, pdg, p(i), m**2)
end do
do i = 5, 6
    call subevt_set_outgoing (expr%subevt_t, i, pdg, p(i), m**2)
end do
expr%sqrts_hat = subevt_get_sqrts_hat (expr%subevt_t)
expr%n_in = 2
expr%n_out = 2
expr%n_tot = 4
expr%subevt_filled = .true.

call expr%evaluate (passed, scale, fac_scale, ren_scale, weight)

write (u, "(A,L1)")      "Event has passed      = ", passed
write (u, "(A," // FMT_12 // ")")  "Scale          = ", scale
write (u, "(A," // FMT_12 // ")")  "Factorization scale = ", fac_scale
write (u, "(A," // FMT_12 // ")")  "Renormalization scale = ", ren_scale
write (u, "(A," // FMT_12 // ")")  "Weight          = ", weight
write (u, "(A)")

call write_separator (u)
call expr%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call expr%final ()

```

```

call model%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: subevt_expr_1"

end subroutine subevt_expr_1

```

Parton-event expressions

```

<Expr tests: execute tests>+≡
call test (subevt_expr_2, "subevt_expr_2", &
  "parton-event expressions", &
  u, results)

<Expr tests: test declarations>+≡
public :: subevt_expr_2

<Expr tests: tests>+≡
subroutine subevt_expr_2 (u)
  integer, intent(in) :: u
  type(string_t) :: expr_text
  type(ifile_t) :: ifile
  type(stream_t) :: stream
  type(parse_tree_t) :: pt_selection
  type(parse_tree_t) :: pt_reweight, pt_analysis
  type(parse_node_t), pointer :: pn_selection
  type(parse_node_t), pointer :: pn_reweight, pn_analysis
  type(os_data_t) :: os_data
  type(model_t), target :: model
  type(eval_tree_factory_t) :: expr_factory
  type(event_expr_t), target :: expr
  real(default) :: E, Ex, m
  type(vector4_t), dimension(6) :: p
  integer :: i, pdg
  logical :: passed
  real(default) :: reweight
  logical :: analysis_flag

  write (u, "(A)")  "* Test output: subevt_expr_2"
  write (u, "(A)")  "* Purpose: Set up a subevt and associated &
    &process-specific expressions"
  write (u, "(A)")

  call syntax_pexpr_init ()

  call syntax_model_file_init ()
  call os_data%init ()
  call model%read (var_str ("Test.mdl"), os_data)

  write (u, "(A)")  "* Expression texts"
  write (u, "(A)")

```

```

expr_text = "all Pt > 100 [s]"
write (u, "(A,A)") "selection = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (pt_selection, stream, .true.)
call stream_final (stream)
pn_selection => pt_selection%get_root_ptr ()

expr_text = "n_tot - n_in - n_out"
write (u, "(A,A)") "reweight = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_reweight, stream, .true.)
call stream_final (stream)
pn_reweight => pt_reweight%get_root_ptr ()

expr_text = "true"
write (u, "(A,A)") "analysis = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (pt_analysis, stream, .true.)
call stream_final (stream)
pn_analysis => pt_analysis%get_root_ptr ()

call ifile_final (ifile)

write (u, "(A)")
write (u, "(A)") "* Initialize process expr"
write (u, "(A)")

call expr%setup_vars (1000._default)
call expr%link_var_list (model%get_var_list_ptr ())
call expr%var_list%append_real (var_str ("tolerance"), 0._default)

call expr_factory%init (pn_selection)
call expr%setup_selection (expr_factory)
call expr_factory%init (pn_analysis)
call expr%setup_analysis (expr_factory)
call expr_factory%init (pn_reweight)
call expr%setup_reweight (expr_factory)

call write_separator (u)
call expr%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)") "* Fill subevt and evaluate expressions"
write (u, "(A)")

call subevt_init (expr%subevt_t, 6)

```

```

E = 500._default
Ex = 400._default
m = 125._default
pdg = 25
p(1) = vector4_moving (E, sqrt (E**2 - m**2), 3)
p(2) = vector4_moving (E, -sqrt (E**2 - m**2), 3)
p(3) = vector4_moving (Ex, sqrt (Ex**2 - m**2), 3)
p(4) = vector4_moving (Ex, -sqrt (Ex**2 - m**2), 3)
p(5) = vector4_moving (Ex, sqrt (Ex**2 - m**2), 1)
p(6) = vector4_moving (Ex, -sqrt (Ex**2 - m**2), 1)

call expr%reset_contents ()
do i = 1, 2
  call subevt_set_beam (expr%subevt_t, i, pdg, p(i), m**2)
end do
do i = 3, 4
  call subevt_set_incoming (expr%subevt_t, i, pdg, p(i), m**2)
end do
do i = 5, 6
  call subevt_set_outgoing (expr%subevt_t, i, pdg, p(i), m**2)
end do
expr%sqrts_hat = subevt_get_sqrts_hat (expr%subevt_t)
expr%n_in = 2
expr%n_out = 2
expr%n_tot = 4
expr%subevt_filled = .true.

call expr%evaluate (passed, reweight, analysis_flag)

write (u, "(A,L1)")      "Event has passed      = ", passed
write (u, "(A," // FMT_12 // ")") "Reweighting factor = ", reweight
write (u, "(A,L1)")      "Analysis flag      = ", analysis_flag
write (u, "(A)")

call write_separator (u)
call expr%write (u)
call write_separator (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call expr%final ()

call model%final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: subevt_expr_2"

end subroutine subevt_expr_2

```

Processes: handle partonic cuts

Initialize a process and process instance, choose a sampling point and fill the process instance, evaluating a given cut configuration.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

```
(Expr tests: execute tests)+≡
    call test (processes_5, "processes_5", &
        "handle cuts (partonic event)", &
        u, results)

(Expr tests: test declarations)+≡
    public :: processes_5

(Expr tests: tests)+≡
    subroutine processes_5 (u)
        integer, intent(in) :: u
        type(string_t) :: cut_expr_text
        type(ifile_t) :: ifile
        type(stream_t) :: stream
        type(parse_tree_t) :: parse_tree
        type(eval_tree_factory_t) :: expr_factory
        type(process_library_t), target :: lib
        type(string_t) :: libname
        type(string_t) :: procname
        type(os_data_t) :: os_data
        type(model_t), pointer :: model_tmp
        type(model_t), pointer :: model
        type(var_list_t), target :: var_list
        type(process_t), allocatable, target :: process
        class(phs_config_t), allocatable :: phs_config_template
        real(default) :: sqrts
        type(process_instance_t), allocatable, target :: process_instance

        write (u, "(A)")  "* Test output: processes_5"
        write (u, "(A)")  "*   Purpose: create a process &
            &and fill a process instance"
        write (u, "(A)")

        write (u, "(A)")  "* Prepare a cut expression"
        write (u, "(A)")

        call syntax_pexpr_init ()
        cut_expr_text = "all Pt > 100 [s]"
        call ifile_append (ifile, cut_expr_text)
        call stream_init (stream, ifile)
        call parse_tree_init_lexpr (parse_tree, stream, .true.)

        write (u, "(A)")  "* Build and initialize a test process"
        write (u, "(A)")

        libname = "processes5"
        procname = libname

        call os_data%init ()
```



```

call prc_test_create_library (libname, lib)

call syntax_model_file_init ()
allocate (model_tmp)
call model_tmp%read (var_str ("Test.mdl"), os_data)
call var_list%init_snapshot (model_tmp%get_var_list_ptr ())
model => model_tmp

call reset_interaction_counter ()

call var_list%append_real (var_str ("tolerance"), 0._default)
call var_list%append_log (var_str ("?alphas_is_fixed"), .true.)
call var_list%append_int (var_str ("seed"), 0)

allocate (process)
call process%init (procname, lib, os_data, model, var_list)

call var_list%final ()

allocate (phs_test_config_t :: phs_config_template)
call process%setup_test_cores ()
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrt_s = 1000
call process%setup_beams_sqrt_s (sqrt_s, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization and set cuts"
write (u, "(A)")

call process%setup_terms ()
call expr_factory%init (parse_tree%get_root_ptr ())
call process%set_cuts (expr_factory)
call process%write (.false., u, &
    show_var_list=.true., show_expressions=.true., show_os_data=.false.)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)

write (u, "(A)")
write (u, "(A)")  "* Inject a set of random numbers"
write (u, "(A)")

call process_instance%choose_mci (1)
call process_instance%set_mcpars ([0._default, 0._default])

```

```

write (u, "(A)")
write (u, "(A)")  "* Set up kinematics and subvt, check cuts (should fail)"
write (u, "(A)")

call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()
call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for another set (should succeed)"
write (u, "(A)")

call process_instance%reset ()
call process_instance%set_mcpair ([0.5_default, 0.125_default])
call process_instance%select_channel (1)
call process_instance%compute_seed_kinematics ()
call process_instance%compute_hard_kinematics ()
call process_instance%compute_eff_kinematics ()
call process_instance%evaluate_expressions ()
call process_instance%compute_other_channels ()
call process_instance%evaluate_trace ()

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for another set using convenience procedure &
                  &(failure)"
write (u, "(A)")

call process_instance%evaluate_sqme (1, [0.0_default, 0.2_default])

call process_instance%write_header (u)

write (u, "(A)")
write (u, "(A)")  "* Evaluate for another set using convenience procedure &
                  &(success)"
write (u, "(A)")

call process_instance%evaluate_sqme (1, [0.1_default, 0.2_default])

call process_instance%write_header (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()

```

```

deallocate (process)

call parse_tree_final (parse_tree)
call stream_final (stream)
call ifile_final (ifile)
call syntax_pexpr_final ()

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_5"

end subroutine processes_5

```

Trivial for testing: do not allocate the MCI record.

```

<Expr tests: test auxiliary>≡
subroutine dispatch_mci_empty (mci, var_list, process_id, is_nlo)
  class(mci_t), allocatable, intent(out) :: mci
  type(var_list_t), intent(in) :: var_list
  type(string_t), intent(in) :: process_id
  logical, intent(in), optional :: is_nlo
end subroutine dispatch_mci_empty

```

Processes: scales and such

Initialize a process and process instance, choose a sampling point and fill the process instance, evaluating a given cut configuration.

We use the same trivial process as for the previous test. All momentum and state dependence is trivial, so we just test basic functionality.

```

<Expr tests: execute tests>+≡
  call test (processes_6, "processes_6", &
    "handle scales and weight (partonic event)", &
    u, results)

<Expr tests: test declarations>+≡
  public :: processes_6

<Expr tests: tests>+≡
subroutine processes_6 (u)
  integer, intent(in) :: u
  type(string_t) :: expr_text
  type(ifile_t) :: ifile
  type(stream_t) :: stream
  type(parse_tree_t) :: pt_scale, pt_fac_scale, pt_ren_scale, pt_weight
  type(process_library_t), target :: lib
  type(string_t) :: libname
  type(string_t) :: procname
  type(os_data_t) :: os_data
  type(model_t), pointer :: model_tmp
  type(model_t), pointer :: model
  type(var_list_t), target :: var_list
  type(process_t), allocatable, target :: process
  class(phs_config_t), allocatable :: phs_config_template

```

```

real(default) :: sqrts
type(process_instance_t), allocatable, target :: process_instance
type(eval_tree_factory_t) :: expr_factory

write (u, "(A)")  "* Test output: processes_6"
write (u, "(A)")  "*   Purpose: create a process &
                    &and fill a process instance"
write (u, "(A)")

write (u, "(A)")  "* Prepare expressions"
write (u, "(A)")

call syntax_pexpr_init ()

expr_text = "sqrts - 100 GeV"
write (u, "(A,A)") "scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_scale, stream, .true.)
call stream_final (stream)

expr_text = "sqrts_hat"
write (u, "(A,A)") "fac_scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_fac_scale, stream, .true.)
call stream_final (stream)

expr_text = "eval sqrt (M2) [collect [s]]"
write (u, "(A,A)") "ren_scale = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_ren_scale, stream, .true.)
call stream_final (stream)

expr_text = "n_tot * n_in * n_out * (eval Phi / pi [s])"
write (u, "(A,A)") "weight = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_weight, stream, .true.)
call stream_final (stream)

call ifile_final (ifile)

write (u, "(A)")
write (u, "(A)")  "* Build and initialize a test process"
write (u, "(A)")

libname = "processes4"
procname = libname

```

```

call os_data%init ()
call prc_test_create_library (libname, lib)

call syntax_model_file_init ()
allocate (model_tmp)
call model_tmp%read (var_str ("Test.mdl"), os_data)
call var_list%init_snapshot (model_tmp%get_var_list_ptr ())
model => model_tmp

call var_list%append_log (var_str ("?alphas_is_fixed"), .true.)
call var_list%append_int (var_str ("seed"), 0)

call reset_interaction_counter ()

allocate (process)
call process%init (procname, lib, os_data, model, var_list)

call var_list%final ()

call process%setup_test_cores ()
allocate (phs_test_config_t :: phs_config_template)
call process%init_components (phs_config_template)

write (u, "(A)")  "* Prepare a trivial beam setup"
write (u, "(A)")

sqrt_s = 1000
call process%setup_beams_sqrt_s (sqrt_s, i_core = 1)
call process%configure_phs ()
call process%setup_mci (dispatch_mci_empty)

write (u, "(A)")  "* Complete process initialization and set cuts"
write (u, "(A)")

call process%setup_terms ()
call expr_factory%init (pt_scale%get_root_ptr ())
call process%set_scale (expr_factory)
call expr_factory%init (pt_fac_scale%get_root_ptr ())
call process%set_fac_scale (expr_factory)
call expr_factory%init (pt_ren_scale%get_root_ptr ())
call process%set_ren_scale (expr_factory)
call expr_factory%init (pt_weight%get_root_ptr ())
call process%set_weight (expr_factory)
call process%write (.false., u, show_expressions=.true.)

write (u, "(A)")
write (u, "(A)")  "* Create a process instance and evaluate"
write (u, "(A)")

allocate (process_instance)
call process_instance%init (process)
call process_instance%choose_mci (1)
call process_instance%evaluate_sqme (1, [0.5_default, 0.125_default])

```

```

call process_instance%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call process_instance%final ()
deallocate (process_instance)

call process%final ()
deallocate (process)

call parse_tree_final (pt_scale)
call parse_tree_final (pt_fac_scale)
call parse_tree_final (pt_ren_scale)
call parse_tree_final (pt_weight)
call syntax_pexpr_final ()

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: processes_6"

end subroutine processes_6

```

Event expressions

After generating an event, fill the `subevt` and evaluate expressions for selection, reweighting, and analysis.

```

<Expr tests: execute tests>+≡
  call test (events_3, "events_3", &
    "expression evaluation", &
    u, results)

<Expr tests: test declarations>+≡
  public :: events_3

<Expr tests: tests>+≡
  subroutine events_3 (u)
    use processes_ut, only: prepare_test_process, cleanup_test_process
    integer, intent(in) :: u
    type(string_t) :: expr_text
    type(ifile_t) :: ifile
    type(stream_t) :: stream
    type(parse_tree_t) :: pt_selection, pt_reweight, pt_analysis
    type(eval_tree_factory_t) :: expr_factory
    type(event_t), allocatable, target :: event
    type(process_t), allocatable, target :: process
    type(process_instance_t), allocatable, target :: process_instance
    type(os_data_t) :: os_data
    type(model_t), pointer :: model
    type(var_list_t), target :: var_list

```

```

write (u, "(A)")  "* Test output: events_3"
write (u, "(A)")  "* Purpose: generate an event and evaluate expressions"
write (u, "(A)")

call syntax_pexpr_init ()

write (u, "(A)")  "* Expression texts"
write (u, "(A)")

expr_text = "all Pt > 100 [s]"
write (u, "(A,A)") "selection = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (pt_selection, stream, .true.)
call stream_final (stream)

expr_text = "1 + sqrt_hat / sqrt"
write (u, "(A,A)") "reweight = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_expr (pt_reweight, stream, .true.)
call stream_final (stream)

expr_text = "true"
write (u, "(A,A)") "analysis = ", char (expr_text)
call ifile_clear (ifile)
call ifile_append (ifile, expr_text)
call stream_init (stream, ifile)
call parse_tree_init_lexpr (pt_analysis, stream, .true.)
call stream_final (stream)

call ifile_final (ifile)

write (u, "(A)")
write (u, "(A)")  "* Initialize test process event"

call os_data%init ()

call syntax_model_file_init ()
allocate (model)
call model%read (var_str ("Test.mdl"), os_data)
call var_list%init_snapshot (model%get_var_list_ptr ())

call var_list%append_log (var_str ("?alphas_is_fixed"), .true.)
call var_list%append_int (var_str ("seed"), 0)

allocate (process)
allocate (process_instance)
call prepare_test_process (process, process_instance, model, var_list)

call var_list%final ()

```

```

call process_instance%setup_event_data ()

write (u, "(A)")
write (u, "(A)")  "* Initialize event object and set expressions"

allocate (event)
call event%basic_init ()

call expr_factory%init (pt_selection%get_root_ptr ())
call event%set_selection (expr_factory)
call expr_factory%init (pt_reweight%get_root_ptr ())
call event%set_reweight (expr_factory)
call expr_factory%init (pt_analysis%get_root_ptr ())
call event%set_analysis (expr_factory)

call event%connect (process_instance, process%get_model_ptr ())
call event%expr%var_list%append_real (var_str ("tolerance"), 0._default)
call event%setup_expressions ()

write (u, "(A)")
write (u, "(A)")  "* Generate test process event"

call process_instance%generate_weighted_event (1)

write (u, "(A)")
write (u, "(A)")  "* Fill event object and evaluate expressions"
write (u, "(A)")

call event%generate (1, [0.4_default, 0.4_default])
call event%set_index (42)
call event%evaluate_expressions ()
call event%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call event%final ()
deallocate (event)

call cleanup_test_process (process, process_instance)
deallocate (process_instance)
deallocate (process)

call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: events_3"

end subroutine events_3

```


Chapter 35

Top Level

The top level consists of

commands Defines generic command-list and command objects, and all specific implementations. Each command type provides a specific functionality. Together with the modules that provide expressions and variables, this module defines the Sindarin language.

whizard This module interprets streams of various kind in terms of the command language. It also contains the unit-test feature. We also define the externally visible procedures here, for the **WHIZARD** as a library.

main The driver for **WHIZARD** as a stand-alone program. Contains the command-line interpreter.

whizard_c_interface Alternative top-level procedures, for use in the context of a C-compatible caller program.

35.1 Commands

This module defines the command language of the main input file.

```
<commands.f90>≡  
  <File header>  
  
  module commands  
  
    <Use kinds>  
    <Use strings>  
    <Use debug>  
    use io_units  
    use string_utils, only: lower_case, split_string, str  
    use format_utils, only: write_indent  
    use format_defs, only: FMT_14, FMT_19  
    use diagnostics  
  
    use constants, only: one  
    use physics_defs  
    use sorting  
    use sf_lhapdf, only: lhpdf_global_reset  
    use os_interface  
    use ifiles  
    use lexers  
    use syntax_rules  
    use parser  
    use analysis  
    use pdg_arrays  
    use variables, only: var_list_t, V_NONE, V_LOG, V_INT, V_REAL, V_CMPLX, V_STR, V_PDG  
    use observables, only: var_list_check_observable  
    use observables, only: var_list_check_result_var  
    use eval_trees  
    use models  
    use auto_components  
    use flavors  
    use polarizations  
    use particle_specifiers  
    use process_libraries  
    use process  
    use instances  
    use prclib_stacks  
    use slha_interface  
    use user_files  
    use eio_data  
    use rt_data  
  
    use process_configurations  
    use compilations, only: compile_library, compile_executable  
    use integrations, only: integrate_process  
    use restricted_subprocesses, only: get_libname_res  
    use restricted_subprocesses, only: spawn_resonant_subprocess_libraries  
    use event_streams  
    use simulations
```

```

    use radiation_generator

    <Use mpi f08>

    <Standard module head>

    <Commands: public>

    <Commands: types>

    <Commands: variables>

    <Commands: parameters>

    <Commands: interfaces>

contains

    <Commands: procedures>

end module commands

```

35.1.1 The command type

The command type is a generic type that holds any command, compiled for execution.

Each command may come with its own local environment. The command list that determines this environment is allocated as `options`, if necessary. (It has to be allocated as a pointer because the type definition is recursive.) The local environment is available as a pointer which either points to the global environment, or is explicitly allocated and initialized.

```

<Commands: types>≡
    type, abstract :: command_t
        type(parse_node_t), pointer :: pn => null ()
        class(command_t), pointer :: next => null ()
        type(parse_node_t), pointer :: pn_opt => null ()
        type(command_list_t), pointer :: options => null ()
        type(rt_data_t), pointer :: local => null ()
    contains
        <Commands: command: TBP>
    end type command_t

```

Finalizer: If there is an option list, finalize the option list and deallocate. If not, the local environment is just a pointer.

```

<Commands: command: TBP>≡
    procedure :: final => command_final

<Commands: procedures>≡
    recursive subroutine command_final (cmd)
        class(command_t), intent(inout) :: cmd
        if (associated (cmd%options)) then
            call cmd%options%final ()
            deallocate (cmd%options)

```

```

        call cmd%local%local_final ()
        deallocate (cmd%local)
    else
        cmd%local => null ()
    end if
end subroutine command_final

```

Allocate a command with the appropriate concrete type. Store the parse node pointer in the command object, so we can reference to it when compiling.

(Commands: procedures)+≡

```

subroutine dispatch_command (command, pn)
    class(command_t), intent(inout), pointer :: command
    type(parse_node_t), intent(in), target :: pn
    select case (char (parse_node_get_rule_key (pn)))
    case ("cmd_model")
        allocate (cmd_model_t :: command)
    case ("cmd_library")
        allocate (cmd_library_t :: command)
    case ("cmd_process")
        allocate (cmd_process_t :: command)
    case ("cmd_nlo")
        allocate (cmd_nlo_t :: command)
    case ("cmd_compile")
        allocate (cmd_compile_t :: command)
    case ("cmd_exec")
        allocate (cmd_exec_t :: command)
    case ("cmd_num", "cmd_complex", "cmd_real", "cmd_int", &
        "cmd_log_decl", "cmd_log", "cmd_string", "cmd_string_decl", &
        "cmd_alias", "cmd_result")
        allocate (cmd_var_t :: command)
    case ("cmd_slha")
        allocate (cmd_slha_t :: command)
    case ("cmd_show")
        allocate (cmd_show_t :: command)
    case ("cmd_clear")
        allocate (cmd_clear_t :: command)
    case ("cmd_expect")
        allocate (cmd_expect_t :: command)
    case ("cmd_beams")
        allocate (cmd_beams_t :: command)
    case ("cmd_beams_pol_density")
        allocate (cmd_beams_pol_density_t :: command)
    case ("cmd_beams_pol_fraction")
        allocate (cmd_beams_pol_fraction_t :: command)
    case ("cmd_beams_momentum")
        allocate (cmd_beams_momentum_t :: command)
    case ("cmd_beams_theta")
        allocate (cmd_beams_theta_t :: command)
    case ("cmd_beams_phi")
        allocate (cmd_beams_phi_t :: command)
    case ("cmd_cuts")
        allocate (cmd_cuts_t :: command)
    case ("cmd_scale")

```

```

        allocate (cmd_scale_t :: command)
case ("cmd_fac_scale")
        allocate (cmd_fac_scale_t :: command)
case ("cmd_ren_scale")
        allocate (cmd_ren_scale_t :: command)
case ("cmd_weight")
        allocate (cmd_weight_t :: command)
case ("cmd_selection")
        allocate (cmd_selection_t :: command)
case ("cmd_reweight")
        allocate (cmd_reweight_t :: command)
case ("cmd_iterations")
        allocate (cmd_iterations_t :: command)
case ("cmd_integrate")
        allocate (cmd_integrate_t :: command)
case ("cmd_observable")
        allocate (cmd_observable_t :: command)
case ("cmd_histogram")
        allocate (cmd_histogram_t :: command)
case ("cmd_plot")
        allocate (cmd_plot_t :: command)
case ("cmd_graph")
        allocate (cmd_graph_t :: command)
case ("cmd_record")
        allocate (cmd_record_t :: command)
case ("cmd_analysis")
        allocate (cmd_analysis_t :: command)
case ("cmd_alt_setup")
        allocate (cmd_alt_setup_t :: command)
case ("cmd_unstable")
        allocate (cmd_unstable_t :: command)
case ("cmd_stable")
        allocate (cmd_stable_t :: command)
case ("cmd_polarized")
        allocate (cmd_polarized_t :: command)
case ("cmd_unpolarized")
        allocate (cmd_unpolarized_t :: command)
case ("cmd_sample_format")
        allocate (cmd_sample_format_t :: command)
case ("cmd_simulate")
        allocate (cmd_simulate_t :: command)
case ("cmd_rescan")
        allocate (cmd_rescan_t :: command)
case ("cmd_write_analysis")
        allocate (cmd_write_analysis_t :: command)
case ("cmd_compile_analysis")
        allocate (cmd_compile_analysis_t :: command)
case ("cmd_open_out")
        allocate (cmd_open_out_t :: command)
case ("cmd_close_out")
        allocate (cmd_close_out_t :: command)
case ("cmd_printf")
        allocate (cmd_printf_t :: command)
case ("cmd_scan")

```

```

        allocate (cmd_scan_t :: command)
case ("cmd_if")
    allocate (cmd_if_t :: command)
case ("cmd_include")
    allocate (cmd_include_t :: command)
case ("cmd_export")
    allocate (cmd_export_t :: command)
case ("cmd_quit")
    allocate (cmd_quit_t :: command)
case default
    print *, char (parse_node_get_rule_key (pn))
    call msg_bug ("Command not implemented")
end select
command%pn => pn
end subroutine dispatch_command

```

Output. We allow for indentation so we can display a command tree.

```

<Commands: command: TBP>+≡
    procedure (command_write), deferred :: write
<Commands: interfaces>≡
    abstract interface
        subroutine command_write (cmd, unit, indent)
            import
            class(command_t), intent(in) :: cmd
            integer, intent(in), optional :: unit, indent
        end subroutine command_write
    end interface

```

Compile a command. The command type is already fixed, so this is a deferred type-bound procedure.

```

<Commands: command: TBP>+≡
    procedure (command_compile), deferred :: compile
<Commands: interfaces>+≡
    abstract interface
        subroutine command_compile (cmd, global)
            import
            class(command_t), intent(inout) :: cmd
            type(rt_data_t), intent(inout), target :: global
        end subroutine command_compile
    end interface

```

Execute a command. This will use and/or modify the runtime data set. If the quit flag is set, the caller should terminate command execution.

```

<Commands: command: TBP>+≡
    procedure (command_execute), deferred :: execute
<Commands: interfaces>+≡
    abstract interface
        subroutine command_execute (cmd, global)
            import
            class(command_t), intent(inout) :: cmd
            type(rt_data_t), intent(inout), target :: global

```

```

        end subroutine command_execute
    end interface

```

35.1.2 Options

The `options` command list is allocated, initialized, and executed, if the command is associated with an option text in curly braces. If present, a separate local runtime data set `local` will be allocated and initialized; otherwise, `local` becomes a pointer to the global dataset.

For output, we indent the options list.

```

<Commands: command: TBP>+≡
    procedure :: write_options => command_write_options

<Commands: procedures>+≡
    recursive subroutine command_write_options (cmd, unit, indent)
        class(command_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: ind
        ind = 1; if (present (indent)) ind = indent + 1
        if (associated (cmd%options)) call cmd%options%write (unit, ind)
    end subroutine command_write_options

```

Compile the options list, if any. This implies initialization of the local environment. Should be done once the `pn_opt` node has been assigned (if applicable), but before the actual command compilation.

```

<Commands: command: TBP>+≡
    procedure :: compile_options => command_compile_options

<Commands: procedures>+≡
    recursive subroutine command_compile_options (cmd, global)
        class(command_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        if (associated (cmd%pn_opt)) then
            allocate (cmd%local)
            call cmd%local%local_init (global)
            call global%copy_globals (cmd%local)
            allocate (cmd%options)
            call cmd%options%compile (cmd%pn_opt, cmd%local)
            call global%restore_globals (cmd%local)
            call cmd%local%deactivate ()
        else
            cmd%local => global
        end if
    end subroutine command_compile_options

```

Execute options. First prepare the local environment, then execute the command list.

```

<Commands: command: TBP>+≡
    procedure :: execute_options => cmd_execute_options

```

```

⟨Commands: procedures⟩+≡
recursive subroutine cmd_execute_options (cmd, global)
  class(command_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  if (associated (cmd%options)) then
    call cmd%local%activate ()
    call cmd%options%execute (cmd%local)
  end if
end subroutine cmd_execute_options

```

This must be called after the parent command has been executed, to undo temporary modifications to the environment. Note that some modifications to `global` can become permanent.

```

⟨Commands: command: TBP⟩+≡
  procedure :: reset_options => cmd_reset_options

⟨Commands: procedures⟩+≡
subroutine cmd_reset_options (cmd, global)
  class(command_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  if (associated (cmd%options)) then
    call cmd%local%deactivate (global)
  end if
end subroutine cmd_reset_options

```

35.1.3 Specific command types

Model configuration

The command declares a model, looks for the specified file and loads it.

```

⟨Commands: types⟩+≡
type, extends (command_t) :: cmd_model_t
  private
  type(string_t) :: name
  type(string_t) :: scheme
  logical :: ufo_model = .false.
  logical :: ufo_path_set = .false.
  type(string_t) :: ufo_path
  contains
  ⟨Commands: cmd model: TBP⟩
end type cmd_model_t

```

Output

```

⟨Commands: cmd model: TBP⟩≡
  procedure :: write => cmd_model_write

⟨Commands: procedures⟩+≡
subroutine cmd_model_write (cmd, unit, indent)
  class(cmd_model_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u
  u = given_output_unit (unit); if (u < 0) return

```



```

call write_indent (u, indent)
write (u, "(1x,A,1x,'"',A,'\"')", advance="no") "model =", char (cmd%name)
if (cmd%ufo_model) then
  if (cmd%ufo_path_set) then
    write (u, "(1x,A,A,A)") "(ufo (", char (cmd%ufo_path), ")")
  else
    write (u, "(1x,A)") "(ufo)"
  end if
else if (cmd%scheme /= "") then
  write (u, "(1x,'(,A,')')") char (cmd%scheme)
else
  write (u, *)
end if
end subroutine cmd_model_write

```

Compile. Get the model name and read the model from file, so it is readily available when the command list is executed. If the model has a scheme argument, take this into account.

Assign the model pointer in the `global` record, so it can be used for (read-only) variable lookup while compiling further commands.

(Commands: cmd model: TBP)+≡

```

procedure :: compile => cmd_model_compile

```

(Commands: procedures)+≡

```

subroutine cmd_model_compile (cmd, global)
  class(cmd_model_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_name, pn_arg, pn_scheme
  type(parse_node_t), pointer :: pn_ufo_arg, pn_path
  type(model_t), pointer :: model
  type(string_t) :: scheme
  pn_name => cmd%pn%get_sub_ptr (3)
  pn_arg => pn_name%get_next_ptr ()
  if (associated (pn_arg)) then
    pn_scheme => pn_arg%get_sub_ptr ()
  else
    pn_scheme => null ()
  end if
  cmd%name = pn_name%get_string ()
  if (associated (pn_scheme)) then
    select case (char (pn_scheme%get_rule_key ()))
    case ("ufo_spec")
      cmd%ufo_model = .true.
      pn_ufo_arg => pn_scheme%get_sub_ptr (2)
      if (associated (pn_ufo_arg)) then
        pn_path => pn_ufo_arg%get_sub_ptr ()
        cmd%ufo_path_set = .true.
        cmd%ufo_path = pn_path%get_string ()
      end if
    case default
      scheme = pn_scheme%get_string ()
    select case (char (lower_case (scheme)))
    case ("ufo"); cmd%ufo_model = .true.
    case default; cmd%scheme = scheme

```

```

        end select
    end select
    if (cmd%ufo_model) then
        if (cmd%ufo_path_set) then
            call preload_ufo_model (model, cmd%name, cmd%ufo_path)
        else
            call preload_ufo_model (model, cmd%name)
        end if
    else
        call preload_model (model, cmd%name, cmd%scheme)
    end if
else
    cmd%scheme = ""
    call preload_model (model, cmd%name)
end if
global%model => model
if (associated (global%model)) then
    call global%model%link_var_list (global%var_list)
end if
contains
subroutine preload_model (model, name, scheme)
    type(model_t), pointer, intent(out) :: model
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: scheme
    model => null ()
    if (associated (global%model)) then
        if (global%model%matches (name, scheme)) then
            model => global%model
        end if
    end if
    if (.not. associated (model)) then
        if (global%model_list%model_exists (name, scheme)) then
            model => global%model_list%get_model_ptr (name, scheme)
        else
            call global%read_model (name, model, scheme)
        end if
    end if
end subroutine preload_model
subroutine preload_ufo_model (model, name, ufo_path)
    type(model_t), pointer, intent(out) :: model
    type(string_t), intent(in) :: name
    type(string_t), intent(in), optional :: ufo_path
    model => null ()
    if (associated (global%model)) then
        if (global%model%matches (name, ufo=.true., ufo_path=ufo_path)) then
            model => global%model
        end if
    end if
    if (.not. associated (model)) then
        if (global%model_list%model_exists (name, &
            ufo=.true., ufo_path=ufo_path)) then
            model => global%model_list%get_model_ptr (name, &
                ufo=.true., ufo_path=ufo_path)
        else

```

```

        call global%read_ufo_model (name, model, ufo_path=ufo_path)
    end if
end if
end subroutine preload_ufo_model
end subroutine cmd_model_compile

```

Execute: Insert a pointer into the global data record and reassign the variable list.

```

⟨Commands: cmd model: TBP⟩+≡
    procedure :: execute => cmd_model_execute

⟨Commands: procedures⟩+≡
    subroutine cmd_model_execute (cmd, global)
        class(cmd_model_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        if (cmd%ufo_model) then
            if (cmd%ufo_path_set) then
                call global%select_model (cmd%name, ufo=.true., ufo_path=cmd%ufo_path)
            else
                call global%select_model (cmd%name, ufo=.true.)
            end if
        else if (cmd%scheme /= "") then
            call global%select_model (cmd%name, cmd%scheme)
        else
            call global%select_model (cmd%name)
        end if
        if (.not. associated (global%model)) &
            call msg_fatal ("Switching to model '" &
                // char (cmd%name) // "': model not found")
    end subroutine cmd_model_execute

```

Library configuration

We configure a process library that should hold the subsequently defined processes. If the referenced library exists already, just make it the currently active one.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_library_t
    private
        type(string_t) :: name
    contains
        ⟨Commands: cmd library: TBP⟩
    end type cmd_library_t

```

Output.

```

⟨Commands: cmd library: TBP⟩≡
    procedure :: write => cmd_library_write

⟨Commands: procedures⟩+≡
    subroutine cmd_library_write (cmd, unit, indent)
        class(cmd_library_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
    end subroutine cmd_library_write

```

```

integer :: u
u = given_output_unit (unit)
call write_indent (u, indent)
write (u, "(1x,A,1x,'"',A,'\"')") "library =", char (cmd%name)
end subroutine cmd_library_write

```

Compile. Get the library name.

```

⟨Commands: cmd library: TBP⟩+≡
  procedure :: compile => cmd_library_compile
⟨Commands: procedures⟩+≡
  subroutine cmd_library_compile (cmd, global)
    class(cmd_library_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_name
    pn_name => parse_node_get_sub_ptr (cmd%pn, 3)
    cmd%name = parse_node_get_string (pn_name)
  end subroutine cmd_library_compile

```

Execute: Initialize a new library and push it on the library stack (if it does not yet exist). Insert a pointer to the library into the global data record. Then, try to load the library unless the rebuild flag is set.

```

⟨Commands: cmd library: TBP⟩+≡
  procedure :: execute => cmd_library_execute
⟨Commands: procedures⟩+≡
  subroutine cmd_library_execute (cmd, global)
    class(cmd_library_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(prclib_entry_t), pointer :: lib_entry
    type(process_library_t), pointer :: lib
    logical :: rebuild_library
    lib => global%prclib_stack%get_library_ptr (cmd%name)
    rebuild_library = &
      global%var_list%get_lval (var_str ("?rebuild_library"))
    if (.not. (associated (lib))) then
      allocate (lib_entry)
      call lib_entry%init (cmd%name)
      lib => lib_entry%process_library_t
      call global%add_prclib (lib_entry)
    else
      call global%update_prclib (lib)
    end if
    if (associated (lib) .and. .not. rebuild_library) then
      call lib%update_status (global%os_data)
    end if
  end subroutine cmd_library_execute

```

Process configuration

We define a process-configuration command as a specific type. The incoming and outgoing particles are given evaluation-trees which we transform to PDG-code arrays. For transferring to O'MEGA, they are reconverted to strings.

For the incoming particles, we store parse nodes individually. We do not yet resolve the outgoing state, so we store just a single parse node.

This also includes the choice of method for the corresponding process: `omega` for O'MEGA matrix elements as Fortran code, `ovm` for O'MEGA matrix elements as a bytecode virtual machine, `test` for special processes, `unit_test` for internal test matrix elements generated by WHIZARD, `template` and `template_unity` for test matrix elements generated by WHIZARD as Fortran code similar to the O'MEGA code. If the one-loop program (OLP) GoSam is linked, also matrix elements from there (at leading and next-to-leading order) can be generated via `gosam`.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_process_t
  private
  type(string_t) :: id
  integer :: n_in = 0
  type(parse_node_p), dimension(:), allocatable :: pn_pdg_in
  type(parse_node_t), pointer :: pn_out => null ()
  contains
  ⟨Commands: cmd process: TBP⟩
end type cmd_process_t

```

Output. The particle expressions are not resolved, so we just list the number of incoming particles.

```

⟨Commands: cmd process: TBP⟩≡
  procedure :: write => cmd_process_write

⟨Commands: procedures⟩+≡
  subroutine cmd_process_write (cmd, unit, indent)
    class(cmd_process_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,A,A,I0,A)") "process: ", char (cmd%id), " (", &
      size (cmd%pn_pdg_in), " -> X)"
    call cmd%write_options (u, indent)
  end subroutine cmd_process_write

```

Compile. Find and assign the parse nodes.

```

⟨Commands: cmd process: TBP⟩+≡
  procedure :: compile => cmd_process_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_process_compile (cmd, global)
    class(cmd_process_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_id, pn_in, pn_codes
    integer :: i
    pn_id => parse_node_get_sub_ptr (cmd%pn, 2)
    pn_in => parse_node_get_next_ptr (pn_id, 2)
    cmd%pn_out => parse_node_get_next_ptr (pn_in, 2)
    cmd%pn_opt => parse_node_get_next_ptr (cmd%pn_out)
    call cmd%compile_options (global)
    cmd%id = parse_node_get_string (pn_id)

```

```

cmd%n_in = parse_node_get_n_sub (pn_in)
pn_codes => parse_node_get_sub_ptr (pn_in)
allocate (cmd%pn_pdg_in (cmd%n_in))
do i = 1, cmd%n_in
    cmd%pn_pdg_in(i)%ptr => pn_codes
    pn_codes => parse_node_get_next_ptr (pn_codes)
end do
end subroutine cmd_process_compile

```

Command execution. Evaluate the subevents, transform PDG codes into strings, and add the current process configuration to the process library.

The initial state will be unique (one or two particles). For the final state, we allow for expressions. The expressions will be expanded until we have a sum of final states. Each distinct final state will get its own process component.

To identify equivalent final states, we transform the final state into an array of PDG codes, which we sort and compare. If a particle entry is actually a PDG array, only the first entry in the array is used for the comparison. The user should make sure that there is no overlap between different particles or arrays which would make the expansion ambiguous.

There are two possibilities that a process contains more than one component: by an explicit component statement by the user for inclusive processes, or by having one process at NLO level. The first option is determined in the chunk `scan components`, and determines `n_components`.

(Commands: cmd process: TBP)+≡

```

procedure :: execute => cmd_process_execute

```

(Commands: procedures)+≡

```

subroutine cmd_process_execute (cmd, global)
    class(cmd_process_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(pdg_array_t) :: pdg_in, pdg_out
    type(pdg_array_t), dimension(:), allocatable :: pdg_out_tab
    type(string_t), dimension(:), allocatable :: prt_in
    type(string_t) :: prt_out, prt_out1
    type(process_configuration_t) :: prc_config
    type(prt_expr_t) :: prt_expr_out
    type(prt_spec_t), dimension(:), allocatable :: prt_spec_in
    type(prt_spec_t), dimension(:), allocatable :: prt_spec_out
    type(var_list_t), pointer :: var_list
    integer, dimension(:), allocatable :: ipdg
    integer, dimension(:), allocatable :: i_term
    integer, dimension(:), allocatable :: nlo_comp
    integer :: i, j, n_in, n_out, n_terms, n_components
    logical :: nlo_fixed_order
    logical :: qcd_corr, qed_corr
    type(string_t), dimension(:), allocatable :: prt_in_nlo, prt_out_nlo
    type(radiation_generator_t) :: radiation_generator
    type(pdg_list_t) :: pl_in, pl_out, pl_excluded_gaugeSplittings
    type(string_t) :: method, born_me_method, loop_me_method, &
        correlation_me_method, real_tree_me_method, dglap_me_method
    integer, dimension(:), allocatable :: i_list
    logical :: use_real_finite
    logical :: gks_active

```

```

logical :: initial_state_colored
logical :: neg_sf
integer :: comp_mult
integer :: gks_multiplicity
integer :: n_components_init
integer :: alpha_power, alphas_power
logical :: requires_soft_mismatch, requires_dglap_remnants
type(string_t) :: nlo_correction_type
type(pdg_array_t), dimension(:), allocatable :: pdg
if (debug_on) call msg_debug (D_CORE, "cmd_process_execute")
var_list => cmd%local%get_var_list_ptr ()

n_in = size (cmd%pn_pdg_in)
allocate (prt_in (n_in), prt_spec_in (n_in))
do i = 1, n_in
    pdg_in = &
        eval_pdg_array (cmd%pn_pdg_in(i)%ptr, var_list)
    prt_in(i) = make_flavor_string (pdg_in, cmd%local%model)
    prt_spec_in(i) = new_prt_spec (prt_in(i))
end do
call compile_prt_expr &
    (prt_expr_out, cmd%pn_out, var_list, cmd%local%model)
call prt_expr_out%expand ()
<Commands: cmd process execute: scan components>
allocate (nlo_comp (n_components))

nlo_fixed_order = cmd%local%nlo_fixed_order
gks_multiplicity = var_list%get_ival (var_str ("gks_multiplicity"))
gks_active = gks_multiplicity > 2
neg_sf = .false.
select case (char (var_list%get_sval (var_str ("negative_sf"))))
case ("default")
    neg_sf = nlo_fixed_order
case ("negative")
    neg_sf = .true.
case ("positive")
    neg_sf = .false.
case default
    call msg_fatal ("Negative PDF handling can only be " // &
        "default, negative or positive.")
end select
<Commands: cmd process execute: check for nlo corrections>

method = var_list%get_sval (var_str ("method"))
born_me_method = var_list%get_sval (var_str ("born_me_method"))
if (born_me_method == var_str ("")) born_me_method = method
select case (char (var_list%get_sval (var_str ("real_partition_mode"))))
case ("default", "off", "singular")
    use_real_finite = .false.
case ("all", "on", "finite")
    use_real_finite = .true.
case default
    call msg_fatal ("The real partition mode can only be " // &
        "default, off, all, on, singular or finite.")

```

```

end select
if (nlo_fixed_order) then
  real_tree_me_method = &
    var_list%get_sval (var_str ("$real_tree_me_method"))
  if (real_tree_me_method == var_str ("")) &
    real_tree_me_method = method
  loop_me_method = var_list%get_sval (var_str ("$loop_me_method"))
  if (loop_me_method == var_str ("")) &
    loop_me_method = method
  correlation_me_method = &
    var_list%get_sval (var_str ("$correlation_me_method"))
  if (correlation_me_method == var_str ("")) &
    correlation_me_method = method
  dglap_me_method = var_list%get_sval (var_str ("$dglap_me_method"))
  if (dglap_me_method == var_str ("")) &
    dglap_me_method = method
  call check_nlo_options (cmd%local)
end if

call determine_needed_components ()
call prc_config%init (cmd%id, n_in, n_components_init, &
  cmd%local%model, cmd%local%var_list, &
  nlo_process = nlo_fixed_order, &
  negative_sf = neg_sf)

alpha_power = var_list%get_ival (var_str ("alpha_power"))
alphas_power = var_list%get_ival (var_str ("alphas_power"))
call prc_config%set_coupling_powers (alpha_power, alphas_power)

call setup_components ()
call prc_config%record (cmd%local)

contains

<Commands: cmd process execute procedures>

end subroutine cmd_process_execute

<Commands: cmd process execute procedures>≡
elemental function is_threshold (method)
  logical :: is_threshold
  type(string_t), intent(in) :: method
  is_threshold = method == var_str ("threshold")
end function is_threshold

subroutine check_threshold_consistency ()
  if (nlo_fixed_order .and. is_threshold (born_me_method)) then
    if (.not. (is_threshold (real_tree_me_method) .and. is_threshold (loop_me_method) &
      .and. is_threshold (correlation_me_method))) then
      print *, 'born: ', char (born_me_method)
      print *, 'real: ', char (real_tree_me_method)
      print *, 'loop: ', char (loop_me_method)
      print *, 'correlation: ', char (correlation_me_method)
      call msg_fatal ("Inconsistent methods: All components need to be threshold")
    end if
  end if
end subroutine

```



```

        end if
    end if
end subroutine check_threshold_consistency

```

(Commands: cmd process execute: check for nlo corrections)≡

```

if (nlo_fixed_order .or. gks_active) then
    nlo_correction_type = &
        var_list%get_sval (var_str ('$nlo_correction_type'))
    select case (char (nlo_correction_type))
    case ("QCD")
        qcd_corr = .true.; qed_corr = .false.
    case ("EW")
        qcd_corr = .false.; qed_corr = .true.
    case ("Full")
        qcd_corr = .true.; qed_corr = .true.
    case default
        call msg_fatal ("Invalid NLO correction type. " // &
            "Valid inputs are: QCD, EW, Full (default: QCD)")
    end select
    call check_for_excluded_gauge_boson_splitting_partners ()
    call setup_radiation_generator ()
end if
if (nlo_fixed_order) then
    call radiation_generator%findSplittings ()
    if (debug2_active (D_CORE)) then
        print *, ''
        print *, 'Found (pdg) splittings: '
        do i = 1, radiation_generator%if_table%get_length ()
            call radiation_generator%if_table%get_pdg_out (i, pdg)
            call pdg_array_write_set (pdg)
            print *, '-----'
        end do
    end if

    nlo_fixed_order = radiation_generator%contains_emissions ()
    if (.not. nlo_fixed_order) call msg_warning &
        (arr = [var_str ("No NLO corrections found for process ") // &
            cmd%id // var_str ("."), var_str ("Proceed with usual " // &
            "leading-order integration and simulation")])
end if

```

(Commands: cmd process execute procedures)+≡

```

subroutine check_for_excluded_gauge_boson_splitting_partners ()
    type(string_t) :: str_excluded_partners
    type(string_t), dimension(:), allocatable :: excluded_partners
    type(pdg_list_t) :: pl_tmp, pl_anti
    integer :: i, n_anti
    str_excluded_partners = var_list%get_sval &
        (var_str ('$exclude_gaugeSplittings'))
    if (str_excluded_partners == "") then
        return
    else
        call split_string (str_excluded_partners, &

```

```

        var_str (":"), excluded_partners)
    call pl_tmp%init (size (excluded_partners))
    do i = 1, size (excluded_partners)
        call pl_tmp%set (i, &
            cmd%local%model%get_pdg (excluded_partners(i), .true.))
    end do
    call pl_tmp%create_antiparticles (pl_anti, n_anti)
    call pl_excluded_gaugeSplittings%init (pl_tmp%get_size () + n_anti)
    do i = 1, pl_tmp%get_size ()
        call pl_excluded_gaugeSplittings%set (i, pl_tmp%get(i))
    end do
    do i = 1, n_anti
        j = i + pl_tmp%get_size ()
        call pl_excluded_gaugeSplittings%set (j, pl_anti%get(i))
    end do
end if
end subroutine check_for_excluded_gauge_boson_splitting_partners

```

(Commands: cmd process execute procedures)+≡

```

subroutine determine_needed_components ()
    type(string_t) :: fks_method
    comp_mult = 1
    if (nlo_fixed_order) then
        fks_method = var_list%get_sval (var_str ('$fks_mapping_type'))
        call check_threshold_consistency ()
        requires_soft_mismatch = fks_method == var_str ('resonances')
        comp_mult = needed_extra_components (requires_dglap_remnants, &
            use_real_finite, requires_soft_mismatch)
        allocate (i_list (comp_mult))
    else if (gks_active) then
        call radiation_generator%generate_multiple &
            (gks_multiplicity, cmd%local%model)
        comp_mult = radiation_generator%get_n_gks_states () + 1
    end if
    n_components_init = n_components * comp_mult
end subroutine determine_needed_components

```

(Commands: cmd process execute procedures)+≡

```

subroutine setup_radiation_generator ()
    call split_prt (prt_spec_in, n_in, pl_in)
    call split_prt (prt_spec_out, n_out, pl_out)
    call radiation_generator%init (pl_in, pl_out, &
        pl_excluded_gaugeSplittings, qcd = qcd_corr, qed = qed_corr)
    call radiation_generator%set_n (n_in, n_out, 0)
    initial_state_colored = pdg_in%has_colored_particles ()
    if ((n_in == 2 .and. initial_state_colored) .or. qed_corr) then
        requires_dglap_remnants = n_in == 2 .and. initial_state_colored
        call radiation_generator%set_initial_state_emissions ()
    else
        requires_dglap_remnants = .false.
    end if
    call radiation_generator%set_constraints (.false., .false., .true., .true.)
    call radiation_generator%setup_if_table (cmd%local%model)

```

```
end subroutine setup_radiation_generator
```

(Commands: cmd process execute: scan components)≡

```

n_terms = prt_expr_out%get_n_terms ()
allocate (pdg_out_tab (n_terms))
allocate (i_term (n_terms), source = 0)
n_components = 0
SCAN: do i = 1, n_terms
  if (allocated (ipdg)) deallocate (ipdg)
  call prt_expr_out%term_to_array (prt_spec_out, i)
  n_out = size (prt_spec_out)
  allocate (ipdg (n_out))
  do j = 1, n_out
    prt_out = prt_spec_out(j)%to_string ()
    call split (prt_out, prt_out1, ":")
    ipdg(j) = cmd%local%model%get_pdg (prt_out1)
  end do
  pdg_out = sort (ipdg)
  do j = 1, n_components
    if (pdg_out == pdg_out_tab(j)) cycle SCAN
  end do
  n_components = n_components + 1
  i_term(n_components) = i
  pdg_out_tab(n_components) = pdg_out
end do SCAN

```

(Commands: cmd process execute procedures)+≡

```

subroutine split_prt (prt, n_out, pl)
  type(prt_spec_t), intent(in), dimension(:), allocatable :: prt
  integer, intent(in) :: n_out
  type(pdg_list_t), intent(out) :: pl
  type(pdg_array_t) :: pdg
  type(string_t) :: prt_string, prt_tmp
  integer, parameter :: max_particle_number = 25
  integer, dimension(max_particle_number) :: i_particle
  integer :: i, j, n
  i_particle = 0
  call pl%init (n_out)
  do i = 1, n_out
    n = 1
    prt_string = prt(i)%to_string ()
    do
      call split (prt_string, prt_tmp, ":")
      if (prt_tmp /= "") then
        i_particle(n) = cmd%local%model%get_pdg (prt_tmp)
        n = n + 1
      else
        exit
      end if
    end do
    call pdg_array_init (pdg, n - 1)
    do j = 1, n - 1
      call pdg%set (j, i_particle(j))
    end do
  end do

```

```

        end do
        call pl%set (i, pdg)
        call pdg_array_delete (pdg)
    end do
end subroutine split_prt

```

(Commands: cmd process execute procedures)+≡

```

subroutine setup_components()
    integer :: k, i_comp, add_index
    i_comp = 0
    add_index = 0
    if (debug_on) call msg_debug (D_CORE, "setup_components")
    do i = 1, n_components
        call prt_expr_out%term_to_array (prt_spec_out, i_term(i))
        if (nlo_fixed_order) then
            associate (selected_nlo_parts => cmd%local%selected_nlo_parts)
                if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
                    i_comp + 1)
                call prc_config%setup_component (i_comp + 1, &
                    prt_spec_in, prt_spec_out, &
                    cmd%local%model, var_list, BORN, &
                    can_be_integrated = selected_nlo_parts (BORN))
                call radiation_generator%generate_real_particle_strings &
                    (prt_in_nlo, prt_out_nlo)
                if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
                    i_comp + 2)
                call prc_config%setup_component (i_comp + 2, &
                    new_prt_spec (prt_in_nlo), new_prt_spec (prt_out_nlo), &
                    cmd%local%model, var_list, NLO_REAL, &
                    can_be_integrated = selected_nlo_parts (NLO_REAL))
                if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
                    i_comp + 3)
                call prc_config%setup_component (i_comp + 3, &
                    prt_spec_in, prt_spec_out, &
                    cmd%local%model, var_list, NLO_VIRTUAL, &
                    can_be_integrated = selected_nlo_parts (NLO_VIRTUAL))
                if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
                    i_comp + 4)
                call prc_config%setup_component (i_comp + 4, &
                    prt_spec_in, prt_spec_out, &
                    cmd%local%model, var_list, NLO_SUBTRACTION, &
                    can_be_integrated = selected_nlo_parts (NLO_SUBTRACTION))
            end associate
            do k = 1, 4
                i_list(k) = i_comp + k
            end do
            if (requires_dglap_remnants) then
                if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
                    i_comp + 5)
                call prc_config%setup_component (i_comp + 5, &
                    prt_spec_in, prt_spec_out, &
                    cmd%local%model, var_list, NLO_DGLAP, &
                    can_be_integrated = selected_nlo_parts (NLO_DGLAP))
                i_list(5) = i_comp + 5
                add_index = add_index + 1
            end if
        end if
    end do
end subroutine

```

```

end if
if (use_real_finite) then
  if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
    i_comp + 5 + add_index)
  call prc_config%setup_component (i_comp + 5 + add_index, &
    new_prt_spec (prt_in_nlo), new_prt_spec (prt_out_nlo), &
    cmd%local%model, var_list, NLO_REAL, &
    can_be_integrated = selected_nlo_parts (NLO_REAL))
  i_list(5 + add_index) = i_comp + 5 + add_index
  add_index = add_index + 1
end if
if (requires_soft_mismatch) then
  if (debug_on) call msg_debug (D_CORE, "Setting up this NLO component:", &
    i_comp + 5 + add_index)
  call prc_config%setup_component (i_comp + 5 + add_index, &
    prt_spec_in, prt_spec_out, &
    cmd%local%model, var_list, NLO_MISMATCH, &
    can_be_integrated = selected_nlo_parts (NLO_MISMATCH))
  i_list(5 + add_index) = i_comp + 5 + add_index
end if
call prc_config%set_component_associations (i_list, &
  requires_dglap_remnants, use_real_finite, &
  requires_soft_mismatch)
end associate
else if (gks_active) then
  call prc_config%setup_component (i_comp + 1, prt_spec_in, &
    prt_spec_out, cmd%local%model, var_list, BORN, &
    can_be_integrated = .true.)
  call radiation_generator%reset_queue ()
  do j = 1, comp_mult
    prt_out_nlo = radiation_generator%get_next_state ()
    call prc_config%setup_component (i_comp + 1 + j, &
      new_prt_spec (prt_in), new_prt_spec (prt_out_nlo), &
      cmd%local%model, var_list, GKS, can_be_integrated = .false.)
  end do
else
  call prc_config%setup_component (i, &
    prt_spec_in, prt_spec_out, &
    cmd%local%model, var_list, can_be_integrated = .true.)
end if
i_comp = i_comp + comp_mult
end do
end subroutine setup_components

```

These three functions should be bundled with the logicals they depend on into an object (the pcm?).

(Commands: procedures)+≡

```

subroutine check_nlo_options (local)
  type(rt_data_t), intent(in) :: local
  type(var_list_t), pointer :: var_list => null ()
  real :: mult_real, mult_virt, mult_dglap
  logical :: combined, powheg
  logical :: case_lo_but_any_other

```

```

logical :: fixed_order_nlo_events
logical :: real_finite_only
var_list => local%get_var_list_ptr ()
combined = var_list%get_lval (var_str ('?combined_nlo_integration'))
powheg = var_list%get_lval (var_str ('?powheg_matching'))
if (powheg .and. .not. combined) then
    call msg_fatal ("POWHEG matching requires the 'combined_nlo_integration' &
        &-option to be set to true.")
end if
fixed_order_nlo_events = &
    var_list%get_lval (var_str ('?fixed_order_nlo_events'))
if (fixed_order_nlo_events .and. .not. combined .and. &
    count (local%selected_nlo_parts) > 1) &
    call msg_fatal ("Option mismatch: Fixed order NLO events of multiple ", &
        [var_str ("components are requested, but ?combined_nlo_integration "), &
        var_str ("is false. You can either switch to the combined NLO "), &
        var_str ("integration mode for the full process or choose one "), &
        var_str ("individual NLO component to generate events with.")])
real_finite_only = local%var_list%get_sval (var_str ("$real_partition_mode")) == "finite"
associate (nlo_parts => local%selected_nlo_parts)
    ! TODO (PS-2020-03-26): This technically leaves the possibility to skip this
    ! message by deactivating the dglap component for a proton collider process.
    ! To circumvent this, the selected_nlo_parts should be refactored.
    if (combined .and. .not. (nlo_parts(BORN) &
        .and. nlo_parts(NLO_VIRTUAL) .and. nlo_parts(NLO_REAL))) then
        call msg_fatal ("A combined integration of anything else than", &
            [var_str ("all NLO components together is not supported.")])
    end if
    if (real_finite_only .and. combined) then
        call msg_fatal ("You cannot do a combined integration without", &
            [var_str ("the real singular component.")])
    end if
    if (real_finite_only .and. count(nlo_parts([BORN,NLO_VIRTUAL,NLO_DGLAP])) > 1) then
        call msg_fatal ("You cannot do a full NLO integration without", &
            [var_str ("the real singular component.")])
    end if
end associate
mult_real = local%var_list%get_rval (var_str ("mult_call_real"))
mult_virt = local%var_list%get_rval (var_str ("mult_call_virt"))
mult_dglap = local%var_list%get_rval (var_str ("mult_call_dglap"))
if (combined .and. (mult_real /= one .or. mult_virt /= one .or. mult_dglap /= one)) then
    call msg_warning ("mult_call_real, mult_call_virt and mult_call_dglap", &
        [var_str (" will be ignored because of ?combined_nlo_integration = true. ")])
end if
end subroutine check_nlo_options

```

There are four components for a general NLO process, namely Born, real, virtual and subtraction. There will be additional components for DGLAP remnant, in case real contributions are split into singular and finite pieces, and for resonance-aware FKS subtraction for the needed soft mismatch component.

(Commands: procedures)+≡

```

pure function needed_extra_components (requires_dglap_remnant, &
    use_real_finite, requires_soft_mismatch) result (n)

```

```

integer :: n
logical, intent(in) :: requires_dglap_remnant, &
    use_real_finite, requires_soft_mismatch
n = 4
if (requires_dglap_remnant) n = n + 1
if (use_real_finite) n = n + 1
if (requires_soft_mismatch) n = n + 1
end function needed_extra_components

```

This is a method of the eval tree, but cannot be coded inside the `expressions` module since it uses the `model` and `flv` types which are not available there.

(Commands: procedures)+≡

```

function make_flavor_string (aval, model) result (prt)
    type(string_t) :: prt
    type(pdg_array_t), intent(in) :: aval
    type(model_t), intent(in), target :: model
    integer, dimension(:), allocatable :: pdg
    type(flavor_t), dimension(:), allocatable :: flv
    integer :: i
    pdg = aval
    allocate (flv (size (pdg)))
    call flv%init (pdg, model)
    if (size (pdg) /= 0) then
        prt = flv(1)%get_name ()
        do i = 2, size (flv)
            prt = prt // ":" // flv(i)%get_name ()
        end do
    else
        prt = "?"
    end if
end function make_flavor_string

```

Create a `pdg` array from a particle-specification array

(Commands: procedures)+≡

```

function make_pdg_array (prt, model) result (pdg_array)
    type(prt_spec_t), intent(in), dimension(:) :: prt
    type(model_t), intent(in) :: model
    integer, dimension(:), allocatable :: aval
    type(pdg_array_t) :: pdg_array
    type(flavor_t) :: flv
    integer :: k
    allocate (aval (size (prt)))
    do k = 1, size (prt)
        call flv%init (prt(k)%to_string (), model)
        aval (k) = flv%get_pdg ()
    end do
    pdg_array = aval
end function make_pdg_array

```

Compile a (possible nested) expression, to obtain a particle-specifier expression which we can process further.

(Commands: procedures)+≡

```

recursive subroutine compile_prt_expr (prt_expr, pn, var_list, model)
  type(prt_expr_t), intent(out) :: prt_expr
  type(parse_node_t), intent(in), target :: pn
  type(var_list_t), intent(in), target :: var_list
  type(model_t), intent(in), target :: model
  type(parse_node_t), pointer :: pn_entry, pn_term, pn_addition
  type(pdg_array_t) :: pdg
  type(string_t) :: prt_string
  integer :: n_entry, n_term, i
  select case (char (parse_node_get_rule_key (pn)))
  case ("prt_state_list")
    n_entry = parse_node_get_n_sub (pn)
    pn_entry => parse_node_get_sub_ptr (pn)
    if (n_entry == 1) then
      call compile_prt_expr (prt_expr, pn_entry, var_list, model)
    else
      call prt_expr%init_list (n_entry)
      select type (x => prt_expr%x)
      type is (prt_spec_list_t)
        do i = 1, n_entry
          call compile_prt_expr (x%expr(i), pn_entry, var_list, model)
          pn_entry => parse_node_get_next_ptr (pn_entry)
        end do
      end select
    end if
  case ("prt_state_sum")
    n_term = parse_node_get_n_sub (pn)
    pn_term => parse_node_get_sub_ptr (pn)
    pn_addition => pn_term
    if (n_term == 1) then
      call compile_prt_expr (prt_expr, pn_term, var_list, model)
    else
      call prt_expr%init_sum (n_term)
      select type (x => prt_expr%x)
      type is (prt_spec_sum_t)
        do i = 1, n_term
          call compile_prt_expr (x%expr(i), pn_term, var_list, model)
          pn_addition => parse_node_get_next_ptr (pn_addition)
          if (associated (pn_addition)) &
            pn_term => parse_node_get_sub_ptr (pn_addition, 2)
        end do
      end select
    end if
  case ("cexpr")
    pdg = eval_pdg_array (pn, var_list)
    prt_string = make_flavor_string (pdg, model)
    call prt_expr%init_spec (new_prt_spec (prt_string))
  case default
    call parse_node_write_rec (pn)
    call msg_bug ("compile prt expr: impossible syntax rule")
  end select
end subroutine compile_prt_expr

```


Initiating a NLO calculation

```
<Commands: types>+≡
  type, extends (command_t) :: cmd_nlo_t
    private
      integer, dimension(:), allocatable :: nlo_component
    contains
      <Commands: cmd nlo: TBP>
    end type cmd_nlo_t
```

```
<Commands: cmd nlo: TBP>≡
  procedure :: write => cmd_nlo_write
```

```
<Commands: procedures>+≡
  subroutine cmd_nlo_write (cmd, unit, indent)
    class(cmd_nlo_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
  end subroutine cmd_nlo_write
```

As it is, the NLO calculation is switched on by putting nlo behind the process definition. This should be made nicer in the future.

```
<Commands: cmd nlo: TBP>+≡
  procedure :: compile => cmd_nlo_compile
```

```
<Commands: procedures>+≡
  subroutine cmd_nlo_compile (cmd, global)
    class(cmd_nlo_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg, pn_comp
    integer :: i, n_comp
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 3)
    if (associated (pn_arg)) then
      n_comp = parse_node_get_n_sub (pn_arg)
      allocate (cmd%nlo_component (n_comp))
      pn_comp => parse_node_get_sub_ptr (pn_arg)
      i = 0
      do while (associated (pn_comp))
        i = i + 1
        cmd%nlo_component(i) = component_status &
          (parse_node_get_rule_key (pn_comp))
        pn_comp => parse_node_get_next_ptr (pn_comp)
      end do
    else
      allocate (cmd%nlo_component (0))
    end if
  end subroutine cmd_nlo_compile
```

```
<Commands: cmd nlo: TBP>+≡
  procedure :: execute => cmd_nlo_execute
```

```
<Commands: procedures>+≡
  subroutine cmd_nlo_execute (cmd, global)
    class(cmd_nlo_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
```

```

type(string_t) :: string
integer :: n, i, j
logical, dimension(0:5) :: selected_nlo_parts
if (debug_on) call msg_debug (D_CORE, "cmd_nlo_execute")
selected_nlo_parts = .false.
if (allocated (cmd%nlo_component)) then
    n = size (cmd%nlo_component)
else
    n = 0
end if
do i = 1, n
    select case (cmd%nlo_component (i))
    case (BORN, NLO_VIRTUAL, NLO_MISMATCH, NLO_DGLAP, NLO_REAL)
        selected_nlo_parts(cmd%nlo_component (i)) = .true.
    case (NLO_FULL)
        selected_nlo_parts = .true.
        selected_nlo_parts (NLO_SUBTRACTION) = .false.
    case default
        string = var_str ("")
        do j = BORN, NLO_DGLAP
            string = string // component_status (j) // ", "
        end do
        string = string // component_status (NLO_FULL)
        call msg_fatal ("Invalid NLO mode. Valid modes are: " // &
            char (string))
    end select
end do
global%nlo_fixed_order = any (selected_nlo_parts)
global%selected_nlo_parts = selected_nlo_parts
allocate (global%nlo_component (size (cmd%nlo_component)))
global%nlo_component = cmd%nlo_component
end subroutine cmd_nlo_execute

```

Process compilation

```

<Commands: types>+≡
type, extends (command_t) :: cmd_compile_t
private
type(string_t), dimension(:), allocatable :: libname
logical :: make_executable = .false.
type(string_t) :: exec_name
contains
<Commands: cmd compile: TBP>
end type cmd_compile_t

```

Output: list all libraries to be compiled.

```

<Commands: cmd compile: TBP>≡
procedure :: write => cmd_compile_write

<Commands: procedures>+≡
subroutine cmd_compile_write (cmd, unit, indent)
class(cmd_compile_t), intent(in) :: cmd
integer, intent(in), optional :: unit, indent

```

```

integer :: u, i
u = given_output_unit (unit); if (u < 0) return
call write_indent (u, indent)
write (u, "(1x,A)", advance="no") "compile ("
if (allocated (cmd%libname)) then
  do i = 1, size (cmd%libname)
    if (i > 1) write (u, "(A,1x)", advance="no") " ,"
    write (u, "("'",A,"'",)", advance="no") char (cmd%libname(i))
  end do
end if
write (u, "(A)") ")"
end subroutine cmd_compile_write

```

Compile the libraries specified in the argument. If the argument is empty, compile all libraries which can be found in the process library stack.

<Commands: cmd compile: TBP>+≡

```

procedure :: compile => cmd_compile_compile

```

<Commands: procedures>+≡

```

subroutine cmd_compile_compile (cmd, global)
  class(cmd_compile_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_cmd, pn_clause, pn_arg, pn_lib
  type(parse_node_t), pointer :: pn_exec_name_spec, pn_exec_name
  integer :: n_lib, i
  pn_cmd => parse_node_get_sub_ptr (cmd%pn)
  pn_clause => parse_node_get_sub_ptr (pn_cmd)
  pn_exec_name_spec => parse_node_get_sub_ptr (pn_clause, 2)
  if (associated (pn_exec_name_spec)) then
    pn_exec_name => parse_node_get_sub_ptr (pn_exec_name_spec, 2)
  else
    pn_exec_name => null ()
  end if
  pn_arg => parse_node_get_next_ptr (pn_clause)
  cmd%pn_opt => parse_node_get_next_ptr (pn_cmd)
  call cmd%compile_options (global)
  if (associated (pn_arg)) then
    n_lib = parse_node_get_n_sub (pn_arg)
  else
    n_lib = 0
  end if
  if (n_lib > 0) then
    allocate (cmd%libname (n_lib))
    pn_lib => parse_node_get_sub_ptr (pn_arg)
    do i = 1, n_lib
      cmd%libname(i) = parse_node_get_string (pn_lib)
      pn_lib => parse_node_get_next_ptr (pn_lib)
    end do
  end if
  if (associated (pn_exec_name)) then
    cmd%make_executable = .true.
    cmd%exec_name = parse_node_get_string (pn_exec_name)
  end if
end subroutine cmd_compile_compile

```

Command execution. Generate code, write driver, compile and link. Do this for all libraries in the list.

If no library names have been given and stored while compiling this command, we collect all libraries from the current stack and compile those.

As a bonus, a compiled library may be able to spawn new process libraries. For instance, a processes may ask for a set of resonant subprocesses which go into their own library, but this can be determined only after the process is available as a compiled object. Therefore, the compilation loop is implemented as a recursive internal subroutine.

We can compile static libraries (which actually just loads them). However, we can't incorporate in a generated executable.

```

<Commands: cmd compile: TBP>+≡
  procedure :: execute => cmd_compile_execute

<Commands: procedures>+≡
  subroutine cmd_compile_execute (cmd, global)
    class(cmd_compile_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(string_t), dimension(:), allocatable :: libname, libname_static
    integer :: i, n_lib
    <Commands: cmd compile execute: extra variables>
    <Commands: cmd compile execute: extra init>
    if (allocated (cmd%libname)) then
      allocate (libname (size (cmd%libname)))
      libname = cmd%libname
    else
      call cmd%local%prclib_stack%get_names (libname)
    end if
    n_lib = size (libname)
    if (cmd%make_executable) then
      call get_prclib_static (libname_static)
      do i = 1, n_lib
        if (any (libname_static == libname(i))) then
          call msg_fatal ("Compile: can't include static library '" &
            // char (libname(i)) // "'")
        end if
      end do
      call compile_executable (cmd%exec_name, libname, cmd%local)
    else
      call compile_libraries (libname)
      call global%update_prclib &
        (global%prclib_stack%get_library_ptr (libname(n_lib)))
    end if
    <Commands: cmd compile execute: extra end init>
  contains
    recursive subroutine compile_libraries (libname)
      type(string_t), dimension(:), intent(in) :: libname
      integer :: i
      type(string_t), dimension(:), allocatable :: libname_extra
      type(process_library_t), pointer :: lib_saved
      do i = 1, size (libname)
        call compile_library (libname(i), cmd%local)

```

```

lib_saved => global%prclib
call spawn_extra_libraries &
    (libname(i), cmd%local, global, libname_extra)
call compile_libraries (libname_extra)
call global%update_prclib (lib_saved)
end do
end subroutine compile_libraries
end subroutine cmd_compile_execute

```

<Commands: cmd compile execute: extra variables>≡

<Commands: cmd compile execute: extra init>≡

<Commands: cmd compile execute: extra end init>≡

The parallelization leads to undefined behavior while writing simultaneously to one file. The master worker has to initialize single-handed the corresponding library files. The slave worker will wait with a blocking MPI.BCAST until they receive a logical flag.

<MPI: Commands: cmd compile execute: extra variables>≡

```

logical :: compile_init
integer :: rank, n_size

```

<MPI: Commands: cmd compile execute: extra init>≡

```

if (debug_on) call msg_debug (D_MPI, "cmd_compile_execute")
compile_init = .false.
call mpi_get_comm_id (n_size, rank)
if (debug_on) call msg_debug (D_MPI, "n_size", rank)
if (debug_on) call msg_debug (D_MPI, "rank", rank)
if (rank /= 0) then
    if (debug_on) call msg_debug (D_MPI, "wait for master")
    call MPI_bcast (compile_init, 1, MPI_LOGICAL, 0, MPI_COMM_WORLD)
else
    compile_init = .true.
end if

if (compile_init) then

```

<MPI: Commands: cmd compile execute: extra end init>≡

```

if (rank == 0) then
    if (debug_on) call msg_debug (D_MPI, "load slaves")
    call MPI_bcast (compile_init, 1, MPI_LOGICAL, 0, MPI_COMM_WORLD)
end if
end if
call MPI_barrier (MPI_COMM_WORLD)

```

This is the interface to the external procedure which returns the names of all static libraries which are part of the executable. (The default is none.) The routine must allocate the array.

<Commands: public>≡

```

public :: get_prclib_static

```

<Commands: interfaces>+≡

```

interface
    subroutine get_prclib_static (libname)
        import
        type(string_t), dimension(:), intent(inout), allocatable :: libname
    end subroutine

```

```

        end subroutine get_prclib_static
    end interface

```

Spawn extra libraries. We can ask the processes within a compiled library, which we have available at this point, whether they need additional processes which should go into their own libraries.

The current implementation only concerns resonant subprocesses.

Note that the libraries should be created (source code), but not be compiled here. This is done afterwards.

<Commands: procedures>+≡

```

subroutine spawn_extra_libraries (libname, local, global, libname_extra)
    type(string_t), intent(in) :: libname
    type(rt_data_t), intent(inout), target :: local
    type(rt_data_t), intent(inout), target :: global
    type(string_t), dimension(:), allocatable, intent(out) :: libname_extra
    type(string_t), dimension(:), allocatable :: libname_res
    allocate (libname_extra (0))
    call spawn_resonant_subprocess_libraries &
        (libname, local, global, libname_res)
    if (allocated (libname_res)) libname_extra = [libname_extra, libname_res]
end subroutine spawn_extra_libraries

```

Execute a shell command

The argument is a string expression.

<Commands: types>+≡

```

type, extends (command_t) :: cmd_exec_t
    private
    type(parse_node_t), pointer :: pn_command => null ()
contains
    <Commands: cmd exec: TBP>
end type cmd_exec_t

```

Simply tell the status.

<Commands: cmd exec: TBP>≡

```

procedure :: write => cmd_exec_write

```

<Commands: procedures>+≡

```

subroutine cmd_exec_write (cmd, unit, indent)
    class(cmd_exec_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    if (associated (cmd%pn_command)) then
        write (u, "(1x,A)") "exec: [command associated]"
    else
        write (u, "(1x,A)") "exec: [undefined]"
    end if
end subroutine cmd_exec_write

```

Compile the exec command.

```
(Commands: cmd exec: TBP)+≡  
  procedure :: compile => cmd_exec_compile  
  
(Commands: procedures)+≡  
  subroutine cmd_exec_compile (cmd, global)  
    class(cmd_exec_t), intent(inout) :: cmd  
    type(rt_data_t), intent(inout), target :: global  
    type(parse_node_t), pointer :: pn_arg, pn_command  
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)  
    pn_command => parse_node_get_sub_ptr (pn_arg)  
    cmd%pn_command => pn_command  
  end subroutine cmd_exec_compile
```

Execute the specified shell command.

```
(Commands: cmd exec: TBP)+≡  
  procedure :: execute => cmd_exec_execute  
  
(Commands: procedures)+≡  
  subroutine cmd_exec_execute (cmd, global)  
    class(cmd_exec_t), intent(inout) :: cmd  
    type(rt_data_t), intent(inout), target :: global  
    type(string_t) :: command  
    logical :: is_known  
    integer :: status  
    command = eval_string (cmd%pn_command, global%var_list, is_known=is_known)  
    if (is_known) then  
      if (command /= "") then  
        call os_system_call (command, status, verbose=.true.)  
        if (status /= 0) then  
          write (msg_buffer, "(A,I0)") "Return code = ", status  
          call msg_message ()  
          call msg_error ("System command returned with nonzero status code")  
        end if  
      end if  
    end if  
  end subroutine cmd_exec_execute
```

Variable declaration

A variable can have various types. Hold the definition as an eval tree.

There are intrinsic variables, user variables, and model variables. The latter are further divided in independent variables and dependent variables.

Regarding model variables: When dealing with them, we always look at two variable lists in parallel. The global (or local) variable list contains the user-visible values. It includes variables that correspond to variables in the current model's list. These, in turn, are pointers to the model's parameter list, so the model is always in sync, internally. To keep the global variable list in sync with the model, the global variables carry the `is_copy` property and contain a separate pointer to the model variable. (The pointer is reassigned whenever the model changes.) Modifying the global variable changes two values simultaneously: the visible value and the model variable, via this extra pointer.

After each modification, we update dependent parameters in the model variable list and re-synchronize the global variable list (again, using these pointers) with the model variable this. In the last step, modifications in the derived parameters become visible.

When we integrate a process, we capture the current variable list of the current model in a separate model instance, which is stored in the process object. Thus, the model parameters associated to this process at this time are preserved for the lifetime of the process object.

When we generate or rescan events, we can again capture a local model variable list in a model instance. This allows us to reweight event by event with different parameter sets simultaneously.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_var_t
  private
    type(string_t) :: name
    integer :: type = V_NONE
    type(parse_node_t), pointer :: pn_value => null ()
    logical :: is_intrinsic = .false.
    logical :: is_model_var = .false.
  contains
    ⟨Commands: cmd var: TBP⟩
  end type cmd_var_t

```

Output. We know name, type, and properties, but not the value.

```

⟨Commands: cmd var: TBP⟩≡
  procedure :: write => cmd_var_write

⟨Commands: procedures⟩+≡
  subroutine cmd_var_write (cmd, unit, indent)
    class(cmd_var_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,A,A)", advance="no") "var: ", char (cmd%name), " ("
    select case (cmd%type)
    case (V_NONE)
      write (u, "(A)", advance="no") "[unknown]"
    case (V_LOG)
      write (u, "(A)", advance="no") "logical"
    case (V_INT)
      write (u, "(A)", advance="no") "int"
    case (V_REAL)
      write (u, "(A)", advance="no") "real"
    case (V_CMPLX)
      write (u, "(A)", advance="no") "complex"
    case (V_STR)
      write (u, "(A)", advance="no") "string"
    case (V_PDG)
      write (u, "(A)", advance="no") "alias"
    end select
    if (cmd%is_intrinsic) then
      write (u, "(A)", advance="no") ", intrinsic"
    end if
  end subroutine cmd_var_write

```



```

end if
if (cmd%is_model_var) then
    write (u, "(A)", advance="no") " ", model"
end if
write (u, "(A)" )"
end subroutine cmd_var_write

```

Compile the lhs and determine the variable name and type. Check whether this variable can be created or modified as requested, and append the value to the variable list, if appropriate. The value is initially undefined. The rhs is assigned to a pointer, to be compiled and evaluated when the command is executed.

```

⟨Commands: cmd var: TBP⟩+≡
    procedure :: compile => cmd_var_compile

⟨Commands: procedures⟩+≡
    subroutine cmd_var_compile (cmd, global)
        class(cmd_var_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_var, pn_name
        type(parse_node_t), pointer :: pn_result, pn_proc
        type(string_t) :: var_name
        type(var_list_t), pointer :: model_vars
        integer :: type
        logical :: new
        pn_result => null ()
        new = .false.
        select case (char (parse_node_get_rule_key (cmd%pn)))
        case ("cmd_log_decl");    type = V_LOG
            pn_var => parse_node_get_sub_ptr (cmd%pn, 2)
            if (.not. associated (pn_var)) then    ! handle masked syntax error
                cmd%type = V_NONE; return
            end if
            pn_name => parse_node_get_sub_ptr (pn_var, 2)
            new = .true.
        case ("cmd_log");        type = V_LOG
            pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
        case ("cmd_int");        type = V_INT
            pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
            new = .true.
        case ("cmd_real");       type = V_REAL
            pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
            new = .true.
        case ("cmd_complex");    type = V_CMPLX
            pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
            new = .true.
        case ("cmd_num");        type = V_NONE
            pn_name => parse_node_get_sub_ptr (cmd%pn)
        case ("cmd_string_decl"); type = V_STR
            pn_var => parse_node_get_sub_ptr (cmd%pn, 2)
            if (.not. associated (pn_var)) then    ! handle masked syntax error
                cmd%type = V_NONE; return
            end if
            pn_name => parse_node_get_sub_ptr (pn_var, 2)
            new = .true.

```

```

case ("cmd_string");      type = V_STR
    pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
case ("cmd_alias");      type = V_PDG
    pn_name => parse_node_get_sub_ptr (cmd%pn, 2)
    new = .true.
case ("cmd_result");     type = V_REAL
    pn_name => parse_node_get_sub_ptr (cmd%pn)
    pn_result => parse_node_get_sub_ptr (pn_name)
    pn_proc => parse_node_get_next_ptr (pn_result)
case default
    call parse_node_mismatch &
        ("logical|int|real|complex|?|${alias}|var_name", cmd%pn) ! $
end select
if (.not. associated (pn_name)) then ! handle masked syntax error
    cmd%type = V_NONE; return
end if
if (.not. associated (pn_result)) then
    var_name = parse_node_get_string (pn_name)
else
    var_name = parse_node_get_key (pn_result) &
        // "(" // parse_node_get_string (pn_proc) // ")"
end if
select case (type)
case (V_LOG); var_name = "?" // var_name
case (V_STR); var_name = "$" // var_name ! $
end select
if (associated (global%model)) then
    model_vars => global%model%get_var_list_ptr ()
else
    model_vars => null ()
end if
call var_list_check_observable (global%var_list, var_name, type)
call var_list_check_result_var (global%var_list, var_name, type)
call global%var_list%check_user_var (var_name, type, new)
cmd%name = var_name
cmd%pn_value => parse_node_get_next_ptr (pn_name, 2)
if (global%var_list%contains (cmd%name, follow_link = .false.)) then
    ! local variable
    cmd%is_intrinsic = &
        global%var_list%is_intrinsic (cmd%name, follow_link = .false.)
    cmd%type = &
        global%var_list%get_type (cmd%name, follow_link = .false.)
else
    if (new) cmd%type = type
    if (global%var_list%contains (cmd%name, follow_link = .true.)) then
        ! global variable
        cmd%is_intrinsic = &
            global%var_list%is_intrinsic (cmd%name, follow_link = .true.)
        if (cmd%type == V_NONE) then
            cmd%type = &
                global%var_list%get_type (cmd%name, follow_link = .true.)
        end if
    else if (associated (model_vars)) then ! check model variable
        cmd%is_model_var = &

```

```

        model_vars%contains (cmd%name)
    if (cmd%type == V_NONE) then
        cmd%type = &
            model_vars%get_type (cmd%name)
    end if
end if
if (cmd%type == V_NONE) then
    call msg_fatal ("Variable '" // char (cmd%name) // "' " &
        // "set without declaration")
    cmd%type = V_NONE; return
end if
if (cmd%is_model_var) then
    if (new) then
        call msg_fatal ("Model variable '" // char (cmd%name) // "' " &
            // "redeclared")
    else if (model_vars%is_locked (cmd%name)) then
        call msg_fatal ("Model variable '" // char (cmd%name) // "' " &
            // "is locked")
    end if
else
    select case (cmd%type)
    case (V_LOG)
        call global%var_list%append_log (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_INT)
        call global%var_list%append_int (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_REAL)
        call global%var_list%append_real (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_CMPLX)
        call global%var_list%append_cmplx (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_PDG)
        call global%var_list%append_pdg_array (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    case (V_STR)
        call global%var_list%append_string (cmd%name, &
            intrinsic=cmd%is_intrinsic, user=.true.)
    end select
end if
end if
end subroutine cmd_var_compile

```

Execute. Evaluate the definition and assign the variable value. If the variable is a model variable, take a snapshot of the model if necessary and set the variable in the local model.

```

<Commands: cmd var: TBP>+≡
    procedure :: execute => cmd_var_execute

<Commands: procedures>+≡
    subroutine cmd_var_execute (cmd, global)
        class(cmd_var_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
    end subroutine

```

```

type(var_list_t), pointer :: var_list
real(default) :: rval
logical :: is_known, pacified
var_list => global%get_var_list_ptr ()
if (cmd%is_model_var) then
    pacified = var_list%get_lval (var_str ("?pacify"))
    rval = eval_real (cmd%pn_value, var_list, is_known=is_known)
    call global%model_set_real &
        (cmd%name, rval, verbose=.true., pacified=pacified)
else if (cmd%type /= V_NONE) then
    call cmd%set_value (var_list, verbose=.true.)
end if
end subroutine cmd_var_execute

```

Copy the value to the variable list, where the variable should already exist.

(Commands: cmd var: TBP)+≡

```

procedure :: set_value => cmd_var_set_value

```

(Commands: procedures)+≡

```

subroutine cmd_var_set_value (var, var_list, verbose, model_name)
class(cmd_var_t), intent(inout) :: var
type(var_list_t), intent(inout), target :: var_list
logical, intent(in), optional :: verbose
type(string_t), intent(in), optional :: model_name
logical :: lval, pacified
integer :: ival
real(default) :: rval
complex(default) :: cval
type(pdg_array_t) :: aval
type(string_t) :: sval
logical :: is_known
pacified = var_list%get_lval (var_str ("?pacify"))
select case (var%type)
case (V_LOG)
    lval = eval_log (var%pn_value, var_list, is_known=is_known)
    call var_list%set_log (var%name, &
        lval, is_known, verbose=verbose, model_name=model_name)
case (V_INT)
    ival = eval_int (var%pn_value, var_list, is_known=is_known)
    call var_list%set_int (var%name, &
        ival, is_known, verbose=verbose, model_name=model_name)
case (V_REAL)
    rval = eval_real (var%pn_value, var_list, is_known=is_known)
    call var_list%set_real (var%name, &
        rval, is_known, verbose=verbose, &
        model_name=model_name, pacified = pacified)
case (V_CMPLX)
    cval = eval_cmplx (var%pn_value, var_list, is_known=is_known)
    call var_list%set_cmplx (var%name, &
        cval, is_known, verbose=verbose, &
        model_name=model_name, pacified = pacified)
case (V_PDG)
    aval = eval_pdg_array (var%pn_value, var_list, is_known=is_known)
    call var_list%set_pdg_array (var%name, &

```

```

        aval, is_known, verbose=verbose, model_name=model_name)
case (V_STR)
    sval = eval_string (var%pn_value, var_list, is_known=is_known)
    call var_list%set_string (var%name, &
        sval, is_known, verbose=verbose, model_name=model_name)
end select
end subroutine cmd_var_set_value

```

SLHA

Read a SLHA (SUSY Les Houches Accord) file to fill the appropriate model parameters. We do not access the current variable record, but directly work on the appropriate SUSY model, which is loaded if necessary.

We may be in read or write mode. In the latter case, we may write just input parameters, or the complete spectrum, or the spectrum with all decays.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_slha_t
private
type(string_t) :: file
logical :: write_mode = .false.
contains
<Commands: cmd slha: TBP>
end type cmd_slha_t

```

Output.

```

<Commands: cmd slha: TBP>≡
procedure :: write => cmd_slha_write

<Commands: procedures>+≡
subroutine cmd_slha_write (cmd, unit, indent)
class(cmd_slha_t), intent(in) :: cmd
integer, intent(in), optional :: unit, indent
integer :: u
u = given_output_unit (unit); if (u < 0) return
call write_indent (u, indent)
write (u, "(1x,A,A)") "slha: file name = ", char (cmd%file)
write (u, "(1x,A,L1)") "slha: write mode = ", cmd%write_mode
end subroutine cmd_slha_write

```

Compile. Read the filename and store it.

```

<Commands: cmd slha: TBP>+≡
procedure :: compile => cmd_slha_compile

<Commands: procedures>+≡
subroutine cmd_slha_compile (cmd, global)
class(cmd_slha_t), intent(inout) :: cmd
type(rt_data_t), intent(inout), target :: global
type(parse_node_t), pointer :: pn_key, pn_arg, pn_file
pn_key => parse_node_get_sub_ptr (cmd%pn)
pn_arg => parse_node_get_next_ptr (pn_key)
pn_file => parse_node_get_sub_ptr (pn_arg)
call cmd%compile_options (global)

```

```

cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
select case (char (parse_node_get_key (pn_key)))
case ("read_slha")
    cmd%write_mode = .false.
case ("write_slha")
    cmd%write_mode = .true.
case default
    call parse_node_mismatch ("read_slha|write_slha", cmd%pn)
end select
cmd%file = parse_node_get_string (pn_file)
end subroutine cmd_slha_compile

```

Execute. Read or write the specified SLHA file. Behind the scenes, this will first read the WHIZARD model file, then read the SLHA file and assign the SLHA parameters as far as determined by `dispatch_slha`. Finally, the global variables are synchronized with the model. This is similar to executing `cmd_model`.

(*Commands: cmd slha: TBP*) \equiv

```

procedure :: execute => cmd_slha_execute

```

(*Commands: procedures*) \equiv

```

subroutine cmd_slha_execute (cmd, global)
class(cmd_slha_t), intent(inout) :: cmd
type(rt_data_t), intent(inout), target :: global
logical :: input, spectrum, decays
if (cmd%write_mode) then
    input = .true.
    spectrum = .false.
    decays = .false.
    if (.not. associated (cmd%local%model)) then
        call msg_fatal ("SLHA: local model not associated")
        return
    end if
    call slha_write_file &
        (cmd%file, cmd%local%model, &
         input = input, spectrum = spectrum, decays = decays)
else
    if (.not. associated (global%model)) then
        call msg_fatal ("SLHA: global model not associated")
        return
    end if
    call dispatch_slha (cmd%local%var_list, &
        input = input, spectrum = spectrum, decays = decays)
    call global%ensure_model_copy ()
    call slha_read_file &
        (cmd%file, cmd%local%os_data, global%model, &
         input = input, spectrum = spectrum, decays = decays)
end if
end subroutine cmd_slha_execute

```

Show values

This command shows the current values of variables or other objects, in a suitably condensed form.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_show_t
  private
    type(string_t), dimension(:), allocatable :: name
  contains
    <Commands: cmd show: TBP>
  end type cmd_show_t

```

Output: list the object names, not values.

```

<Commands: cmd show: TBP>≡
  procedure :: write => cmd_show_write

<Commands: procedures>+≡
  subroutine cmd_show_write (cmd, unit, indent)
    class(cmd_show_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)", advance="no") "show: "
    if (allocated (cmd%name)) then
      do i = 1, size (cmd%name)
        write (u, "(1x,A)", advance="no") char (cmd%name(i))
      end do
      write (u, *)
    else
      write (u, "(5x,A)") "[undefined]"
    end if
  end subroutine cmd_show_write

```

Compile. Allocate an array which is filled with the names of the variables to show.

```

<Commands: cmd show: TBP>+≡
  procedure :: compile => cmd_show_compile

<Commands: procedures>+≡
  subroutine cmd_show_compile (cmd, global)
    class(cmd_show_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg, pn_var, pn_prefix, pn_name
    type(string_t) :: key
    integer :: i, n_args
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
    if (associated (pn_arg)) then
      select case (char (parse_node_get_rule_key (pn_arg)))
        case ("show_arg")
          cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
        case default
          cmd%pn_opt => pn_arg
          pn_arg => null ()
      end select
    end if
    call cmd%compile_options (global)
    if (associated (pn_arg)) then

```

```

n_args = parse_node_get_n_sub (pn_arg)
allocate (cmd%name (n_args))
pn_var => parse_node_get_sub_ptr (pn_arg)
i = 0
do while (associated (pn_var))
  i = i + 1
  select case (char (parse_node_get_rule_key (pn_var)))
  case ("model", "library", "beams", "iterations", &
        "cuts", "weight", "int", "real", "complex", &
        "scale", "factorization_scale", "renormalization_scale", &
        "selection", "reweight", "analysis", "pdg", &
        "stable", "unstable", "polarized", "unpolarized", &
        "results", "expect", "intrinsic", "string", "logical")
    cmd%name(i) = parse_node_get_key (pn_var)
  case ("result_var")
    pn_prefix => parse_node_get_sub_ptr (pn_var)
    pn_name => parse_node_get_next_ptr (pn_prefix)
    if (associated (pn_name)) then
      cmd%name(i) = parse_node_get_key (pn_prefix) &
        // "(" // parse_node_get_string (pn_name) // ")"
    else
      cmd%name(i) = parse_node_get_key (pn_prefix)
    end if
  case ("log_var", "string_var", "alias_var")
    pn_prefix => parse_node_get_sub_ptr (pn_var)
    pn_name => parse_node_get_next_ptr (pn_prefix)
    key = parse_node_get_key (pn_prefix)
    if (associated (pn_name)) then
      select case (char (parse_node_get_rule_key (pn_name)))
      case ("var_name")
        select case (char (key))
        case ("?", "$") ! $ sign
          cmd%name(i) = key // parse_node_get_string (pn_name)
        case ("alias")
          cmd%name(i) = parse_node_get_string (pn_name)
        end select
      case default
        call parse_node_mismatch &
          ("var_name", pn_name)
      end select
    else
      cmd%name(i) = key
    end if
  case default
    cmd%name(i) = parse_node_get_string (pn_var)
  end select
  pn_var => parse_node_get_next_ptr (pn_var)
end do
else
  allocate (cmd%name (0))
end if
end subroutine cmd_show_compile

```

Execute. Scan the list of objects to show.


```

{Commands: parameters}≡
    integer, parameter, public :: SHOW_BUFFER_SIZE = 4096

{Commands: cmd show: TBP}+≡
    procedure :: execute => cmd_show_execute

{Commands: procedures}+≡
    subroutine cmd_show_execute (cmd, global)
        class(cmd_show_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list, model_vars
        type(model_t), pointer :: model
        type(string_t) :: name
        integer :: n, pdg
        type(flavor_t) :: flv
        type(process_library_t), pointer :: prc_lib
        type(process_t), pointer :: process
        logical :: pacified
        character(SHOW_BUFFER_SIZE) :: buffer
        type(string_t) :: out_file
        integer :: i, j, u, u_log, u_out, u_ext
        u = free_unit ()
        var_list => cmd%local%var_list
        if (associated (cmd%local%model)) then
            model_vars => cmd%local%model%get_var_list_ptr ()
        else
            model_vars => null ()
        end if
        pacified = var_list%get_lval (var_str ("?pacify"))
        out_file = var_list%get_sval (var_str ("$out_file"))
        if (file_list_is_open (global%out_files, out_file, action="write")) then
            call msg_message ("show: copying output to file '" &
                // char (out_file) // "'")
            u_ext = file_list_get_unit (global%out_files, out_file)
        else
            u_ext = -1
        end if
        open (u, status = "scratch", action = "readwrite")
        if (associated (cmd%local%model)) then
            name = cmd%local%model%get_name ()
        end if
        if (size (cmd%name) == 0) then
            if (associated (model_vars)) then
                call model_vars%write (model_name = name, &
                    unit = u, pacified = pacified, follow_link = .false.)
            end if
            call var_list%write (unit = u, pacified = pacified)
        else
            do i = 1, size (cmd%name)
                select case (char (cmd%name(i)))
                case ("model")
                    if (associated (cmd%local%model)) then
                        call cmd%local%model%show (u)
                    else
                        write (u, "(A)") "Model: [undefined]"
                    end if
                end select
            end do
        end if
    end subroutine

```

```

        end if
    case ("library")
        if (associated (cmd%local%prclib)) then
            call cmd%local%prclib%show (u)
        else
            write (u, "(A)") "Process library: [undefined]"
        end if
    case ("beams")
        call cmd%local%show_beams (u)
    case ("iterations")
        call cmd%local%it_list%write (u)
    case ("results")
        call cmd%local%process_stack%show (u, fifo=.true.)
    case ("stable")
        call cmd%local%model%show_stable (u)
    case ("polarized")
        call cmd%local%model%show_polarized (u)
    case ("unpolarized")
        call cmd%local%model%show_unpolarized (u)
    case ("unstable")
        model => cmd%local%model
        call model%show_unstable (u)
        n = model%get_n_field ()
        do j = 1, n
            pdg = model%get_pdg (j)
            call flv%init (pdg, model)
            if (.not. flv%is_stable ()) &
                call show_unstable (cmd%local, pdg, u)
            if (flv%has_antiparticle ()) then
                associate (anti => flv%anti ())
                if (.not. anti%is_stable ()) &
                    call show_unstable (cmd%local, -pdg, u)
                end associate
            end if
        end do
    case ("cuts", "weight", "scale", &
        "factorization_scale", "renormalization_scale", &
        "selection", "reweight", "analysis")
        call cmd%local%pn%show (cmd%name(i), u)
    case ("expect")
        call expect_summary (force = .true.)
    case ("intrinsic")
        call var_list%write (intrinsic=.true., unit=u, &
            pacified = pacified)
    case ("logical")
        if (associated (model_vars)) then
            call model_vars%write (only_type=V_LOG, &
                model_name = name, unit=u, pacified = pacified, &
                follow_link=.false.)
        end if
        call var_list%write (&
            only_type=V_LOG, unit=u, pacified = pacified)
    case ("int")
        if (associated (model_vars)) then

```

```

        call model_vars%write (only_type=V_INT, &
            model_name = name, unit=u, pacified = pacified, &
            follow_link=.false.)
    end if
    call var_list%write (only_type=V_INT, &
        unit=u, pacified = pacified)
case ("real")
    if (associated (model_vars)) then
        call model_vars%write (only_type=V_REAL, &
            model_name = name, unit=u, pacified = pacified, &
            follow_link=.false.)
    end if
    call var_list%write (only_type=V_REAL, &
        unit=u, pacified = pacified)
case ("complex")
    if (associated (model_vars)) then
        call model_vars%write (only_type=V_CMPLX, &
            model_name = name, unit=u, pacified = pacified, &
            follow_link=.false.)
    end if
    call var_list%write (only_type=V_CMPLX, &
        unit=u, pacified = pacified)
case ("pdg")
    if (associated (model_vars)) then
        call model_vars%write (only_type=V_PDG, &
            model_name = name, unit=u, pacified = pacified, &
            follow_link=.false.)
    end if
    call var_list%write (only_type=V_PDG, &
        unit=u, pacified = pacified)
case ("string")
    if (associated (model_vars)) then
        call model_vars%write (only_type=V_STR, &
            model_name = name, unit=u, pacified = pacified, &
            follow_link=.false.)
    end if
    call var_list%write (only_type=V_STR, &
        unit=u, pacified = pacified)
case default
    if (analysis_exists (cmd%name(i))) then
        call analysis_write (cmd%name(i), u)
    else if (cmd%local%process_stack%exists (cmd%name(i))) then
        process => cmd%local%process_stack%get_process_ptr (cmd%name(i))
        call process%show (u)
    else if (associated (cmd%local%prclib_stack%get_library_ptr &
        (cmd%name(i)))) then
        prc_lib => cmd%local%prclib_stack%get_library_ptr (cmd%name(i))
        call prc_lib%show (u)
    else if (associated (model_vars)) then
        if (model_vars%contains (cmd%name(i), follow_link=.false.)) then
            call model_vars%write_var (cmd%name(i), &
                unit = u, model_name = name, pacified = pacified)
        else if (var_list%contains (cmd%name(i))) then
            call var_list%write_var (cmd%name(i), &

```

```

        unit = u, pacified = pacified)
    else
        call msg_error ("show: object '" // char (cmd%name(i)) &
            // "' not found")
    end if
    else if (var_list%contains (cmd%name(i))) then
        call var_list%write_var (cmd%name(i), &
            unit = u, pacified = pacified)
    else
        call msg_error ("show: object '" // char (cmd%name(i)) &
            // "' not found")
    end if
end select
end do
end if
rewind (u)
u_log = logfile_unit ()
u_out = given_output_unit ()
do
    read (u, "(A)", end = 1) buffer
    if (u_log > 0) write (u_log, "(A)") trim (buffer)
    if (u_out > 0) write (u_out, "(A)") trim (buffer)
    if (u_ext > 0) write (u_ext, "(A)") trim (buffer)
end do
1 close (u)
if (u_log > 0) flush (u_log)
if (u_out > 0) flush (u_out)
if (u_ext > 0) flush (u_ext)
end subroutine cmd_show_execute

```

Clear values

This command clears the current values of variables or other objects, where this makes sense. It parallels the `show` command. The objects are cleared, but not deleted.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_clear_t
    private
        type(string_t), dimension(:), allocatable :: name
    contains
        <Commands: cmd_clear: TBP>
    end type cmd_clear_t

```

Output: list the names of the objects to be cleared.

```

<Commands: cmd_clear: TBP>≡
    procedure :: write => cmd_clear_write

<Commands: procedures>+≡
    subroutine cmd_clear_write (cmd, unit, indent)
        class(cmd_clear_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u, i
    end subroutine

```

```

u = given_output_unit (unit); if (u < 0) return
call write_indent (u, indent)
write (u, "(1x,A)", advance="no") "clear: "
if (allocated (cmd%name)) then
  do i = 1, size (cmd%name)
    write (u, "(1x,A)", advance="no") char (cmd%name(i))
  end do
  write (u, *)
else
  write (u, "(5x,A)") "[undefined]"
end if
end subroutine cmd_clear_write

```

Compile. Allocate an array which is filled with the names of the objects to be cleared.

Note: there is currently no need to account for options, but we prepare for that possibility.

```

<Commands: cmd clear: TBP>+≡
  procedure :: compile => cmd_clear_compile

<Commands: procedures>+≡
  subroutine cmd_clear_compile (cmd, global)
    class(cmd_clear_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg, pn_var, pn_prefix, pn_name
    type(string_t) :: key
    integer :: i, n_args
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
    if (associated (pn_arg)) then
      select case (char (parse_node_get_rule_key (pn_arg)))
        case ("clear_arg")
          cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
        case default
          cmd%pn_opt => pn_arg
          pn_arg => null ()
      end select
    end if
    call cmd%compile_options (global)
    if (associated (pn_arg)) then
      n_args = parse_node_get_n_sub (pn_arg)
      allocate (cmd%name (n_args))
      pn_var => parse_node_get_sub_ptr (pn_arg)
      i = 0
      do while (associated (pn_var))
        i = i + 1
        select case (char (parse_node_get_rule_key (pn_var)))
          case ("beams", "iterations", &
                "cuts", "weight", &
                "scale", "factorization_scale", "renormalization_scale", &
                "selection", "reweight", "analysis", &
                "unstable", "polarized", &
                "expect")
          cmd%name(i) = parse_node_get_key (pn_var)
          case ("log_var", "string_var")

```

```

pn_prefix => parse_node_get_sub_ptr (pn_var)
pn_name => parse_node_get_next_ptr (pn_prefix)
key = parse_node_get_key (pn_prefix)
if (associated (pn_name)) then
  select case (char (parse_node_get_rule_key (pn_name)))
  case ("var_name")
    select case (char (key))
    case ("?", "$") ! $ sign
      cmd%name(i) = key // parse_node_get_string (pn_name)
    end select
  case default
    call parse_node_mismatch &
      ("var_name", pn_name)
  end select
else
  cmd%name(i) = key
end if
case default
  cmd%name(i) = parse_node_get_string (pn_var)
end select
pn_var => parse_node_get_next_ptr (pn_var)
end do
else
  allocate (cmd%name (0))
end if
end subroutine cmd_clear_compile

```

Execute. Scan the list of objects to clear.

Objects that can be shown but not cleared: model, library, results

<Commands: cmd clear: TBP>+≡

```

procedure :: execute => cmd_clear_execute

```

<Commands: procedures>+≡

```

subroutine cmd_clear_execute (cmd, global)
  class(cmd_clear_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  integer :: i
  logical :: success
  type(var_list_t), pointer :: model_vars
  if (size (cmd%name) == 0) then
    call msg_warning ("clear: no object specified")
  else
    do i = 1, size (cmd%name)
      success = .true.
      select case (char (cmd%name(i)))
      case ("beams")
        call cmd%local%clear_beams ()
      case ("iterations")
        call cmd%local%it_list%clear ()
      case ("polarized")
        call cmd%local%model%clear_polarized ()
      case ("unstable")
        call cmd%local%model%clear_unstable ()
      case ("cuts", "weight", "scale", &

```

```

        "factorization_scale", "renormalization_scale", &
        "selection", "reweight", "analysis")
    call cmd%local%pn%clear (cmd%name(i))
case ("expect")
    call expect_clear ()
case default
    if (analysis_exists (cmd%name(i))) then
        call analysis_clear (cmd%name(i))
    else if (cmd%local%var_list%contains (cmd%name(i))) then
        if (.not. cmd%local%var_list%is_locked (cmd%name(i))) then
            call cmd%local%var_list%unset (cmd%name(i))
        else
            call msg_error ("clear: variable '" // char (cmd%name(i)) &
                // "' is locked and can't be cleared")
            success = .false.
        end if
    else if (associated (cmd%local%model)) then
        model_vars => cmd%local%model%get_var_list_ptr ()
        if (model_vars%contains (cmd%name(i), follow_link=.false.)) then
            call msg_error ("clear: variable '" // char (cmd%name(i)) &
                // "' is a model variable and can't be cleared")
        else
            call msg_error ("clear: object '" // char (cmd%name(i)) &
                // "' not found")
        end if
        success = .false.
    else
        call msg_error ("clear: object '" // char (cmd%name(i)) &
            // "' not found")
        success = .false.
    end if
end select
if (success) call msg_message ("cleared: " // char (cmd%name(i)))
end do
end if
end subroutine cmd_clear_execute

```

Compare values of variables to expectation

The implementation is similar to the `show` command. There are just two arguments: two values that should be compared. For providing local values for the numerical tolerance, the command has a local argument list.

If the expectation fails, an error condition is recorded.

```

<Commands: types>+≡
type, extends (command_t) :: cmd_expect_t
    private
    type(parse_node_t), pointer :: pn_lexpr => null ()
contains
    <Commands: cmd expect: TBP>
end type cmd_expect_t

```

Simply tell the status.

```

⟨Commands: cmd expect: TBP⟩≡
  procedure :: write => cmd_expect_write

⟨Commands: procedures⟩+≡
  subroutine cmd_expect_write (cmd, unit, indent)
    class(cmd_expect_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    if (associated (cmd%pn_lexpr)) then
      write (u, "(1x,A)") "expect: [expression associated]"
    else
      write (u, "(1x,A)") "expect: [undefined]"
    end if
  end subroutine cmd_expect_write

```

Compile. This merely assigns the parse node, the actual compilation is done at execution. This is necessary because the origin of variables (local/global) may change during execution.

```

⟨Commands: cmd expect: TBP⟩+≡
  procedure :: compile => cmd_expect_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_expect_compile (cmd, global)
    class(cmd_expect_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
    cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
    cmd%pn_lexpr => parse_node_get_sub_ptr (pn_arg)
    call cmd%compile_options (global)
  end subroutine cmd_expect_compile

```

Execute. Evaluate both arguments, print them and their difference (if numerical), and whether they agree. Record the result.

```

⟨Commands: cmd expect: TBP⟩+≡
  procedure :: execute => cmd_expect_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_expect_execute (cmd, global)
    class(cmd_expect_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    logical :: success, is_known
    var_list => cmd%local%get_var_list_ptr ()
    success = eval_log (cmd%pn_lexpr, var_list, is_known=is_known)
    if (is_known) then
      if (success) then
        call msg_message ("expect: success")
      else
        call msg_error ("expect: failure")
      end if
    end if
  end subroutine cmd_expect_execute

```



```

    else
        call msg_error ("expect: undefined result")
        success = .false.
    end if
    call expect_record (success)
end subroutine cmd_expect_execute

```

Beams

The beam command includes both beam and structure-function definition.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_beams_t
    private
        integer :: n_in = 0
        type(parse_node_p), dimension(:), allocatable :: pn_pdg
        integer :: n_sf_record = 0
        integer, dimension(:), allocatable :: n_entry
        type(parse_node_p), dimension(:, :), allocatable :: pn_sf_entry
    contains
        ⟨Commands: cmd beams: TBP⟩
    end type cmd_beams_t

```

Output. The particle expressions are not resolved.

```

⟨Commands: cmd beams: TBP⟩≡
    procedure :: write => cmd_beams_write

⟨Commands: procedures⟩+≡
    subroutine cmd_beams_write (cmd, unit, indent)
        class(cmd_beams_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        select case (cmd%n_in)
        case (1)
            write (u, "(1x,A)") "beams: 1 [decay]"
        case (2)
            write (u, "(1x,A)") "beams: 2 [scattering]"
        case default
            write (u, "(1x,A)") "beams: [undefined]"
        end select
        if (allocated (cmd%n_entry)) then
            if (cmd%n_sf_record > 0) then
                write (u, "(1x,A,99(1x,I0))") "structure function entries:", &
                    cmd%n_entry
            end if
        end if
    end subroutine cmd_beams_write

```

Compile. Find and assign the parse nodes.

Note: local environments are not yet supported.

```

⟨Commands: cmd beams: TBP⟩+≡

```

```

    procedure :: compile => cmd_beams_compile
  (Commands: procedures)+≡
    subroutine cmd_beams_compile (cmd, global)
      class(cmd_beams_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
      type(parse_node_t), pointer :: pn_beam_def, pn_beam_spec
      type(parse_node_t), pointer :: pn_beam_list
      type(parse_node_t), pointer :: pn_codes
      type(parse_node_t), pointer :: pn_strfun_seq, pn_strfun_pair
      type(parse_node_t), pointer :: pn_strfun_def
      integer :: i
      pn_beam_def => parse_node_get_sub_ptr (cmd%pn, 3)
      pn_beam_spec => parse_node_get_sub_ptr (pn_beam_def)
      pn_strfun_seq => parse_node_get_next_ptr (pn_beam_spec)
      pn_beam_list => parse_node_get_sub_ptr (pn_beam_spec)
      call cmd%compile_options (global)
      cmd%n_in = parse_node_get_n_sub (pn_beam_list)
      allocate (cmd%pn_pdg (cmd%n_in))
      pn_codes => parse_node_get_sub_ptr (pn_beam_list)
      do i = 1, cmd%n_in
        cmd%pn_pdg(i)%ptr => pn_codes
        pn_codes => parse_node_get_next_ptr (pn_codes)
      end do
      if (associated (pn_strfun_seq)) then
        cmd%n_sf_record = parse_node_get_n_sub (pn_beam_def) - 1
        allocate (cmd%n_entry (cmd%n_sf_record), source = 1)
        allocate (cmd%pn_sf_entry (2, cmd%n_sf_record))
        do i = 1, cmd%n_sf_record
          pn_strfun_pair => parse_node_get_sub_ptr (pn_strfun_seq, 2)
          pn_strfun_def => parse_node_get_sub_ptr (pn_strfun_pair)
          cmd%pn_sf_entry(1,i)%ptr => pn_strfun_def
          pn_strfun_def => parse_node_get_next_ptr (pn_strfun_def)
          cmd%pn_sf_entry(2,i)%ptr => pn_strfun_def
          if (associated (pn_strfun_def)) cmd%n_entry(i) = 2
          pn_strfun_seq => parse_node_get_next_ptr (pn_strfun_seq)
        end do
      else
        allocate (cmd%n_entry (0))
        allocate (cmd%pn_sf_entry (0, 0))
      end if
    end subroutine cmd_beams_compile

```

Command execution: Determine beam particles and structure-function names, if any. The results are stored in the `beam_structure` component of the `global` data block.

```

  (Commands: cmd beams: TBP)+≡
    procedure :: execute => cmd_beams_execute
  (Commands: procedures)+≡
    subroutine cmd_beams_execute (cmd, global)
      class(cmd_beams_t), intent(inout) :: cmd
      type(rt_data_t), intent(inout), target :: global
      type(var_list_t), pointer :: var_list

```

```

type(pdg_array_t) :: pdg_array
integer, dimension(:), allocatable :: pdg
type(flavor_t), dimension(:), allocatable :: flv
type(parse_node_t), pointer :: pn_key
type(string_t) :: sf_name
integer :: i, j
call lhpdf_global_reset ()
var_list => cmd%local%get_var_list_ptr ()
allocate (flv (cmd%n_in))
do i = 1, cmd%n_in
    pdg_array = eval_pdg_array (cmd%pn_pdg(i)%ptr, var_list)
    pdg = pdg_array
    select case (size (pdg))
    case (1)
        call flv(i)%init ( pdg(1), cmd%local%model)
    case default
        call msg_fatal ("Beams: beam particles must be unique")
    end select
end do
select case (cmd%n_in)
case (1)
    if (cmd%n_sf_record > 0) then
        call msg_fatal ("Beam setup: no structure functions allowed &
            &for decay")
    end if
    call global%beam_structure%init_sf (flv%get_name ())
case (2)
    call global%beam_structure%init_sf (flv%get_name (), cmd%n_entry)
    do i = 1, cmd%n_sf_record
        do j = 1, cmd%n_entry(i)
            pn_key => parse_node_get_sub_ptr (cmd%pn_sf_entry(j,i)%ptr)
            sf_name = parse_node_get_key (pn_key)
            call global%beam_structure%set_sf (i, j, sf_name)
        end do
    end do
end select
end subroutine cmd_beams_execute

```

Density matrices for beam polarization

For holding beam polarization, we define a notation and a data structure for sparse matrices. The entries (and the index expressions) are numerical expressions, so we use evaluation trees.

Each entry in the sparse matrix is an n-tuple of expressions. The first tuple elements represent index values, the last one is an arbitrary (complex) number. Absent expressions are replaced by default-value rules.

Note: Here, and in some other commands, we would like to store an evaluation tree, not just a parse node pointer. However, the current expression handler wants all variables defined, so the evaluation tree can only be built by `evaluate`, i.e., compiled just-in-time and evaluated immediately.

(Commands: types)+≡

```

type :: sentry_expr_t

```

```

        type(parse_node_p), dimension(:), allocatable :: expr
contains
    <Commands: sentry expr: TBP>
end type sentry_expr_t

```

Compile parse nodes into evaluation trees.

```

<Commands: sentry expr: TBP>≡
    procedure :: compile => sentry_expr_compile

<Commands: procedures>+≡
    subroutine sentry_expr_compile (sentry, pn)
        class(sentry_expr_t), intent(out) :: sentry
        type(parse_node_t), intent(in), target :: pn
        type(parse_node_t), pointer :: pn_expr, pn_extra
        integer :: n_expr, i
        n_expr = parse_node_get_n_sub (pn)
        allocate (sentry%expr (n_expr))
        if (n_expr > 0) then
            i = 0
            pn_expr => parse_node_get_sub_ptr (pn)
            pn_extra => parse_node_get_next_ptr (pn_expr)
            do i = 1, n_expr
                sentry%expr(i)%ptr => pn_expr
                if (associated (pn_extra)) then
                    pn_expr => parse_node_get_sub_ptr (pn_extra, 2)
                    pn_extra => parse_node_get_next_ptr (pn_extra)
                end if
            end do
        end if
    end subroutine sentry_expr_compile

```

Evaluate the expressions and return an index array of predefined length together with a complex value. If the value (as the last expression) is undefined, set it to unity. If index values are undefined, repeat the previous index value.

```

<Commands: sentry expr: TBP>+≡
    procedure :: evaluate => sentry_expr_evaluate

<Commands: procedures>+≡
    subroutine sentry_expr_evaluate (sentry, index, value, global)
        class(sentry_expr_t), intent(inout) :: sentry
        integer, dimension(:), intent(out) :: index
        complex(default), intent(out) :: value
        type(rt_data_t), intent(in), target :: global
        type(var_list_t), pointer :: var_list
        integer :: i, n_expr, n_index
        type(eval_tree_t) :: eval_tree
        var_list => global%get_var_list_ptr ()
        n_expr = size (sentry%expr)
        n_index = size (index)
        if (n_expr <= n_index + 1) then
            do i = 1, min (n_expr, n_index)
                associate (expr => sentry%expr(i))
                    call eval_tree%init_expr (expr%ptr, var_list)
                    call eval_tree%evaluate ()
                end associate
            end do
        end if
    end subroutine sentry_expr_evaluate

```

```

        if (eval_tree%is_known ()) then
            index(i) = eval_tree%get_int ()
        else
            call msg_fatal ("Evaluating density matrix: undefined index")
        end if
    end associate
end do
do i = n_expr + 1, n_index
    index(i) = index(n_expr)
end do
if (n_expr == n_index + 1) then
    associate (expr => sentry%expr(n_expr))
        call eval_tree%init_expr (expr%ptr, var_list)
        call eval_tree%evaluate ()
        if (eval_tree%is_known ()) then
            value = eval_tree%get_cmplx ()
        else
            call msg_fatal ("Evaluating density matrix: undefined index")
        end if
        call eval_tree%final ()
    end associate
else
    value = 1
end if
else
    call msg_fatal ("Evaluating density matrix: index expression too long")
end if
end subroutine sentry_expr_evaluate

```

The sparse matrix itself consists of an arbitrary number of entries.

```

⟨Commands: types⟩+≡
    type :: smatrix_expr_t
        type(sentry_expr_t), dimension(:), allocatable :: entry
        contains
        ⟨Commands: smatrix_expr: TBP⟩
    end type smatrix_expr_t

```

Compile: assign sub-nodes to sentry-expressions and compile those.

```

⟨Commands: smatrix_expr: TBP⟩≡
    procedure :: compile => smatrix_expr_compile

⟨Commands: procedures⟩+≡
    subroutine smatrix_expr_compile (smatrix_expr, pn)
        class(smatrix_expr_t), intent(out) :: smatrix_expr
        type(parse_node_t), intent(in), target :: pn
        type(parse_node_t), pointer :: pn_arg, pn_entry
        integer :: n_entry, i
        pn_arg => parse_node_get_sub_ptr (pn, 2)
        if (associated (pn_arg)) then
            n_entry = parse_node_get_n_sub (pn_arg)
            allocate (smatrix_expr%entry (n_entry))
            pn_entry => parse_node_get_sub_ptr (pn_arg)
            do i = 1, n_entry

```

```

        call smatrix_expr%entry(i)%compile (pn_entry)
        pn_entry => parse_node_get_next_ptr (pn_entry)
    end do
else
    allocate (smatrix_expr%entry (0))
end if
end subroutine smatrix_expr_compile

```

Evaluate the entries and build a new `smatrix` object, which contains just the numerical results.

```

<Commands: smatrix expr: TBP>+≡
    procedure :: evaluate => smatrix_expr_evaluate

<Commands: procedures>+≡
    subroutine smatrix_expr_evaluate (smatrix_expr, smatrix, global)
        class(smatrix_expr_t), intent(inout) :: smatrix_expr
        type(smatrix_t), intent(out) :: smatrix
        type(rt_data_t), intent(in), target :: global
        integer, dimension(2) :: idx
        complex(default) :: value
        integer :: i, n_entry
        n_entry = size (smatrix_expr%entry)
        call smatrix%init (2, n_entry)
        do i = 1, n_entry
            call smatrix_expr%entry(i)%evaluate (idx, value, global)
            call smatrix%set_entry (i, idx, value)
        end do
    end subroutine smatrix_expr_evaluate

```

Beam polarization density

The beam polarization command defines spin density matrix for one or two beams (scattering or decay).

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_beams_pol_density_t
        private
        integer :: n_in = 0
        type(smatrix_expr_t), dimension(:), allocatable :: smatrix
    contains
        <Commands: cmd beams pol density: TBP>
    end type cmd_beams_pol_density_t

```

Output.

```

<Commands: cmd beams pol density: TBP>≡
    procedure :: write => cmd_beams_pol_density_write

<Commands: procedures>+≡
    subroutine cmd_beams_pol_density_write (cmd, unit, indent)
        class(cmd_beams_pol_density_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
    end subroutine cmd_beams_pol_density_write

```

```

call write_indent (u, indent)
select case (cmd%n_in)
case (1)
  write (u, "(1x,A)") "beams polarization setup: 1 [decay]"
case (2)
  write (u, "(1x,A)") "beams polarization setup: 2 [scattering]"
case default
  write (u, "(1x,A)") "beams polarization setup: [undefined]"
end select
end subroutine cmd_beams_pol_density_write

```

Compile. Find and assign the parse nodes.

Note: local environments are not yet supported.

```

⟨Commands: cmd beams pol density: TBP⟩+≡
  procedure :: compile => cmd_beams_pol_density_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_beams_pol_density_compile (cmd, global)
    class(cmd_beams_pol_density_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_pol_spec, pn_smatrix
    integer :: i
    pn_pol_spec => parse_node_get_sub_ptr (cmd%pn, 3)
    call cmd%compile_options (global)
    cmd%n_in = parse_node_get_n_sub (pn_pol_spec)
    allocate (cmd%smatrix (cmd%n_in))
    pn_smatrix => parse_node_get_sub_ptr (pn_pol_spec)
    do i = 1, cmd%n_in
      call cmd%smatrix(i)%compile (pn_smatrix)
      pn_smatrix => parse_node_get_next_ptr (pn_smatrix)
    end do
  end subroutine cmd_beams_pol_density_compile

```

Command execution: Fill polarization density matrices. No check yet, the matrices are checked and normalized when the actual beam object is created, just before integration. For intermediate storage, we use the `beam_structure` object in the `global` data set.

```

⟨Commands: cmd beams pol density: TBP⟩+≡
  procedure :: execute => cmd_beams_pol_density_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_beams_pol_density_execute (cmd, global)
    class(cmd_beams_pol_density_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(smatrix_t) :: smatrix
    integer :: i
    call global%beam_structure%init_pol (cmd%n_in)
    do i = 1, cmd%n_in
      call cmd%smatrix(i)%evaluate (smatrix, global)
      call global%beam_structure%set_smatrix (i, smatrix)
    end do
  end subroutine cmd_beams_pol_density_execute

```

Beam polarization fraction

In addition to the polarization density matrix, we can independently specify the polarization fraction for one or both beams.

```
<Commands: types>+≡
  type, extends (command_t) :: cmd_beams_pol_fraction_t
    private
    integer :: n_in = 0
    type(parse_node_p), dimension(:), allocatable :: expr
  contains
    <Commands: cmd beams pol fraction: TBP>
  end type cmd_beams_pol_fraction_t
```

Output.

```
<Commands: cmd beams pol fraction: TBP>≡
  procedure :: write => cmd_beams_pol_fraction_write

<Commands: procedures>+≡
  subroutine cmd_beams_pol_fraction_write (cmd, unit, indent)
    class(cmd_beams_pol_fraction_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    select case (cmd%n_in)
    case (1)
      write (u, "(1x,A)") "beams polarization fraction: 1 [decay]"
    case (2)
      write (u, "(1x,A)") "beams polarization fraction: 2 [scattering]"
    case default
      write (u, "(1x,A)") "beams polarization fraction: [undefined]"
    end select
  end subroutine cmd_beams_pol_fraction_write
```

Compile. Find and assign the parse nodes.

Note: local environments are not yet supported.

```
<Commands: cmd beams pol fraction: TBP>+≡
  procedure :: compile => cmd_beams_pol_fraction_compile

<Commands: procedures>+≡
  subroutine cmd_beams_pol_fraction_compile (cmd, global)
    class(cmd_beams_pol_fraction_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_frac_spec, pn_expr
    integer :: i
    pn_frac_spec => parse_node_get_sub_ptr (cmd%pn, 3)
    call cmd%compile_options (global)
    cmd%n_in = parse_node_get_n_sub (pn_frac_spec)
    allocate (cmd%expr (cmd%n_in))
    pn_expr => parse_node_get_sub_ptr (pn_frac_spec)
    do i = 1, cmd%n_in
      cmd%expr(i)%ptr => pn_expr
      pn_expr => parse_node_get_next_ptr (pn_expr)
    end do
```



```
end subroutine cmd_beams_pol_fraction_compile
```

Command execution: Retrieve the numerical values of the beam polarization fractions. The results are stored in the `beam_structure` component of the global data block.

```
<Commands: cmd_beams_pol_fraction: TBP>+≡
  procedure :: execute => cmd_beams_pol_fraction_execute

<Commands: procedures>+≡
  subroutine cmd_beams_pol_fraction_execute (cmd, global)
    class(cmd_beams_pol_fraction_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    real(default), dimension(:), allocatable :: pol_f
    type(eval_tree_t) :: expr
    integer :: i
    var_list => global%get_var_list_ptr ()
    allocate (pol_f (cmd%n_in))
    do i = 1, cmd%n_in
      call expr%init_expr (cmd%expr(i)%ptr, var_list)
      call expr%evaluate ()
      if (expr%is_known ()) then
        pol_f(i) = expr%get_real ()
      else
        call msg_fatal ("beams polarization fraction: undefined value")
      end if
      call expr%final ()
    end do
    call global%beam_structure%set_pol_f (pol_f)
  end subroutine cmd_beams_pol_fraction_execute
```

Beam momentum

This is completely analogous to the previous command, hence we can use inheritance.

```
<Commands: types>+≡
  type, extends (cmd_beams_pol_fraction_t) :: cmd_beams_momentum_t
  contains
    <Commands: cmd_beams_momentum: TBP>
  end type cmd_beams_momentum_t
```

Output.

```
<Commands: cmd_beams_momentum: TBP>≡
  procedure :: write => cmd_beams_momentum_write

<Commands: procedures>+≡
  subroutine cmd_beams_momentum_write (cmd, unit, indent)
    class(cmd_beams_momentum_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
```

```

select case (cmd%n_in)
case (1)
  write (u, "(1x,A)") "beams momentum: 1 [decay]"
case (2)
  write (u, "(1x,A)") "beams momentum: 2 [scattering]"
case default
  write (u, "(1x,A)") "beams momentum: [undefined]"
end select
end subroutine cmd_beams_momentum_write

```

Compile: inherited.

Command execution: Not inherited, but just the error string and the final command are changed.

```

⟨Commands: cmd beams momentum: TBP⟩+≡
  procedure :: execute => cmd_beams_momentum_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_beams_momentum_execute (cmd, global)
    class(cmd_beams_momentum_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    real(default), dimension(:), allocatable :: p
    type(eval_tree_t) :: expr
    integer :: i
    var_list => global%get_var_list_ptr ()
    allocate (p (cmd%n_in))
    do i = 1, cmd%n_in
      call expr%init_expr (cmd%expr(i)%ptr, var_list)
      call expr%evaluate ()
      if (expr%is_known ()) then
        p(i) = expr%get_real ()
      else
        call msg_fatal ("beams momentum: undefined value")
      end if
      call expr%final ()
    end do
    call global%beam_structure%set_momentum (p)
  end subroutine cmd_beams_momentum_execute

```

Beam angles

Again, this is analogous. There are two angles, polar angle θ and azimuthal angle ϕ , which can be set independently for both beams.

```

⟨Commands: types⟩+≡
  type, extends (cmd_beams_pol_fraction_t) :: cmd_beams_theta_t
  contains
  ⟨Commands: cmd beams theta: TBP⟩
  end type cmd_beams_theta_t

  type, extends (cmd_beams_pol_fraction_t) :: cmd_beams_phi_t
  contains
  ⟨Commands: cmd beams phi: TBP⟩

```

```
end type cmd_beams_phi_t
```

Output.

```
<Commands: cmd beams theta: TBP>≡
  procedure :: write => cmd_beams_theta_write

<Commands: cmd beams phi: TBP>≡
  procedure :: write => cmd_beams_phi_write

<Commands: procedures>+≡
  subroutine cmd_beams_theta_write (cmd, unit, indent)
    class(cmd_beams_theta_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    select case (cmd%n_in)
    case (1)
      write (u, "(1x,A)") "beams theta: 1 [decay]"
    case (2)
      write (u, "(1x,A)") "beams theta: 2 [scattering]"
    case default
      write (u, "(1x,A)") "beams theta: [undefined]"
    end select
  end subroutine cmd_beams_theta_write

  subroutine cmd_beams_phi_write (cmd, unit, indent)
    class(cmd_beams_phi_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    select case (cmd%n_in)
    case (1)
      write (u, "(1x,A)") "beams phi: 1 [decay]"
    case (2)
      write (u, "(1x,A)") "beams phi: 2 [scattering]"
    case default
      write (u, "(1x,A)") "beams phi: [undefined]"
    end select
  end subroutine cmd_beams_phi_write
```

Compile: inherited.

Command execution: Not inherited, but just the error string and the final command are changed.

```
<Commands: cmd beams theta: TBP>+≡
  procedure :: execute => cmd_beams_theta_execute

<Commands: cmd beams phi: TBP>+≡
  procedure :: execute => cmd_beams_phi_execute

<Commands: procedures>+≡
  subroutine cmd_beams_theta_execute (cmd, global)
    class(cmd_beams_theta_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
```

```

type(var_list_t), pointer :: var_list
real(default), dimension(:), allocatable :: theta
type(eval_tree_t) :: expr
integer :: i
var_list => global%get_var_list_ptr ()
allocate (theta (cmd%n_in))
do i = 1, cmd%n_in
  call expr%init_expr (cmd%expr(i)%ptr, var_list)
  call expr%evaluate ()
  if (expr%is_known ()) then
    theta(i) = expr%get_real ()
  else
    call msg_fatal ("beams theta: undefined value")
  end if
  call expr%final ()
end do
call global%beam_structure%set_theta (theta)
end subroutine cmd_beams_theta_execute

subroutine cmd_beams_phi_execute (cmd, global)
class(cmd_beams_phi_t), intent(inout) :: cmd
type(rt_data_t), intent(inout), target :: global
type(var_list_t), pointer :: var_list
real(default), dimension(:), allocatable :: phi
type(eval_tree_t) :: expr
integer :: i
var_list => global%get_var_list_ptr ()
allocate (phi (cmd%n_in))
do i = 1, cmd%n_in
  call expr%init_expr (cmd%expr(i)%ptr, var_list)
  call expr%evaluate ()
  if (expr%is_known ()) then
    phi(i) = expr%get_real ()
  else
    call msg_fatal ("beams phi: undefined value")
  end if
  call expr%final ()
end do
call global%beam_structure%set_phi (phi)
end subroutine cmd_beams_phi_execute

```

Cuts

Define a cut expression. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the process environment where the cut expression is used.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_cuts_t
  private
  type(parse_node_t), pointer :: pn_lexpr => null ()
  contains
  ⟨Commands: cmd cuts: TBP⟩

```

```
end type cmd_cuts_t
```

Output. Do not print the parse tree, since this may get cluttered. Just a message that cuts have been defined.

```
<Commands: cmd cuts: TBP>≡
  procedure :: write => cmd_cuts_write

<Commands: procedures>+≡
  subroutine cmd_cuts_write (cmd, unit, indent)
    class(cmd_cuts_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "cuts: [defined]"
  end subroutine cmd_cuts_write
```

Compile. Simply store the parse (sub)tree.

```
<Commands: cmd cuts: TBP>+≡
  procedure :: compile => cmd_cuts_compile

<Commands: procedures>+≡
  subroutine cmd_cuts_compile (cmd, global)
    class(cmd_cuts_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_lexpr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_cuts_compile
```

Instead of evaluating the cut expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```
<Commands: cmd cuts: TBP>+≡
  procedure :: execute => cmd_cuts_execute

<Commands: procedures>+≡
  subroutine cmd_cuts_execute (cmd, global)
    class(cmd_cuts_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%cuts_lexpr => cmd%pn_lexpr
  end subroutine cmd_cuts_execute
```

General, Factorization and Renormalization Scales

Define a scale expression for either the renormalization or the factorization scale. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the process environment where the expression is used.

```
<Commands: types>+≡
  type, extends (command_t) :: cmd_scale_t
  private
  type(parse_node_t), pointer :: pn_expr => null ()
  contains
```

```

    <Commands: cmd scale: TBP>
end type cmd_scale_t

```

```

<Commands: types>+=
type, extends (command_t) :: cmd_fac_scale_t
    private
    type(parse_node_t), pointer :: pn_expr => null ()
contains
    <Commands: cmd fac scale: TBP>
end type cmd_fac_scale_t

```

```

<Commands: types>+=
type, extends (command_t) :: cmd_ren_scale_t
    private
    type(parse_node_t), pointer :: pn_expr => null ()
contains
    <Commands: cmd ren scale: TBP>
end type cmd_ren_scale_t

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that scale, renormalization and factorization have been defined, respectively.

```

<Commands: cmd scale: TBP>=
    procedure :: write => cmd_scale_write

<Commands: procedures>+=
    subroutine cmd_scale_write (cmd, unit, indent)
        class(cmd_scale_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)") "scale: [defined]"
    end subroutine cmd_scale_write

<Commands: cmd fac scale: TBP>=
    procedure :: write => cmd_fac_scale_write

<Commands: procedures>+=
    subroutine cmd_fac_scale_write (cmd, unit, indent)
        class(cmd_fac_scale_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A)") "factorization scale: [defined]"
    end subroutine cmd_fac_scale_write

<Commands: cmd ren scale: TBP>=
    procedure :: write => cmd_ren_scale_write

```

```

<Commands: procedures>+≡
  subroutine cmd_ren_scale_write (cmd, unit, indent)
    class(cmd_ren_scale_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "renormalization scale: [defined]"
  end subroutine cmd_ren_scale_write

```

Compile. Simply store the parse (sub)tree.

```

<Commands: cmd scale: TBP>+≡
  procedure :: compile => cmd_scale_compile

<Commands: procedures>+≡
  subroutine cmd_scale_compile (cmd, global)
    class(cmd_scale_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_scale_compile

```

```

<Commands: cmd fac scale: TBP>+≡
  procedure :: compile => cmd_fac_scale_compile

<Commands: procedures>+≡
  subroutine cmd_fac_scale_compile (cmd, global)
    class(cmd_fac_scale_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_fac_scale_compile

```

```

<Commands: cmd ren scale: TBP>+≡
  procedure :: compile => cmd_ren_scale_compile

<Commands: procedures>+≡
  subroutine cmd_ren_scale_compile (cmd, global)
    class(cmd_ren_scale_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_ren_scale_compile

```

Instead of evaluating the scale expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

<Commands: cmd scale: TBP>+≡
  procedure :: execute => cmd_scale_execute

<Commands: procedures>+≡
  subroutine cmd_scale_execute (cmd, global)
    class(cmd_scale_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%scale_expr => cmd%pn_expr
  end subroutine cmd_scale_execute

```

```

<Commands: cmd fac scale: TBP>+≡
  procedure :: execute => cmd_fac_scale_execute

<Commands: procedures>+≡
  subroutine cmd_fac_scale_execute (cmd, global)
    class(cmd_fac_scale_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%fac_scale_expr => cmd%pn_expr
  end subroutine cmd_fac_scale_execute

<Commands: cmd ren scale: TBP>+≡
  procedure :: execute => cmd_ren_scale_execute

<Commands: procedures>+≡
  subroutine cmd_ren_scale_execute (cmd, global)
    class(cmd_ren_scale_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%ren_scale_expr => cmd%pn_expr
  end subroutine cmd_ren_scale_execute

```

Weight

Define a weight expression. The weight is applied to a process to be integrated, event by event. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the process environment where the expression is used.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_weight_t
    private
    type(parse_node_t), pointer :: pn_expr => null ()
  contains
    <Commands: cmd weight: TBP>
  end type cmd_weight_t

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that scale, renormalization and factorization have been defined, respectively.

```

<Commands: cmd weight: TBP>≡
  procedure :: write => cmd_weight_write

<Commands: procedures>+≡
  subroutine cmd_weight_write (cmd, unit, indent)
    class(cmd_weight_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "weight expression: [defined]"
  end subroutine cmd_weight_write

```

Compile. Simply store the parse (sub)tree.

```

<Commands: cmd weight: TBP>+≡
  procedure :: compile => cmd_weight_compile

```



```

<Commands: procedures>+≡
  subroutine cmd_weight_compile (cmd, global)
    class(cmd_weight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_weight_compile

```

Instead of evaluating the expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

<Commands: cmd weight: TBP>+≡
  procedure :: execute => cmd_weight_execute

<Commands: procedures>+≡
  subroutine cmd_weight_execute (cmd, global)
    class(cmd_weight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%weight_expr => cmd%pn_expr
  end subroutine cmd_weight_execute

```

Selection

Define a selection expression. This is to be applied upon simulation or event-file rescanning, event by event. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the environment where the expression is used.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_selection_t
  private
    type(parse_node_t), pointer :: pn_expr => null ()
  contains
    <Commands: cmd selection: TBP>
  end type cmd_selection_t

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that scale, renormalization and factorization have been defined, respectively.

```

<Commands: cmd selection: TBP>≡
  procedure :: write => cmd_selection_write

<Commands: procedures>+≡
  subroutine cmd_selection_write (cmd, unit, indent)
    class(cmd_selection_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "selection expression: [defined]"
  end subroutine cmd_selection_write

```

Compile. Simply store the parse (sub)tree.

```

<Commands: cmd selection: TBP>+≡
  procedure :: compile => cmd_selection_compile

```

```

⟨Commands: procedures⟩+≡
  subroutine cmd_selection_compile (cmd, global)
    class(cmd_selection_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_selection_compile

```

Instead of evaluating the expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

⟨Commands: cmd selection: TBP⟩+≡
  procedure :: execute => cmd_selection_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_selection_execute (cmd, global)
    class(cmd_selection_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%selection_lexpr => cmd%pn_expr
  end subroutine cmd_selection_execute

```

Reweight

Define a reweight expression. This is to be applied upon simulation or event-file rescanning, event by event. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the environment where the expression is used.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_reweight_t
  private
    type(parse_node_t), pointer :: pn_expr => null ()
  contains
    ⟨Commands: cmd reweight: TBP⟩
  end type cmd_reweight_t

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that scale, renormalization and factorization have been defined, respectively.

```

⟨Commands: cmd reweight: TBP⟩≡
  procedure :: write => cmd_reweight_write

⟨Commands: procedures⟩+≡
  subroutine cmd_reweight_write (cmd, unit, indent)
    class(cmd_reweight_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "reweight expression: [defined]"
  end subroutine cmd_reweight_write

```

Compile. Simply store the parse (sub)tree.

```

⟨Commands: cmd reweight: TBP⟩+≡
  procedure :: compile => cmd_reweight_compile

```

```

<Commands: procedures>+≡
  subroutine cmd_reweight_compile (cmd, global)
    class(cmd_reweight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_expr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_reweight_compile

```

Instead of evaluating the expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

<Commands: cmd reweight: TBP>+≡
  procedure :: execute => cmd_reweight_execute

<Commands: procedures>+≡
  subroutine cmd_reweight_execute (cmd, global)
    class(cmd_reweight_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%reweight_expr => cmd%pn_expr
  end subroutine cmd_reweight_execute

```

Alternative Simulation Setups

Together with simulation, we can re-evaluate event weights in the context of alternative setups. The `cmd_alt_setup_t` object is designed to hold these setups, which are brace-enclosed command lists. Compilation is deferred to the simulation environment where the setup expression is used.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_alt_setup_t
  private
    type(parse_node_p), dimension(:), allocatable :: setup
  contains
    <Commands: cmd alt setup: TBP>
  end type cmd_alt_setup_t

```

Output. Print just a message that the alternative setup list has been defined.

```

<Commands: cmd alt setup: TBP>≡
  procedure :: write => cmd_alt_setup_write

<Commands: procedures>+≡
  subroutine cmd_alt_setup_write (cmd, unit, indent)
    class(cmd_alt_setup_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,I0,A)") "alt_setup: ", size (cmd%setup), " entries"
  end subroutine cmd_alt_setup_write

```

Compile. Store the parse sub-trees in an array.

```

<Commands: cmd alt setup: TBP>+≡
  procedure :: compile => cmd_alt_setup_compile

```

```

<Commands: procedures>+=
subroutine cmd_alt_setup_compile (cmd, global)
  class(cmd_alt_setup_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_list, pn_setup
  integer :: i
  pn_list => parse_node_get_sub_ptr (cmd%pn, 3)
  if (associated (pn_list)) then
    allocate (cmd%setup (parse_node_get_n_sub (pn_list)))
    i = 1
    pn_setup => parse_node_get_sub_ptr (pn_list)
    do while (associated (pn_setup))
      cmd%setup(i)%ptr => pn_setup
      i = i + 1
      pn_setup => parse_node_get_next_ptr (pn_setup)
    end do
  else
    allocate (cmd%setup (0))
  end if
end subroutine cmd_alt_setup_compile

```

Execute. Transfer the array of command lists to the global environment.

```

<Commands: cmd alt setup: TBP>+=
procedure :: execute => cmd_alt_setup_execute

<Commands: procedures>+=
subroutine cmd_alt_setup_execute (cmd, global)
  class(cmd_alt_setup_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  if (allocated (global%pn%alt_setup)) deallocate (global%pn%alt_setup)
  allocate (global%pn%alt_setup (size (cmd%setup)))
  global%pn%alt_setup = cmd%setup
end subroutine cmd_alt_setup_execute

```

Integration

Integrate several processes, consecutively with identical parameters.

```

<Commands: types>+=
type, extends (command_t) :: cmd_integrate_t
  private
  integer :: n_proc = 0
  type(string_t), dimension(:), allocatable :: process_id
contains
  <Commands: cmd integrate: TBP>
end type cmd_integrate_t

```

Output: we know the process IDs.

```

<Commands: cmd integrate: TBP>=
procedure :: write => cmd_integrate_write

```

```

⟨Commands: procedures⟩+≡
  subroutine cmd_integrate_write (cmd, unit, indent)
    class(cmd_integrate_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)", advance="no") "integrate ("
    do i = 1, cmd%n_proc
      if (i > 1) write (u, "(A,1x)", advance="no") ", "
      write (u, "(A)", advance="no") char (cmd%process_id(i))
    end do
    write (u, "(A)") ")"
  end subroutine cmd_integrate_write

```

Compile.

```

⟨Commands: cmd integrate: TBP⟩+≡
  procedure :: compile => cmd_integrate_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_integrate_compile (cmd, global)
    class(cmd_integrate_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_proclist, pn_proc
    integer :: i
    pn_proclist => parse_node_get_sub_ptr (cmd%pn, 2)
    cmd%pn_opt => parse_node_get_next_ptr (pn_proclist)
    call cmd%compile_options (global)
    cmd%n_proc = parse_node_get_n_sub (pn_proclist)
    allocate (cmd%process_id (cmd%n_proc))
    pn_proc => parse_node_get_sub_ptr (pn_proclist)
    do i = 1, cmd%n_proc
      cmd%process_id(i) = parse_node_get_string (pn_proc)
      call global%process_stack%init_result_vars (cmd%process_id(i))
      pn_proc => parse_node_get_next_ptr (pn_proc)
    end do
  end subroutine cmd_integrate_compile

```

Command execution. Integrate the process(es) with the predefined number of passes, iterations and calls. For structure functions, cuts, weight and scale, use local definitions if present; by default, the local definitions are initialized with the global ones.

The `integrate` procedure should take its input from the currently active local environment, but produce a process record in the stack of the global environment.

Since the process acquires a snapshot of the variable list, so if the global list (or the local one) is deleted, this does no harm. This implies that later changes of the variable list do not affect the stored process.

```

⟨Commands: cmd integrate: TBP⟩+≡
  procedure :: execute => cmd_integrate_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_integrate_execute (cmd, global)

```

```

class(cmd_integrate_t), intent(inout) :: cmd
type(rt_data_t), intent(inout), target :: global
integer :: i
if (debug_on) call msg_debug (D_CORE, "cmd_integrate_execute")
do i = 1, cmd%n_proc
  if (debug_on) call msg_debug (D_CORE, "cmd%process_id(i) ", cmd%process_id(i))
  call integrate_process (cmd%process_id(i), cmd%local, global)
  call global%process_stack%fill_result_vars (cmd%process_id(i))
  call global%process_stack%update_result_vars &
    (cmd%process_id(i), global%var_list)
  if (signal_is_pending ()) return
end do
end subroutine cmd_integrate_execute

```

Observables

Declare an observable. After the declaration, it can be used to record data, and at the end one can retrieve average and error.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_observable_t
  private
  type(string_t) :: id
  contains
  ⟨Commands: cmd observable: TBP⟩
end type cmd_observable_t

```

Output. We know the ID.

```

⟨Commands: cmd observable: TBP⟩≡
  procedure :: write => cmd_observable_write

⟨Commands: procedures⟩+≡
  subroutine cmd_observable_write (cmd, unit, indent)
    class(cmd_observable_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,A)" "observable: ", char (cmd%id)
  end subroutine cmd_observable_write

```

Compile. Just record the observable ID.

```

⟨Commands: cmd observable: TBP⟩+≡
  procedure :: compile => cmd_observable_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_observable_compile (cmd, global)
    class(cmd_observable_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_tag
    pn_tag => parse_node_get_sub_ptr (cmd%pn, 2)
    if (associated (pn_tag)) then
      cmd%pn_opt => parse_node_get_next_ptr (pn_tag)
    end if
  end subroutine cmd_observable_compile

```

```

end if
call cmd%compile_options (global)
select case (char (parse_node_get_rule_key (pn_tag)))
case ("analysis_id")
    cmd%id = parse_node_get_string (pn_tag)
case default
    call msg_bug ("observable: name expression not implemented (yet)")
end select
end subroutine cmd_observable_compile

```

Command execution. This declares the observable and allocates it in the analysis store.

```

⟨Commands: cmd observable: TBP⟩+≡
    procedure :: execute => cmd_observable_execute

⟨Commands: procedures⟩+≡
    subroutine cmd_observable_execute (cmd, global)
        class(cmd_observable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(graph_options_t) :: graph_options
        type(string_t) :: label, unit
        var_list => cmd%local%get_var_list_ptr ()
        label = var_list%get_sval (var_str ("$_obs_label"))
        unit = var_list%get_sval (var_str ("$_obs_unit"))
        call graph_options_init (graph_options)
        call set_graph_options (graph_options, var_list)
        call analysis_init_observable (cmd%id, label, unit, graph_options)
    end subroutine cmd_observable_execute

```

Histograms

Declare a histogram. At minimum, we have to set lower and upper bound and bin width.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_histogram_t
    private
        type(string_t) :: id
        type(parse_node_t), pointer :: pn_lower_bound => null ()
        type(parse_node_t), pointer :: pn_upper_bound => null ()
        type(parse_node_t), pointer :: pn_bin_width => null ()
    contains
        ⟨Commands: cmd histogram: TBP⟩
    end type cmd_histogram_t

```

Output. Just print the ID.

```

⟨Commands: cmd histogram: TBP⟩≡
    procedure :: write => cmd_histogram_write

⟨Commands: procedures⟩+≡
    subroutine cmd_histogram_write (cmd, unit, indent)
        class(cmd_histogram_t), intent(in) :: cmd

```

```

integer, intent(in), optional :: unit, indent
integer :: u
u = given_output_unit (unit); if (u < 0) return
call write_indent (u, indent)
write (u, "(1x,A,A)") "histogram: ", char (cmd%id)
end subroutine cmd_histogram_write

```

Compile. Record the histogram ID and initialize lower, upper bound and bin width.

```

⟨Commands: cmd histogram: TBP⟩+≡
  procedure :: compile => cmd_histogram_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_histogram_compile (cmd, global)
    class(cmd_histogram_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_tag, pn_args, pn_arg1, pn_arg2, pn_arg3
    character(*), parameter :: e_illegal_use = &
      "illegal usage of 'histogram': insufficient number of arguments"
    pn_tag => parse_node_get_sub_ptr (cmd%pn, 2)
    pn_args => parse_node_get_next_ptr (pn_tag)
    if (associated (pn_args)) then
      pn_arg1 => parse_node_get_sub_ptr (pn_args)
      if (.not. associated (pn_arg1)) call msg_fatal (e_illegal_use)
      pn_arg2 => parse_node_get_next_ptr (pn_arg1)
      if (.not. associated (pn_arg2)) call msg_fatal (e_illegal_use)
      pn_arg3 => parse_node_get_next_ptr (pn_arg2)
      cmd%pn_opt => parse_node_get_next_ptr (pn_args)
    end if
    call cmd%compile_options (global)
    select case (char (parse_node_get_rule_key (pn_tag)))
    case ("analysis_id")
      cmd%id = parse_node_get_string (pn_tag)
    case default
      call msg_bug ("histogram: name expression not implemented (yet)")
    end select
    cmd%pn_lower_bound => pn_arg1
    cmd%pn_upper_bound => pn_arg2
    cmd%pn_bin_width => pn_arg3
  end subroutine cmd_histogram_compile

```

Command execution. This declares the histogram and allocates it in the analysis store.

```

⟨Commands: cmd histogram: TBP⟩+≡
  procedure :: execute => cmd_histogram_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_histogram_execute (cmd, global)
    class(cmd_histogram_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    real(default) :: lower_bound, upper_bound, bin_width
    integer :: bin_number
    logical :: bin_width_is_used, normalize_bins

```



```

type(string_t) :: obs_label, obs_unit
type(graph_options_t) :: graph_options
type(drawing_options_t) :: drawing_options

var_list => cmd%local%get_var_list_ptr ()
lower_bound = eval_real (cmd%pn_lower_bound, var_list)
upper_bound = eval_real (cmd%pn_upper_bound, var_list)
if (associated (cmd%pn_bin_width)) then
    bin_width = eval_real (cmd%pn_bin_width, var_list)
    bin_width_is_used = .true.
else if (var_list%is_known (var_str ("n_bins"))) then
    bin_number = &
        var_list%get_ival (var_str ("n_bins"))
    bin_width_is_used = .false.
else
    call msg_error ("Cmd '" // char (cmd%id) // &
        "' : neither bin width nor number is defined")
end if
normalize_bins = &
    var_list%get_lval (var_str ("?normalize_bins"))
obs_label = &
    var_list%get_sval (var_str ("$obs_label"))
obs_unit = &
    var_list%get_sval (var_str ("$obs_unit"))

call graph_options_init (graph_options)
call set_graph_options (graph_options, var_list)
call drawing_options_init_histogram (drawing_options)
call set_drawing_options (drawing_options, var_list)

if (bin_width_is_used) then
    call analysis_init_histogram &
        (cmd%id, lower_bound, upper_bound, bin_width, &
            normalize_bins, &
            obs_label, obs_unit, &
            graph_options, drawing_options)
else
    call analysis_init_histogram &
        (cmd%id, lower_bound, upper_bound, bin_number, &
            normalize_bins, &
            obs_label, obs_unit, &
            graph_options, drawing_options)
end if
end subroutine cmd_histogram_execute

```

Set the graph options from a variable list.

(Commands: procedures)+≡

```

subroutine set_graph_options (gro, var_list)
    type(graph_options_t), intent(inout) :: gro
    type(var_list_t), intent(in) :: var_list
    call graph_options_set (gro, title = &
        var_list%get_sval (var_str ("$title")))
    call graph_options_set (gro, description = &

```

```

        var_list%get_sval (var_str ("description"))
call graph_options_set (gro, x_label = &
    var_list%get_sval (var_str ("x_label")))
call graph_options_set (gro, y_label = &
    var_list%get_sval (var_str ("y_label")))
call graph_options_set (gro, width_mm = &
    var_list%get_ival (var_str ("graph_width_mm")))
call graph_options_set (gro, height_mm = &
    var_list%get_ival (var_str ("graph_height_mm")))
call graph_options_set (gro, x_log = &
    var_list%get_lval (var_str ("x_log")))
call graph_options_set (gro, y_log = &
    var_list%get_lval (var_str ("y_log")))
if (var_list%is_known (var_str ("x_min"))) &
    call graph_options_set (gro, x_min = &
        var_list%get_rval (var_str ("x_min")))
if (var_list%is_known (var_str ("x_max"))) &
    call graph_options_set (gro, x_max = &
        var_list%get_rval (var_str ("x_max")))
if (var_list%is_known (var_str ("y_min"))) &
    call graph_options_set (gro, y_min = &
        var_list%get_rval (var_str ("y_min")))
if (var_list%is_known (var_str ("y_max"))) &
    call graph_options_set (gro, y_max = &
        var_list%get_rval (var_str ("y_max")))
call graph_options_set (gro, gmlcode_bg = &
    var_list%get_sval (var_str ("gmlcode_bg")))
call graph_options_set (gro, gmlcode_fg = &
    var_list%get_sval (var_str ("gmlcode_fg")))
end subroutine set_graph_options

```

Set the drawing options from a variable list.

(Commands: procedures)+≡

```

subroutine set_drawing_options (dro, var_list)
type(drawing_options_t), intent(inout) :: dro
type(var_list_t), intent(in) :: var_list
if (var_list%is_known (var_str ("draw_histogram"))) then
    if (var_list%get_lval (var_str ("draw_histogram"))) then
        call drawing_options_set (dro, with_hbars = .true.)
    else
        call drawing_options_set (dro, with_hbars = .false., &
            with_base = .false., fill = .false., piecewise = .false.)
    end if
end if
if (var_list%is_known (var_str ("draw_base"))) then
    if (var_list%get_lval (var_str ("draw_base"))) then
        call drawing_options_set (dro, with_base = .true.)
    else
        call drawing_options_set (dro, with_base = .false., fill = .false.)
    end if
end if
if (var_list%is_known (var_str ("draw_piecewise"))) then
    if (var_list%get_lval (var_str ("draw_piecewise"))) then
        call drawing_options_set (dro, piecewise = .true.)
    end if
end if

```

```

else
    call drawing_options_set (dro, piecewise = .false.)
end if
end if
if (var_list%is_known (var_str ("?fill_curve"))) then
    if (var_list%get_lval (var_str ("?fill_curve"))) then
        call drawing_options_set (dro, fill = .true., with_base = .true.)
    else
        call drawing_options_set (dro, fill = .false.)
    end if
end if
if (var_list%is_known (var_str ("?draw_curve"))) then
    if (var_list%get_lval (var_str ("?draw_curve"))) then
        call drawing_options_set (dro, draw = .true.)
    else
        call drawing_options_set (dro, draw = .false.)
    end if
end if
if (var_list%is_known (var_str ("?draw_errors"))) then
    if (var_list%get_lval (var_str ("?draw_errors"))) then
        call drawing_options_set (dro, err = .true.)
    else
        call drawing_options_set (dro, err = .false.)
    end if
end if
if (var_list%is_known (var_str ("?draw_symbols"))) then
    if (var_list%get_lval (var_str ("?draw_symbols"))) then
        call drawing_options_set (dro, symbols = .true.)
    else
        call drawing_options_set (dro, symbols = .false.)
    end if
end if
if (var_list%is_known (var_str (" $fill_options"))) then
    call drawing_options_set (dro, fill_options = &
        var_list%get_sval (var_str (" $fill_options")))
end if
if (var_list%is_known (var_str (" $draw_options"))) then
    call drawing_options_set (dro, draw_options = &
        var_list%get_sval (var_str (" $draw_options")))
end if
if (var_list%is_known (var_str (" $err_options"))) then
    call drawing_options_set (dro, err_options = &
        var_list%get_sval (var_str (" $err_options")))
end if
if (var_list%is_known (var_str (" $symbol"))) then
    call drawing_options_set (dro, symbol = &
        var_list%get_sval (var_str (" $symbol")))
end if
if (var_list%is_known (var_str (" $gmlcode_bg"))) then
    call drawing_options_set (dro, gmlcode_bg = &
        var_list%get_sval (var_str (" $gmlcode_bg")))
end if
if (var_list%is_known (var_str (" $gmlcode_fg"))) then
    call drawing_options_set (dro, gmlcode_fg = &

```

```

        var_list%get_sval (var_str ("$gmlcode_fg"))
    end if
end subroutine set_drawing_options

```

Plots

Declare a plot. No mandatory arguments, just options.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_plot_t
        private
        type(string_t) :: id
    contains
        ⟨Commands: cmd plot: TBP⟩
    end type cmd_plot_t

```

Output. Just print the ID.

```

⟨Commands: cmd plot: TBP⟩≡
    procedure :: write => cmd_plot_write

⟨Commands: procedures⟩+≡
    subroutine cmd_plot_write (cmd, unit, indent)
        class(cmd_plot_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A,A)") "plot: ", char (cmd%id)
    end subroutine cmd_plot_write

```

Compile. Record the plot ID and initialize lower, upper bound and bin width.

```

⟨Commands: cmd plot: TBP⟩+≡
    procedure :: compile => cmd_plot_compile

⟨Commands: procedures⟩+≡
    subroutine cmd_plot_compile (cmd, global)
        class(cmd_plot_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(parse_node_t), pointer :: pn_tag
        pn_tag => parse_node_get_sub_ptr (cmd%pn, 2)
        cmd%pn_opt => parse_node_get_next_ptr (pn_tag)
        call cmd%init (pn_tag, global)
    end subroutine cmd_plot_compile

```

This init routine is separated because it is reused below for graph initialization.

```

⟨Commands: cmd plot: TBP⟩+≡
    procedure :: init => cmd_plot_init

⟨Commands: procedures⟩+≡
    subroutine cmd_plot_init (plot, pn_tag, global)
        class(cmd_plot_t), intent(inout) :: plot
        type(parse_node_t), intent(in), pointer :: pn_tag
        type(rt_data_t), intent(inout), target :: global

```

```

call plot%compile_options (global)
select case (char (parse_node_get_rule_key (pn_tag)))
case ("analysis_id")
    plot%id = parse_node_get_string (pn_tag)
case default
    call msg_bug ("plot: name expression not implemented (yet)")
end select
end subroutine cmd_plot_init

```

Command execution. This declares the plot and allocates it in the analysis store.

```

⟨Commands: cmd plot: TBP⟩+≡
    procedure :: execute => cmd_plot_execute

⟨Commands: procedures⟩+≡
    subroutine cmd_plot_execute (cmd, global)
        class(cmd_plot_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(graph_options_t) :: graph_options
        type(drawing_options_t) :: drawing_options

        var_list => cmd%local%get_var_list_ptr ()
        call graph_options_init (graph_options)
        call set_graph_options (graph_options, var_list)
        call drawing_options_init_plot (drawing_options)
        call set_drawing_options (drawing_options, var_list)

        call analysis_init_plot (cmd%id, graph_options, drawing_options)
    end subroutine cmd_plot_execute

```

Graphs

Declare a graph. The graph is defined in terms of its contents. Both the graph and its contents may carry options.

The graph object contains its own ID as well as the IDs of its elements. For the elements, we reuse the `cmd_plot_t` defined above.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_graph_t
        private
        type(string_t) :: id
        integer :: n_elements = 0
        type(cmd_plot_t), dimension(:), allocatable :: el
        type(string_t), dimension(:), allocatable :: element_id
    contains
        ⟨Commands: cmd graph: TBP⟩
    end type cmd_graph_t

```

Output. Just print the ID.

```

⟨Commands: cmd graph: TBP⟩≡
    procedure :: write => cmd_graph_write

```

```

⟨Commands: procedures⟩+≡
subroutine cmd_graph_write (cmd, unit, indent)
  class(cmd_graph_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  write (u, "(1x,A,A,A,IO,A)") "graph: ", char (cmd%id), &
    " (" , cmd%n_elements, " entries)"
end subroutine cmd_graph_write

```

Compile. Record the graph ID and initialize lower, upper bound and bin width. For compiling the graph element syntax, we use part of the `cmd_plot_t` compiler.

Note: currently, we do not respect options, therefore just IDs on the RHS.

```

⟨Commands: cmd graph: TBP⟩+≡
  procedure :: compile => cmd_graph_compile

⟨Commands: procedures⟩+≡
subroutine cmd_graph_compile (cmd, global)
  class(cmd_graph_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_term, pn_tag, pn_def, pn_app
  integer :: i

  pn_term => parse_node_get_sub_ptr (cmd%pn, 2)
  pn_tag => parse_node_get_sub_ptr (pn_term)
  cmd%pn_opt => parse_node_get_next_ptr (pn_tag)
  call cmd%compile_options (global)
  select case (char (parse_node_get_rule_key (pn_tag)))
  case ("analysis_id")
    cmd%id = parse_node_get_string (pn_tag)
  case default
    call msg_bug ("graph: name expression not implemented (yet)")
  end select
  pn_def => parse_node_get_next_ptr (pn_term, 2)
  cmd%n_elements = parse_node_get_n_sub (pn_def)
  allocate (cmd%element_id (cmd%n_elements))
  allocate (cmd%el (cmd%n_elements))
  pn_term => parse_node_get_sub_ptr (pn_def)
  pn_tag => parse_node_get_sub_ptr (pn_term)
  cmd%el(1)%pn_opt => parse_node_get_next_ptr (pn_tag)
  call cmd%el(1)%init (pn_tag, global)
  cmd%element_id(1) = parse_node_get_string (pn_tag)
  pn_app => parse_node_get_next_ptr (pn_term)
  do i = 2, cmd%n_elements
    pn_term => parse_node_get_sub_ptr (pn_app, 2)
    pn_tag => parse_node_get_sub_ptr (pn_term)
    cmd%el(i)%pn_opt => parse_node_get_next_ptr (pn_tag)
    call cmd%el(i)%init (pn_tag, global)
    cmd%element_id(i) = parse_node_get_string (pn_tag)
    pn_app => parse_node_get_next_ptr (pn_app)
  end do
end subroutine cmd_graph_compile

```

Command execution. This declares the graph, allocates it in the analysis store, and copies the graph elements.

For the graph, we set graph and default drawing options. For the elements, we reset individual drawing options.

This accesses internals of the contained elements of type `cmd_plot_t`, see above. We might disentangle such an interdependency when this code is rewritten using proper type extension.

```

⟨Commands: cmd graph: TBP⟩+≡
  procedure :: execute => cmd_graph_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_graph_execute (cmd, global)
    class(cmd_graph_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    type(graph_options_t) :: graph_options
    type(drawing_options_t) :: drawing_options
    integer :: i, type

    var_list => cmd%local%get_var_list_ptr ()
    call graph_options_init (graph_options)
    call set_graph_options (graph_options, var_list)
    call analysis_init_graph (cmd%id, cmd%n_elements, graph_options)

    do i = 1, cmd%n_elements
      if (associated (cmd%el(i)%options)) then
        call cmd%el(i)%options%execute (cmd%el(i)%local)
      end if
      type = analysis_store_get_object_type (cmd%element_id(i))
      select case (type)
        case (AN_HISTOGRAM)
          call drawing_options_init_histogram (drawing_options)
        case (AN_PLOT)
          call drawing_options_init_plot (drawing_options)
        end select
      call set_drawing_options (drawing_options, var_list)
      if (associated (cmd%el(i)%options)) then
        call set_drawing_options (drawing_options, cmd%el(i)%local%var_list)
      end if
      call analysis_fill_graph (cmd%id, i, cmd%element_id(i), drawing_options)
    end do
  end subroutine cmd_graph_execute

```

Analysis

Hold the analysis ID either as a string or as an expression:

```

⟨Commands: types⟩+≡
  type :: analysis_id_t
    type(string_t) :: tag
    type(parse_node_t), pointer :: pn_sexpr => null ()
  end type analysis_id_t

```

Define the analysis expression. We store the parse tree for the right-hand side instead of compiling it. Compilation is deferred to the process environment where the analysis expression is used.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_analysis_t
  private
    type(parse_node_t), pointer :: pn_lexpr => null ()
  contains
    ⟨Commands: cmd analysis: TBP⟩
  end type cmd_analysis_t

```

Output. Print just a message that analysis has been defined.

```

⟨Commands: cmd analysis: TBP⟩≡
  procedure :: write => cmd_analysis_write

⟨Commands: procedures⟩+≡
  subroutine cmd_analysis_write (cmd, unit, indent)
    class(cmd_analysis_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "analysis: [defined]"
  end subroutine cmd_analysis_write

```

Compile. Simply store the parse (sub)tree.

```

⟨Commands: cmd analysis: TBP⟩+≡
  procedure :: compile => cmd_analysis_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_analysis_compile (cmd, global)
    class(cmd_analysis_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%pn_lexpr => parse_node_get_sub_ptr (cmd%pn, 3)
  end subroutine cmd_analysis_compile

```

Instead of evaluating the cut expression, link the parse tree to the global data set, such that it is compiled and executed in the appropriate process context.

```

⟨Commands: cmd analysis: TBP⟩+≡
  procedure :: execute => cmd_analysis_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_analysis_execute (cmd, global)
    class(cmd_analysis_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    global%pn%analysis_lexpr => cmd%pn_lexpr
  end subroutine cmd_analysis_execute

```


Write histograms and plots

The data type encapsulating the command:

```
<Commands: types>+≡
  type, extends (command_t) :: cmd_write_analysis_t
    private
    type(analysis_id_t), dimension(:), allocatable :: id
    type(string_t), dimension(:), allocatable :: tag
  contains
    <Commands: cmd write analysis: TBP>
  end type cmd_write_analysis_t
```

Output. Just the keyword.

```
<Commands: cmd write analysis: TBP>≡
  procedure :: write => cmd_write_analysis_write

<Commands: procedures>+≡
  subroutine cmd_write_analysis_write (cmd, unit, indent)
    class(cmd_write_analysis_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "write_analysis"
  end subroutine cmd_write_analysis_write
```

Compile.

```
<Commands: cmd write analysis: TBP>+≡
  procedure :: compile => cmd_write_analysis_compile

<Commands: procedures>+≡
  subroutine cmd_write_analysis_compile (cmd, global)
    class(cmd_write_analysis_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_clause, pn_args, pn_id
    integer :: n, i
    pn_clause => parse_node_get_sub_ptr (cmd%pn)
    pn_args => parse_node_get_sub_ptr (pn_clause, 2)
    cmd%pn_opt => parse_node_get_next_ptr (pn_clause)
    call cmd%compile_options (global)
    if (associated (pn_args)) then
      n = parse_node_get_n_sub (pn_args)
      allocate (cmd%id (n))
      do i = 1, n
        pn_id => parse_node_get_sub_ptr (pn_args, i)
        if (char (parse_node_get_rule_key (pn_id)) == "analysis_id") then
          cmd%id(i)%tag = parse_node_get_string (pn_id)
        else
          cmd%id(i)%pn_sexpr => pn_id
        end if
      end do
    else
      allocate (cmd%id (0))
    end if
```

```
end subroutine cmd_write_analysis_compile
```

The output format for real data values:

```
<Commands: parameters>+≡
character(*), parameter, public :: &
  DEFAULT_ANALYSIS_FILENAME = "whizard_analysis.dat"
character(len=1), dimension(2), parameter, public :: &
  FORBIDDEN_ENDINGS1 = [ "o", "a" ]
character(len=2), dimension(6), parameter, public :: &
  FORBIDDEN_ENDINGS2 = [ "mp", "ps", "vg", "pg", "lo", "la" ]
character(len=3), dimension(18), parameter, public :: &
  FORBIDDEN_ENDINGS3 = [ "aux", "dvi", "evt", "evx", "f03", "f90", &
    "f95", "log", "ltp", "mpx", "olc", "olp", "pdf", "phs", "sin", &
    "tex", "vg2", "vgx" ]
```

As this contains a lot of similar code to `cmd.compile.analysis.execute` we outsource the main code to a subroutine.

```
<Commands: cmd write analysis: TBP>+≡
procedure :: execute => cmd_write_analysis_execute

<Commands: procedures>+≡
subroutine cmd_write_analysis_execute (cmd, global)
  class(cmd_write_analysis_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  var_list => cmd%local%get_var_list_ptr ()
  call write_analysis_wrap (var_list, global%out_files, &
    cmd%id, tag = cmd%tag)
end subroutine cmd_write_analysis_execute
```

If the `data_file` optional argument is present, this is called from `cmd.compile.analysis.execute`, which needs the file name for further processing, and requires the default format. For the moment, parameters and macros for custom data processing are disabled.

```
<Commands: procedures>+≡
subroutine write_analysis_wrap (var_list, out_files, id, tag, data_file)
  type(var_list_t), intent(inout), target :: var_list
  type(file_list_t), intent(inout), target :: out_files
  type(analysis_id_t), dimension(:), intent(in), target :: id
  type(string_t), dimension(:), allocatable, intent(out) :: tag
  type(string_t), intent(out), optional :: data_file
  type(string_t) :: defaultfile, file
  integer :: i
  logical :: keep_open
  type(string_t) :: extension
  logical :: one_file
  defaultfile = var_list%get_sval (var_str ("out_file"))
  if (present (data_file)) then
    if (defaultfile == "" .or. defaultfile == ".") then
      defaultfile = DEFAULT_ANALYSIS_FILENAME
    else
      if (scan (".", defaultfile) > 0) then
```

```

        call split (defaultfile, extension, ".", back=.true.)
        if (any (lower_case (char(extension)) == FORBIDDEN_ENDINGS1) .or. &
            any (lower_case (char(extension)) == FORBIDDEN_ENDINGS2) .or. &
            any (lower_case (char(extension)) == FORBIDDEN_ENDINGS3)) &
            call msg_fatal ("The ending " // char(extension) // &
                " is internal and not allowed as data file.")
        if (extension /= "") then
            if (defaultfile /= "") then
                defaultfile = defaultfile // "." // extension
            else
                defaultfile = "whizard_analysis." // extension
            end if
        else
            defaultfile = defaultfile // ".dat"
        endif
        endif
        else
            defaultfile = defaultfile // ".dat"
        end if
    end if
    data_file = defaultfile
end if
one_file = defaultfile /= ""
if (one_file) then
    file = defaultfile
    keep_open = file_list_is_open (out_files, file, &
        action = "write")
    if (keep_open) then
        if (present (data_file)) then
            call msg_fatal ("Compiling analysis: File '" &
                // char (data_file) &
                // "' can't be used, it is already open.")
        else
            call msg_message ("Appending analysis data to file '" &
                // char (file) // "'")
        end if
    else
        call file_list_open (out_files, file, &
            action = "write", status = "replace", position = "asis")
        call msg_message ("Writing analysis data to file '" &
            // char (file) // "'")
    end if
end if

call get_analysis_tags (tag, id, var_list)
do i = 1, size (tag)
    call file_list_write_analysis &
        (out_files, file, tag(i))
end do
if (one_file .and. .not. keep_open) then
    call file_list_close (out_files, file)
end if
contains

```

```

subroutine get_analysis_tags (analysis_tag, id, var_list)
  type(string_t), dimension(:), intent(out), allocatable :: analysis_tag
  type(analysis_id_t), dimension(:), intent(in) :: id
  type(var_list_t), intent(in), target :: var_list
  if (size (id) /= 0) then
    allocate (analysis_tag (size (id)))
    do i = 1, size (id)
      if (associated (id(i)%pn_sexpr)) then
        analysis_tag(i) = eval_string (id(i)%pn_sexpr, var_list)
      else
        analysis_tag(i) = id(i)%tag
      end if
    end do
  else
    call analysis_store_get_ids (tag)
  end if
end subroutine get_analysis_tags

end subroutine write_analysis_wrap

```

Compile analysis results

This command writes files in a form suitable for GAMELAN and executes the appropriate commands to compile them. The first part is identical to `cmd_write_analysis`.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_compile_analysis_t
  private
  type(analysis_id_t), dimension(:), allocatable :: id
  type(string_t), dimension(:), allocatable :: tag
  contains
  <Commands: cmd compile analysis: TBP>
end type cmd_compile_analysis_t

```

Output. Just the keyword.

```

<Commands: cmd compile analysis: TBP>≡
  procedure :: write => cmd_compile_analysis_write

<Commands: procedures>+≡
  subroutine cmd_compile_analysis_write (cmd, unit, indent)
    class(cmd_compile_analysis_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "compile_analysis"
  end subroutine cmd_compile_analysis_write

```

Compile.

```

<Commands: cmd compile analysis: TBP>+≡
  procedure :: compile => cmd_compile_analysis_compile

```

```

⟨Commands: procedures⟩+=
subroutine cmd_compile_analysis_compile (cmd, global)
  class(cmd_compile_analysis_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_clause, pn_args, pn_id
  integer :: n, i
  pn_clause => parse_node_get_sub_ptr (cmd%pn)
  pn_args => parse_node_get_sub_ptr (pn_clause, 2)
  cmd%pn_opt => parse_node_get_next_ptr (pn_clause)
  call cmd%compile_options (global)
  if (associated (pn_args)) then
    n = parse_node_get_n_sub (pn_args)
    allocate (cmd%id (n))
    do i = 1, n
      pn_id => parse_node_get_sub_ptr (pn_args, i)
      if (char (parse_node_get_rule_key (pn_id)) == "analysis_id") then
        cmd%id(i)%tag = parse_node_get_string (pn_id)
      else
        cmd%id(i)%pn_sexpr => pn_id
      end if
    end do
  else
    allocate (cmd%id (0))
  end if
end subroutine cmd_compile_analysis_compile

```

First write the analysis data to file, then write a GAMELAN driver and produce MetaPost and T_EX output.

```

⟨Commands: cmd compile analysis: TBP⟩+=
procedure :: execute => cmd_compile_analysis_execute

⟨Commands: procedures⟩+=
subroutine cmd_compile_analysis_execute (cmd, global)
  class(cmd_compile_analysis_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  type(string_t) :: file, basename, extension, driver_file, &
    makefile
  integer :: u_driver, u_makefile
  logical :: has_gmlcode, only_file
  var_list => cmd%local%get_var_list_ptr ()
  call write_analysis_wrap (var_list, &
    global%out_files, cmd%id, tag = cmd%tag, &
    data_file = file)
  basename = file
  if (scan (".", basename) > 0) then
    call split (basename, extension, ".", back=.true.)
  else
    extension = ""
  end if
  driver_file = basename // ".tex"
  makefile = basename // "_ana.makefile"
  u_driver = free_unit ()
  open (unit=u_driver, file=char(driver_file), &

```

```

        action="write", status="replace")
if (allocated (cmd%tag)) then
    call analysis_write_driver (file, cmd%tag, unit=u_driver)
    has_gmlcode = analysis_has_plots (cmd%tag)
else
    call analysis_write_driver (file, unit=u_driver)
    has_gmlcode = analysis_has_plots ()
end if
close (u_driver)
u_makefile = free_unit ()
open (unit=u_makefile, file=char(makefile), &
      action="write", status="replace")
call analysis_write_makefile (basename, u_makefile, &
      has_gmlcode, global%os_data)
close (u_makefile)
call msg_message ("Compiling analysis results display in '" &
      // char (driver_file) // "'")
call msg_message ("Providing analysis steering makefile '" &
      // char (makefile) // "'")
only_file = global%var_list%get_lval &
      (var_str ("?analysis_file_only"))
if (.not. only_file) call analysis_compile_tex &
      (basename, has_gmlcode, global%os_data)
end subroutine cmd_compile_analysis_execute

```

35.1.4 User-controlled output to data files

Open file (output)

Open a file for output.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_open_out_t
        private
            type(parse_node_t), pointer :: file_expr => null ()
        contains
            <Commands: cmd open out: TBP>
        end type cmd_open_out_t

```

Finalizer for the embedded eval tree.

```

<Commands: procedures>+≡
    subroutine cmd_open_out_final (object)
        class(cmd_open_out_t), intent(inout) :: object
    end subroutine cmd_open_out_final

```

Output (trivial here).

```

<Commands: cmd open out: TBP>≡
    procedure :: write => cmd_open_out_write

<Commands: procedures>+≡
    subroutine cmd_open_out_write (cmd, unit, indent)
        class(cmd_open_out_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent

```

```

integer :: u
u = given_output_unit (unit); if (u < 0) return
call write_indent (u, indent)
write (u, "(1x,A)", advance="no") "open_out: <filename>"
end subroutine cmd_open_out_write

```

Compile: create an eval tree for the filename expression.

```

⟨Commands: cmd open out: TBP⟩+≡
  procedure :: compile => cmd_open_out_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_open_out_compile (cmd, global)
    class(cmd_open_out_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    cmd%file_expr => parse_node_get_sub_ptr (cmd%pn, 2)
    if (associated (cmd%file_expr)) then
      cmd%pn_opt => parse_node_get_next_ptr (cmd%file_expr)
    end if
    call cmd%compile_options (global)
  end subroutine cmd_open_out_compile

```

Execute: append the file to the global list of open files.

```

⟨Commands: cmd open out: TBP⟩+≡
  procedure :: execute => cmd_open_out_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_open_out_execute (cmd, global)
    class(cmd_open_out_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    type(eval_tree_t) :: file_expr
    type(string_t) :: file
    var_list => cmd%local%get_var_list_ptr ()
    call file_expr%init_sexpr (cmd%file_expr, var_list)
    call file_expr%evaluate ()
    if (file_expr%is_known ()) then
      file = file_expr%get_string ()
      call file_list_open (global%out_files, file, &
        action = "write", status = "replace", position = "asis")
    else
      call msg_fatal ("open_out: file name argument evaluates to unknown")
    end if
    call file_expr%final ()
  end subroutine cmd_open_out_execute

```

Open file (output)

Close an output file. Except for the `execute` method, everything is analogous to the open command, so we can just inherit.

```

⟨Commands: types⟩+≡
  type, extends (cmd_open_out_t) :: cmd_close_out_t
  private

```

```

contains
  <Commands: cmd close out: TBP>
end type cmd_close_out_t

```

Execute: remove the file from the global list of output files.

```

<Commands: cmd close out: TBP>≡
  procedure :: execute => cmd_close_out_execute

<Commands: procedures>+≡
  subroutine cmd_close_out_execute (cmd, global)
    class(cmd_close_out_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    type(eval_tree_t) :: file_expr
    type(string_t) :: file
    var_list => cmd%local%var_list
    call file_expr%init_sexpr (cmd%file_expr, var_list)
    call file_expr%evaluate ()
    if (file_expr%is_known ()) then
      file = file_expr%get_string ()
      call file_list_close (global%out_files, file)
    else
      call msg_fatal ("close_out: file name argument evaluates to unknown")
    end if
    call file_expr%final ()
  end subroutine cmd_close_out_execute

```

35.1.5 Print custom-formatted values

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_printf_t
  private
    type(parse_node_t), pointer :: sexpr => null ()
    type(parse_node_t), pointer :: sprintf_fun => null ()
    type(parse_node_t), pointer :: sprintf_clause => null ()
    type(parse_node_t), pointer :: sprintf => null ()
  contains
    <Commands: cmd printf: TBP>
  end type cmd_printf_t

```

Finalize.

```

<Commands: cmd printf: TBP>≡
  procedure :: final => cmd_printf_final

<Commands: procedures>+≡
  subroutine cmd_printf_final (cmd)
    class(cmd_printf_t), intent(inout) :: cmd
    call parse_node_final (cmd%sexpr, recursive = .false.)
    deallocate (cmd%sexpr)
    call parse_node_final (cmd%sprintf_fun, recursive = .false.)
    deallocate (cmd%sprintf_fun)
    call parse_node_final (cmd%sprintf_clause, recursive = .false.)

```



```

deallocate (cmd%sprintf_clause)
call parse_node_final (cmd%sprintf, recursive = .false.)
deallocate (cmd%sprintf)
end subroutine cmd_printf_final

```

Output. Do not print the parse tree, since this may get cluttered. Just a message that cuts have been defined.

```

⟨Commands: cmd printf: TBP⟩+≡
  procedure :: write => cmd_printf_write

⟨Commands: procedures⟩+≡
  subroutine cmd_printf_write (cmd, unit, indent)
    class(cmd_printf_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "printf:"
  end subroutine cmd_printf_write

```

Compile. We create a fake parse node (subtree) with a `sprintf` command with identical arguments which can then be handled by the corresponding evaluation procedure.

```

⟨Commands: cmd printf: TBP⟩+≡
  procedure :: compile => cmd_printf_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_printf_compile (cmd, global)
    class(cmd_printf_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_cmd, pn_clause, pn_args, pn_format
    pn_cmd => parse_node_get_sub_ptr (cmd%pn)
    pn_clause => parse_node_get_sub_ptr (pn_cmd)
    pn_format => parse_node_get_sub_ptr (pn_clause, 2)
    pn_args => parse_node_get_next_ptr (pn_clause)
    cmd%pn_opt => parse_node_get_next_ptr (pn_cmd)
    call cmd%compile_options (global)
    allocate (cmd%sexpr)
    call parse_node_create_branch (cmd%sexpr, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("sexpr")))
    allocate (cmd%sprintf_fun)
    call parse_node_create_branch (cmd%sprintf_fun, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("sprintf_fun")))
    allocate (cmd%sprintf_clause)
    call parse_node_create_branch (cmd%sprintf_clause, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("sprintf_clause")))
    allocate (cmd%sprintf)
    call parse_node_create_key (cmd%sprintf, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("sprintf")))
    call parse_node_append_sub (cmd%sprintf_clause, cmd%sprintf)
    call parse_node_append_sub (cmd%sprintf_clause, pn_format)
    call parse_node_freeze_branch (cmd%sprintf_clause)
    call parse_node_append_sub (cmd%sprintf_fun, cmd%sprintf_clause)
    if (associated (pn_args)) then

```

```

        call parse_node_append_sub (cmd%sprintf_fun, pn_args)
    end if
    call parse_node_freeze_branch (cmd%sprintf_fun)
    call parse_node_append_sub (cmd%sexpr, cmd%sprintf_fun)
    call parse_node_freeze_branch (cmd%sexpr)
end subroutine cmd_printf_compile

```

Execute. Evaluate the string (pretending this is a `sprintf` expression) and print it.

```

⟨Commands: cmd printf: TBP⟩+≡
    procedure :: execute => cmd_printf_execute

⟨Commands: procedures⟩+≡
    subroutine cmd_printf_execute (cmd, global)
        class(cmd_printf_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(string_t) :: string, file
        type(eval_tree_t) :: sprintf_expr
        logical :: advance
        var_list => cmd%local%get_var_list_ptr ()
        advance = var_list%get_lval (&
            var_str ("?out_advance"))
        file = var_list%get_sval (&
            var_str ("out_file"))
        call sprintf_expr%init_sexpr (cmd%sexpr, var_list)
        call sprintf_expr%evaluate ()
        if (sprintf_expr%is_known ()) then
            string = sprintf_expr%get_string ()
            if (len (file) == 0) then
                call msg_result (char (string))
            else
                call file_list_write (global%out_files, file, string, advance)
            end if
        end if
    end if
end subroutine cmd_printf_execute

```

Record data

The expression syntax already contains a `record` keyword; this evaluates to a logical which is always true, but it has the side-effect of recording data into analysis objects. Here we define a command as an interface to this construct.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_record_t
        private
        type(parse_node_t), pointer :: pn_lexpr => null ()
    contains
        ⟨Commands: cmd record: TBP⟩
    end type cmd_record_t

```

Output. With the compile hack below, there is nothing of interest to print here.

```

⟨Commands: cmd record: TBP⟩≡
  procedure :: write => cmd_record_write

⟨Commands: procedures⟩+≡
  subroutine cmd_record_write (cmd, unit, indent)
    class(cmd_record_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)") "record"
  end subroutine cmd_record_write

```

Compile. This is a hack which transforms the `record` command into a `record` expression, which we handle in the `expressions` module.

```

⟨Commands: cmd record: TBP⟩+≡
  procedure :: compile => cmd_record_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_record_compile (cmd, global)
    class(cmd_record_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_lexpr, pn_lsinglet, pn_lterm, pn_record
    call parse_node_create_branch (pn_lexpr, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("lexpr")))
    call parse_node_create_branch (pn_lsinglet, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("lsinglet")))
    call parse_node_append_sub (pn_lexpr, pn_lsinglet)
    call parse_node_create_branch (pn_lterm, &
      syntax_get_rule_ptr (syntax_cmd_list, var_str ("lterm")))
    call parse_node_append_sub (pn_lsinglet, pn_lterm)
    pn_record => parse_node_get_sub_ptr (cmd%pn)
    call parse_node_append_sub (pn_lterm, pn_record)
    cmd%pn_lexpr => pn_lexpr
  end subroutine cmd_record_compile

```

Command execution. Again, transfer this to the embedded expression and just forget the logical result.

```

⟨Commands: cmd record: TBP⟩+≡
  procedure :: execute => cmd_record_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_record_execute (cmd, global)
    class(cmd_record_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    logical :: lval
    var_list => global%get_var_list_ptr ()
    lval = eval_log (cmd%pn_lexpr, var_list)
  end subroutine cmd_record_execute

```

Unstable particles

Mark a particle as unstable. For each unstable particle, we store a number of decay channels and compute their respective BRs.

```
<Commands: types>+≡
  type, extends (command_t) :: cmd_unstable_t
  private
  integer :: n_proc = 0
  type(string_t), dimension(:), allocatable :: process_id
  type(parse_node_t), pointer :: pn_prt_in => null ()
  contains
  <Commands: cmd unstable: TBP>
end type cmd_unstable_t
```

Output: we know the process IDs.

```
<Commands: cmd unstable: TBP>≡
  procedure :: write => cmd_unstable_write

<Commands: procedures>+≡
  subroutine cmd_unstable_write (cmd, unit, indent)
    class(cmd_unstable_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,1x,I0,1x,A)", advance="no") &
      "unstable:", 1, "("
    do i = 1, cmd%n_proc
      if (i > 1) write (u, "(A,1x)", advance="no") ", "
      write (u, "(A)", advance="no") char (cmd%process_id(i))
    end do
    write (u, "(A)") ")"
  end subroutine cmd_unstable_write
```

Compile. Initiate an eval tree for the decaying particle and determine the decay channel process IDs.

```
<Commands: cmd unstable: TBP>+≡
  procedure :: compile => cmd_unstable_compile

<Commands: procedures>+≡
  subroutine cmd_unstable_compile (cmd, global)
    class(cmd_unstable_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_list, pn_proc
    integer :: i
    cmd%pn_prt_in => parse_node_get_sub_ptr (cmd%pn, 2)
    pn_list => parse_node_get_next_ptr (cmd%pn_prt_in)
    if (associated (pn_list)) then
      select case (char (parse_node_get_rule_key (pn_list)))
      case ("unstable_arg")
        cmd%n_proc = parse_node_get_n_sub (pn_list)
        cmd%pn_opt => parse_node_get_next_ptr (pn_list)
      case default
        cmd%n_proc = 0
      end select
    end if
  end subroutine cmd_unstable_compile
```

```

        cmd%pn_opt => pn_list
        pn_list => null ()
    end select
end if
call cmd%compile_options (global)
if (associated (pn_list)) then
    allocate (cmd%process_id (cmd%n_proc))
    pn_proc => parse_node_get_sub_ptr (pn_list)
    do i = 1, cmd%n_proc
        cmd%process_id(i) = parse_node_get_string (pn_proc)
        call cmd%local%process_stack%init_result_vars (cmd%process_id(i))
        pn_proc => parse_node_get_next_ptr (pn_proc)
    end do
else
    allocate (cmd%process_id (0))
end if
end if
end subroutine cmd_unstable_compile

```

Command execution. Evaluate the decaying particle and mark the decays in the current model object.

```

<Commands: cmd_unstable: TBP>+≡
    procedure :: execute => cmd_unstable_execute

<Commands: procedures>+≡
    subroutine cmd_unstable_execute (cmd, global)
        class(cmd_unstable_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        logical :: auto_decays, auto_decays_radiative
        integer :: auto_decays_multiplicity
        logical :: isotropic_decay, diagonal_decay, polarized_decay
        integer :: decay_helicity
        type(pdg_array_t) :: pa_in
        integer :: pdg_in
        type(string_t) :: libname_cur, libname_dec
        type(string_t), dimension(:), allocatable :: auto_id, tmp_id
        integer :: n_proc_user
        integer :: i, u_tmp
        character(80) :: buffer
        var_list => cmd%local%get_var_list_ptr ()
        auto_decays = &
            var_list%get_lval (var_str ("?auto_decays"))
        if (auto_decays) then
            auto_decays_multiplicity = &
                var_list%get_ival (var_str ("auto_decays_multiplicity"))
            auto_decays_radiative = &
                var_list%get_lval (var_str ("?auto_decays_radiative"))
        end if
        isotropic_decay = &
            var_list%get_lval (var_str ("?isotropic_decay"))
        if (isotropic_decay) then
            diagonal_decay = .false.
            polarized_decay = .false.
        else

```

```

diagonal_decay = &
    var_list%get_lval (var_str ("?diagonal_decay"))
if (diagonal_decay) then
    polarized_decay = .false.
else
    polarized_decay = &
        var_list%is_known (var_str ("decay_helicity"))
    if (polarized_decay) then
        decay_helicity = var_list%get_lval (var_str ("decay_helicity"))
    end if
end if
end if
pa_in = eval_pdg_array (cmd%pn_prt_in, var_list)
if (pdg_array_get_length (pa_in) /= 1) &
    call msg_fatal ("Unstable: decaying particle must be unique")
pdg_in = pdg_array_get (pa_in, 1)
n_proc_user = cmd%n_proc
if (auto_decays) then
    call create_auto_decays (pdg_in, &
        auto_decays_multiplicity, auto_decays_radiative, &
        libname_dec, auto_id, cmd%local)
    allocate (tmp_id (cmd%n_proc + size (auto_id)))
    tmp_id(:cmd%n_proc) = cmd%process_id
    tmp_id(cmd%n_proc+1:) = auto_id
    call move_alloc (from = tmp_id, to = cmd%process_id)
    cmd%n_proc = size (cmd%process_id)
end if
libname_cur = cmd%local%prclib%get_name ()
do i = 1, cmd%n_proc
    if (i == n_proc_user + 1) then
        call cmd%local%update_prclib &
            (cmd%local%prclib_stack%get_library_ptr (libname_dec))
    end if
    if (.not. global%process_stack%exists (cmd%process_id(i))) then
        call var_list%set_log &
            (var_str ("?decay_rest_frame"), .false., is_known = .true.)
        call integrate_process (cmd%process_id(i), cmd%local, global)
        call global%process_stack%fill_result_vars (cmd%process_id(i))
    end if
end do
call cmd%local%update_prclib &
    (cmd%local%prclib_stack%get_library_ptr (libname_cur))
if (cmd%n_proc > 0) then
    if (polarized_decay) then
        call global%modify_particle (pdg_in, stable = .false., &
            decay = cmd%process_id, &
            isotropic_decay = .false., &
            diagonal_decay = .false., &
            decay_helicity = decay_helicity, &
            polarized = .false.)
    else
        call global%modify_particle (pdg_in, stable = .false., &
            decay = cmd%process_id, &
            isotropic_decay = isotropic_decay, &

```

```

        diagonal_decay = diagonal_decay, &
        polarized = .false.)
    end if
    u_tmp = free_unit ()
    open (u_tmp, status = "scratch", action = "readwrite")
    call show_unstable (global, pdg_in, u_tmp)
    rewind (u_tmp)
    do
        read (u_tmp, "(A)", end = 1) buffer
        write (msg_buffer, "(A)") trim (buffer)
        call msg_message ()
    end do
1    continue
    close (u_tmp)
else
    call err_unstable (global, pdg_in)
end if
end subroutine cmd_unstable_execute

```

Show data for the current unstable particle. This is called both by the `unstable` and by the `show` command.

To determine decay branching ratios, we look at the decay process IDs and inspect the corresponding `integral()` result variables.

(Commands: procedures)+≡

```

subroutine show_unstable (global, pdg, u)
    type(rt_data_t), intent(in), target :: global
    integer, intent(in) :: pdg, u
    type(flavor_t) :: flv
    type(string_t), dimension(:), allocatable :: decay
    real(default), dimension(:), allocatable :: br
    real(default) :: width
    type(process_t), pointer :: process
    type(process_component_def_t), pointer :: prc_def
    type(string_t), dimension(:), allocatable :: prt_out, prt_out_str
    integer :: i, j
    logical :: opened
    call flv%init (pdg, global%model)
    call flv%get_decays (decay)
    if (.not. allocated (decay)) return
    allocate (prt_out_str (size (decay)))
    allocate (br (size (decay)))
    do i = 1, size (br)
        process => global%process_stack%get_process_ptr (decay(i))
        prc_def => process%get_component_def_ptr (1)
        call prc_def%get_prt_out (prt_out)
        prt_out_str(i) = prt_out(1)
        do j = 2, size (prt_out)
            prt_out_str(i) = prt_out_str(i) // ", " // prt_out(j)
        end do
        br(i) = global%get_rval ("integral(" // decay(i) // ")")
    end do
    if (all (br >= 0)) then
        if (any (br > 0)) then

```

```

width = sum (br)
br = br / sum (br)
write (u, "(A)") "Unstable particle " &
    // char (flv%get_name ()) &
    // ": computed branching ratios:"
do i = 1, size (br)
    write (u, "(2x,A,':'," // FMT_14 // ",3x,A)") &
        char (decay(i)), br(i), char (prt_out_str(i))
end do
write (u, "(2x,'Total width ='," // FMT_14 // ", ' GeV (computed)'))" width
write (u, "(2x,'          ='," // FMT_14 // ", ' GeV (preset)'))" &
    flv%get_width ()
if (flv%decays_isotropically ()) then
    write (u, "(2x,A)") "Decay options: isotropic"
else if (flv%decays_diagonal ()) then
    write (u, "(2x,A)") "Decay options: &
        &projection on diagonal helicity states"
else if (flv%has_decay_helicity ()) then
    write (u, "(2x,A,1x,I0)") "Decay options: projection onto helicity =", &
        flv%get_decay_helicity ()
else
    write (u, "(2x,A)") "Decay options: helicity treated exactly"
end if
else
    inquire (unit = u, opened = opened)
    if (opened .and. .not. mask_fatal_errors) close (u)
    call msg_fatal ("Unstable particle " &
        // char (flv%get_name ()) &
        // ": partial width vanishes for all decay channels")
    end if
else
    inquire (unit = u, opened = opened)
    if (opened .and. .not. mask_fatal_errors) close (u)
    call msg_fatal ("Unstable particle " &
        // char (flv%get_name ()) &
        // ": partial width is negative")
    end if
end if
end subroutine show_unstable

```

If no decays have been found, issue a non-fatal error.

<Commands: procedures>+≡

```

subroutine err_unstable (global, pdg)
    type(rt_data_t), intent(in), target :: global
    integer, intent(in) :: pdg
    type(flavor_t) :: flv
    call flv%init (pdg, global%model)
    call msg_error ("Unstable: no allowed decays found for particle " &
        // char (flv%get_name ()) // ", keeping as stable")
end subroutine err_unstable

```

Auto decays: create process IDs and make up process configurations, using the PDG codes generated by the `ds_table` make method.

We allocate and use a self-contained process library that contains only the

decay processes of the current particle. When done, we revert the global library pointer to the original library but return the name of the new one. The new library becomes part of the global library stack and can thus be referred to at any time.

(Commands: procedures)+≡

```

subroutine create_auto_decays &
  (pdg_in, mult, rad, libname_dec, process_id, global)
  integer, intent(in) :: pdg_in
  integer, intent(in) :: mult
  logical, intent(in) :: rad
  type(string_t), intent(out) :: libname_dec
  type(string_t), dimension(:), allocatable, intent(out) :: process_id
  type(rt_data_t), intent(inout) :: global
  type(prclib_entry_t), pointer :: lib_entry
  type(process_library_t), pointer :: lib
  type(ds_table_t) :: ds_table
  type(split_constraints_t) :: constraints
  type(pdg_array_t), dimension(:), allocatable :: pa_out
  character(80) :: buffer
  character :: p_or_a
  type(string_t) :: process_string, libname_cur
  type(flavor_t) :: flv_in, flv_out
  type(string_t) :: prt_in
  type(string_t), dimension(:), allocatable :: prt_out
  type(process_configuration_t) :: prc_config
  integer :: i, j, k
  call flv_in%init (pdg_in, global%model)
  if (rad) then
    call constraints%init (2)
  else
    call constraints%init (3)
    call constraints%set (3, constrain_radiation ())
  end if
  call constraints%set (1, constrain_n_tot (mult))
  call constraints%set (2, &
    constrain_mass_sum (flv_in%get_mass (), margin = 0._default))
  call ds_table%make (global%model, pdg_in, constraints)
  prt_in = flv_in%get_name ()
  if (pdg_in > 0) then
    p_or_a = "p"
  else
    p_or_a = "a"
  end if
  if (ds_table%get_length () == 0) then
    call msg_warning ("Auto-decays: Particle " // char (prt_in) // ": " &
      // "no decays found")
    libname_dec = ""
    allocate (process_id (0))
  else
    call msg_message ("Creating decay process library for particle " &
      // char (prt_in))
    libname_cur = global%prclib%get_name ()
    write (buffer, "(A,A,I0)" " _d", p_or_a, abs (pdg_in))
    libname_dec = libname_cur // trim (buffer)
  end if
end subroutine create_auto_decays

```

```

lib => global%prclib_stack%get_library_ptr (libname_dec)
if (.not. (associated (lib))) then
  allocate (lib_entry)
  call lib_entry%init (libname_dec)
  lib => lib_entry%process_library_t
  call global%add_prclib (lib_entry)
else
  call global%update_prclib (lib)
end if
allocate (process_id (ds_table%get_length ()))
do i = 1, size (process_id)
  write (buffer, "(A,'_',A,I0,'_',I0)" &
    "decay", p_or_a, abs (pdg_in), i)
  process_id(i) = trim (buffer)
  process_string = process_id(i) // ": " // prt_in // " =>"
  call ds_table%get_pdg_out (i, pa_out)
  allocate (prt_out (size (pa_out)))
  do j = 1, size (pa_out)
    do k = 1, pa_out(j)%get_length ()
      call flv_out%init (pa_out(j)%get (k), global%model)
      if (k == 1) then
        prt_out(j) = flv_out%get_name ()
      else
        prt_out(j) = prt_out(j) // ":" // flv_out%get_name ()
      end if
    end do
    process_string = process_string // " " // prt_out(j)
  end do
  call msg_message (char (process_string))
  call prc_config%init (process_id(i), 1, 1, &
    global%model, global%var_list, &
    nlo_process = global%nlo_fixed_order)
  call prc_config%setup_component (1, new_prt_spec ([prt_in]), &
    new_prt_spec (prt_out), global%model, global%var_list)
  call prc_config%record (global)
  deallocate (prt_out)
  deallocate (pa_out)
end do
lib => global%prclib_stack%get_library_ptr (libname_cur)
call global%update_prclib (lib)
end if
call ds_table%final ()
end subroutine create_auto_decays

```

(Stable particles

Revert the unstable declaration for a list of particles.

```

<Commands: types>+≡
  type, extends (command_t) :: cmd_stable_t
  private
  type(parse_node_p), dimension(:), allocatable :: pn_pdg
  contains
  <Commands: cmd stable: TBP>

```

```
end type cmd_stable_t
```

Output: we know only the number of particles.

```
<Commands: cmd stable: TBP>≡
  procedure :: write => cmd_stable_write

<Commands: procedures>+≡
  subroutine cmd_stable_write (cmd, unit, indent)
    class(cmd_stable_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,1x,I0)") "stable:", size (cmd%pn_pdg)
  end subroutine cmd_stable_write
```

Compile. Assign parse nodes for the particle IDs.

```
<Commands: cmd stable: TBP>+≡
  procedure :: compile => cmd_stable_compile

<Commands: procedures>+≡
  subroutine cmd_stable_compile (cmd, global)
    class(cmd_stable_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_list, pn_prt
    integer :: n, i
    pn_list => parse_node_get_sub_ptr (cmd%pn, 2)
    cmd%pn_opt => parse_node_get_next_ptr (pn_list)
    call cmd%compile_options (global)
    n = parse_node_get_n_sub (pn_list)
    allocate (cmd%pn_pdg (n))
    pn_prt => parse_node_get_sub_ptr (pn_list)
    i = 1
    do while (associated (pn_prt))
      cmd%pn_pdg(i)%ptr => pn_prt
      pn_prt => parse_node_get_next_ptr (pn_prt)
      i = i + 1
    end do
  end subroutine cmd_stable_compile
```

Execute: apply the modifications to the current model.

```
<Commands: cmd stable: TBP>+≡
  procedure :: execute => cmd_stable_execute

<Commands: procedures>+≡
  subroutine cmd_stable_execute (cmd, global)
    class(cmd_stable_t), intent(inout) :: cmd
    type(rt_data_t), target, intent(inout) :: global
    type(var_list_t), pointer :: var_list
    type(pdg_array_t) :: pa
    integer :: pdg
    type(flavor_t) :: flv
    integer :: i
    var_list => cmd%local%get_var_list_ptr ()
```

```

do i = 1, size (cmd%pn_pdg)
  pa = eval_pdg_array (cmd%pn_pdg(i)%ptr, var_list)
  if (pdg_array_get_length (pa) /= 1) &
    call msg_fatal ("Stable: listed particles must be unique")
  pdg = pdg_array_get (pa, 1)
  call global%modify_particle (pdg, stable = .true., &
    isotropic_decay = .false., &
    diagonal_decay = .false., &
    polarized = .false.)
  call flv%init (pdg, cmd%local%model)
  call msg_message ("Particle " &
    // char (flv%get_name ()) &
    // " declared as stable")
end do
end subroutine cmd_stable_execute

```

Polarized particles

These commands mark particles as (un)polarized, to be applied in subsequent simulation passes. Since this is technically the same as the `stable` command, we take a shortcut and make this an extension, just overriding methods.

```

⟨Commands: types⟩+≡
  type, extends (cmd_stable_t) :: cmd_polarized_t
    contains
    ⟨Commands: cmd polarized: TBP⟩
  end type cmd_polarized_t

  type, extends (cmd_stable_t) :: cmd_unpolarized_t
    contains
    ⟨Commands: cmd unpolarized: TBP⟩
  end type cmd_unpolarized_t

```

Output: we know only the number of particles.

```

⟨Commands: cmd polarized: TBP⟩≡
  procedure :: write => cmd_polarized_write

⟨Commands: cmd unpolarized: TBP⟩≡
  procedure :: write => cmd_unpolarized_write

⟨Commands: procedures⟩+≡
  subroutine cmd_polarized_write (cmd, unit, indent)
    class(cmd_polarized_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,1x,I0)") "polarized:", size (cmd%pn_pdg)
  end subroutine cmd_polarized_write

  subroutine cmd_unpolarized_write (cmd, unit, indent)
    class(cmd_unpolarized_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u

```

```

u = given_output_unit (unit); if (u < 0) return
call write_indent (u, indent)
write (u, "(1x,A,1x,I0)") "unpolarized:", size (cmd%pn_pdg)
end subroutine cmd_unpolarized_write

```

Compile: accounted for by the base command.

Execute: apply the modifications to the current model.

```

⟨Commands: cmd polarized: TBP⟩+≡
  procedure :: execute => cmd_polarized_execute

⟨Commands: cmd unpolarized: TBP⟩+≡
  procedure :: execute => cmd_unpolarized_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_polarized_execute (cmd, global)
    class(cmd_polarized_t), intent(inout) :: cmd
    type(rt_data_t), target, intent(inout) :: global
    type(var_list_t), pointer :: var_list
    type(pdg_array_t) :: pa
    integer :: pdg
    type(flavor_t) :: flv
    integer :: i
    var_list => cmd%local%get_var_list_ptr ()
    do i = 1, size (cmd%pn_pdg)
      pa = eval_pdg_array (cmd%pn_pdg(i)%ptr, var_list)
      if (pdg_array_get_length (pa) /= 1) &
        call msg_fatal ("Polarized: listed particles must be unique")
      pdg = pdg_array_get (pa, 1)
      call global%modify_particle (pdg, polarized = .true., &
        stable = .true., &
        isotropic_decay = .false., &
        diagonal_decay = .false.)
      call flv%init (pdg, cmd%local%model)
      call msg_message ("Particle " &
        // char (flv%get_name ()) &
        // " declared as polarized")
    end do
  end subroutine cmd_polarized_execute

  subroutine cmd_unpolarized_execute (cmd, global)
    class(cmd_unpolarized_t), intent(inout) :: cmd
    type(rt_data_t), target, intent(inout) :: global
    type(var_list_t), pointer :: var_list
    type(pdg_array_t) :: pa
    integer :: pdg
    type(flavor_t) :: flv
    integer :: i
    var_list => cmd%local%get_var_list_ptr ()
    do i = 1, size (cmd%pn_pdg)
      pa = eval_pdg_array (cmd%pn_pdg(i)%ptr, var_list)
      if (pdg_array_get_length (pa) /= 1) &
        call msg_fatal ("Unpolarized: listed particles must be unique")
      pdg = pdg_array_get (pa, 1)
      call global%modify_particle (pdg, polarized = .false., &
        stable = .true., &

```

```

        isotropic_decay = .false., &
        diagonal_decay = .false.)
    call flv%init (pdg, cmd%local%model)
    call msg_message ("Particle " &
        // char (flv%get_name ()) &
        // " declared as unpolarized")
end do
end subroutine cmd_unpolarized_execute

```

Parameters: formats for event-sample output

Specify all event formats that are to be used for output files in the subsequent simulation run. (The raw format is on by default and can be turned off here.)

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_sample_format_t
    private
    type(string_t), dimension(:), allocatable :: format
    contains
    ⟨Commands: cmd sample format: TBP⟩
end type cmd_sample_format_t

```

Output: here, everything is known.

```

⟨Commands: cmd sample format: TBP⟩≡
    procedure :: write => cmd_sample_format_write

⟨Commands: procedures⟩+≡
    subroutine cmd_sample_format_write (cmd, unit, indent)
    class(cmd_sample_format_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)", advance="no") "sample_format = "
    do i = 1, size (cmd%format)
        if (i > 1) write (u, "(A,1x)", advance="no") ", "
        write (u, "(A)", advance="no") char (cmd%format(i))
    end do
    write (u, "(A)")
end subroutine cmd_sample_format_write

```

Compile. Initialize evaluation trees.

```

⟨Commands: cmd sample format: TBP⟩+≡
    procedure :: compile => cmd_sample_format_compile

⟨Commands: procedures⟩+≡
    subroutine cmd_sample_format_compile (cmd, global)
    class(cmd_sample_format_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg
    type(parse_node_t), pointer :: pn_format
    integer :: i, n_format
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 3)

```

```

if (associated (pn_arg)) then
  n_format = parse_node_get_n_sub (pn_arg)
  allocate (cmd%format (n_format))
  pn_format => parse_node_get_sub_ptr (pn_arg)
  i = 0
  do while (associated (pn_format))
    i = i + 1
    cmd%format(i) = parse_node_get_string (pn_format)
    pn_format => parse_node_get_next_ptr (pn_format)
  end do
else
  allocate (cmd%format (0))
end if
end subroutine cmd_sample_format_compile

```

Execute. Transfer the list of format specifications to the corresponding array in the runtime data set.

```

⟨Commands: cmd sample format: TBP⟩+≡
  procedure :: execute => cmd_sample_format_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_sample_format_execute (cmd, global)
    class(cmd_sample_format_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    if (allocated (global%sample_fmt)) deallocate (global%sample_fmt)
    allocate (global%sample_fmt (size (cmd%format)), source = cmd%format)
  end subroutine cmd_sample_format_execute

```

The simulate command

This is the actual SINDARIN command.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_simulate_t
    ! not private anymore as required by the whizard-c-interface
    integer :: n_proc = 0
    type(string_t), dimension(:), allocatable :: process_id
  contains
    ⟨Commands: cmd simulate: TBP⟩
  end type cmd_simulate_t

```

Output: we know the process IDs.

```

⟨Commands: cmd simulate: TBP⟩≡
  procedure :: write => cmd_simulate_write

⟨Commands: procedures⟩+≡
  subroutine cmd_simulate_write (cmd, unit, indent)
    class(cmd_simulate_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)", advance="no") "simulate ("

```

```

do i = 1, cmd%n_proc
  if (i > 1) write (u, "(A,1x)", advance="no") " ,"
  write (u, "(A)", advance="no") char (cmd%process_id(i))
end do
write (u, "(A)") " )"
end subroutine cmd_simulate_write

```

Compile. In contrast to WHIZARD 1 the confusing option to give the number of unweighted events for weighted events as if unweighting were to take place has been abandoned. (We both use `n_events` for weighted and unweighted events, the variable `n_calls` from WHIZARD 1 has been discarded.

```

⟨Commands: cmd simulate: TBP⟩+≡
  procedure :: compile => cmd_simulate_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_simulate_compile (cmd, global)
    class(cmd_simulate_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_proclist, pn_proc
    integer :: i
    pn_proclist => parse_node_get_sub_ptr (cmd%pn, 2)
    cmd%pn_opt => parse_node_get_next_ptr (pn_proclist)
    call cmd%compile_options (global)
    cmd%n_proc = parse_node_get_n_sub (pn_proclist)
    allocate (cmd%process_id (cmd%n_proc))
    pn_proc => parse_node_get_sub_ptr (pn_proclist)
    do i = 1, cmd%n_proc
      cmd%process_id(i) = parse_node_get_string (pn_proc)
      call global%process_stack%init_result_vars (cmd%process_id(i))
      pn_proc => parse_node_get_next_ptr (pn_proc)
    end do
  end subroutine cmd_simulate_compile

```

Execute command: Simulate events. This is done via a `simulation_t` object and its associated methods.

Signal handling: the `generate` method may exit abnormally if there is a pending signal. The current logic ensures that the `es_array` output channels are closed before the `execute` routine returns. The program will terminate then in `command_list_execute`.

```

⟨Commands: cmd simulate: TBP⟩+≡
  procedure :: execute => cmd_simulate_execute

⟨Commands: procedures⟩+≡
  subroutine cmd_simulate_execute (cmd, global)
    class(cmd_simulate_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    type(rt_data_t), dimension(:), allocatable, target :: alt_env
    integer :: n_events
    type(simulation_t), target :: sim
    type(event_stream_array_t) :: es_array
    integer :: i, checkpoint, callback
    var_list => cmd%local%var_list

```



```

if (cmd%local%nlo_fixed_order) then
  call check_nlo_options (cmd%local)
end if
if (allocated (cmd%local%pn%alt_setup)) then
  allocate (alt_env (size (cmd%local%pn%alt_setup)))
  do i = 1, size (alt_env)
    call build_alt_setup (alt_env(i), cmd%local, &
      cmd%local%pn%alt_setup(i)%ptr)
  end do
  call sim%init (cmd%process_id, .true., .true., cmd%local, global, &
    alt_env)
else
  call sim%init (cmd%process_id, .true., .true., cmd%local, global)
end if
if (signal_is_pending ()) return
if (sim%is_valid ()) then
  call sim%init_process_selector ()
  call sim%setup_openmp ()
  call sim%compute_n_events (n_events)
  call sim%set_n_events_requested (n_events)
  call sim%activate_extra_logging ()
  call sim%prepare_event_streams (es_array)
  if (es_array%is_valid ()) then
    call sim%generate (es_array)
  else
    call sim%generate ()
  end if
  call es_array%final ()
  if (allocated (alt_env)) then
    do i = 1, size (alt_env)
      call alt_env(i)%local_final ()
    end do
  end if
end if
call sim%final ()
end subroutine cmd_simulate_execute

```

Build an alternative setup: the parse tree is stored in the global environment. We create a temporary command list to compile and execute this; the result is an alternative local environment `alt_env` which we can hand over to the `simulate` command.

(Commands: procedures)+≡

```

recursive subroutine build_alt_setup (alt_env, global, pn)
  type(rt_data_t), intent(inout), target :: alt_env
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), intent(in), target :: pn
  type(command_list_t), allocatable :: alt_options
  allocate (alt_options)
  call alt_env%local_init (global)
  call alt_env%activate ()
  call alt_options%compile (pn, alt_env)
  call alt_options%execute (alt_env)
  call alt_env%deactivate (global, keep_local = .true.)

```

```

        call alt_options%final ()
    end subroutine build_alt_setup

```

The rescan command

This is the actual SINDARIN command.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_rescan_t
    ! private
    type(parse_node_t), pointer :: pn_filename => null ()
    integer :: n_proc = 0
    type(string_t), dimension(:), allocatable :: process_id
    contains
    ⟨Commands: cmd rescan: TBP⟩
end type cmd_rescan_t

```

Output: we know the process IDs.

```

⟨Commands: cmd rescan: TBP⟩≡
    procedure :: write => cmd_rescan_write

⟨Commands: procedures⟩+≡
    subroutine cmd_rescan_write (cmd, unit, indent)
    class(cmd_rescan_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u, i
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A)", advance="no") "rescan ("
    do i = 1, cmd%n_proc
        if (i > 1) write (u, "(A,1x)", advance="no") " ,"
        write (u, "(A)", advance="no") char (cmd%process_id(i))
    end do
    write (u, "(A)") ")"
end subroutine cmd_rescan_write

```

Compile. The command takes a suffix argument, namely the file name of requested event file.

```

⟨Commands: cmd rescan: TBP⟩+≡
    procedure :: compile => cmd_rescan_compile

⟨Commands: procedures⟩+≡
    subroutine cmd_rescan_compile (cmd, global)
    class(cmd_rescan_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_filename, pn_proclist, pn_proc
    integer :: i
    pn_filename => parse_node_get_sub_ptr (cmd%pn, 2)
    pn_proclist => parse_node_get_next_ptr (pn_filename)
    cmd%pn_opt => parse_node_get_next_ptr (pn_proclist)
    call cmd%compile_options (global)
    cmd%pn_filename => pn_filename
    cmd%n_proc = parse_node_get_n_sub (pn_proclist)

```

```

allocate (cmd%process_id (cmd%n_proc))
pn_proc => parse_node_get_sub_ptr (pn_proclist)
do i = 1, cmd%n_proc
  cmd%process_id(i) = parse_node_get_string (pn_proc)
  pn_proc => parse_node_get_next_ptr (pn_proc)
end do
end subroutine cmd_rescan_compile

```

Execute command: Rescan events. This is done via a `simulation_t` object and its associated methods.

<Commands: cmd rescan: TBP>+≡

```

procedure :: execute => cmd_rescan_execute

```

<Commands: procedures>+≡

```

subroutine cmd_rescan_execute (cmd, global)
  class(cmd_rescan_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  type(rt_data_t), dimension(:), allocatable, target :: alt_env
  type(string_t) :: sample, sample_suffix
  logical :: exist, write_raw, update_event, update_sqme
  type(simulation_t), target :: sim
  type(event_sample_data_t) :: input_data, data
  type(string_t) :: input_sample
  integer :: n_fmt
  type(string_t), dimension(:), allocatable :: sample_fmt
  type(string_t) :: input_format, input_ext, input_file
  type(string_t) :: lhef_extension, extension_hepmc, extension_lcio
  type(event_stream_array_t) :: es_array
  integer :: i, n_events

```

<Commands: cmd rescan execute: extra variables>

```

  var_list => cmd%local%var_list
  if (allocated (cmd%local%pn%alt_setup)) then
    allocate (alt_env (size (cmd%local%pn%alt_setup)))
    do i = 1, size (alt_env)
      call build_alt_setup (alt_env(i), cmd%local, &
        cmd%local%pn%alt_setup(i)%ptr)
    end do
    call sim%init (cmd%process_id, .false., .false., cmd%local, global, &
      alt_env)
  else
    call sim%init (cmd%process_id, .false., .false., cmd%local, global)
  end if
  call sim%compute_n_events (n_events)
  input_sample = eval_string (cmd%pn_filename, var_list)
  input_format = var_list%get_sval (&
    var_str ("$_rescan_input_format"))
  sample_suffix = ""

```

<Commands: cmd rescan execute: extra init>

```

  sample = var_list%get_sval (var_str ("$_sample"))
  if (sample == "") then
    sample = sim%get_default_sample_name () // sample_suffix
  else
    sample = var_list%get_sval (var_str ("$_sample")) // sample_suffix
  end if

```

```

end if
write_raw = var_list%get_lval (var_str ("?write_raw"))
if (allocated (cmd%local%sample_fmt)) then
    n_fmt = size (cmd%local%sample_fmt)
else
    n_fmt = 0
end if
if (write_raw) then
    if (sample == input_sample) then
        call msg_error ("Rescan: ?write_raw = true: " &
            // "suppressing raw event output (filename clashes with input)")
        allocate (sample_fmt (n_fmt))
        if (n_fmt > 0) sample_fmt = cmd%local%sample_fmt
    else
        allocate (sample_fmt (n_fmt + 1))
        if (n_fmt > 0) sample_fmt (:n_fmt) = cmd%local%sample_fmt
        sample_fmt(n_fmt+1) = var_str ("raw")
    end if
else
    allocate (sample_fmt (n_fmt))
    if (n_fmt > 0) sample_fmt = cmd%local%sample_fmt
end if
update_event = &
    var_list%get_lval (var_str ("?update_event"))
update_sqme = &
    var_list%get_lval (var_str ("?update_sqme"))
if (update_event .or. update_sqme) then
    call msg_message ("Recalculating observables")
    if (update_sqme) then
        call msg_message ("Recalculating squared matrix elements")
    end if
end if
lhef_extension = &
    var_list%get_sval (var_str ("$lhef_extension"))
extension_hepmc = &
    var_list%get_sval (var_str ("$extension_hepmc"))
extension_lcio = &
    var_list%get_sval (var_str ("$extension_lcio"))
select case (char (input_format))
case ("raw"); input_ext = "evx"
    call cmd%local%set_log &
        (var_str ("?recover_beams"), .false., is_known=.true.)
case ("lhef"); input_ext = lhef_extension
case ("hepmc"); input_ext = extension_hepmc
case ("lcio"); input_ext = extension_lcio
case default
    call msg_fatal ("rescan: input sample format '" // char (input_format) &
        // "' not supported")
end select
input_file = input_sample // "." // input_ext
inquire (file = char (input_file), exist = exist)
if (exist) then
    input_data = sim%get_data (alt = .false.)
    input_data%n_evt = n_events

```

```

data = sim%get_data ()
data%n_evt = n_events
input_data%md5sum_cfg = ""
call es_array%init (sample, &
    sample_fmt, cmd%local, data, &
    input = input_format, input_sample = input_sample, &
    input_data = input_data, &
    allow_switch = .false.)
call sim%rescan (n_events, es_array, global = cmd%local)
call es_array%final ()
else
    call msg_fatal ("Rescan: event file '" &
        // char (input_file) // "' not found")
end if
if (allocated (alt_env)) then
    do i = 1, size (alt_env)
        call alt_env(i)%local_final ()
    end do
end if
call sim%final ()
end subroutine cmd_rescan_execute

```

MPI: Append rank id to sample name.

<Commands: cmd rescan execute: extra variables>≡

<MPI: Commands: cmd rescan execute: extra variables>≡

```

logical :: mpi_logging
integer :: rank, n_size

```

<Commands: cmd rescan execute: extra init>≡

<MPI: Commands: cmd rescan execute: extra init>≡

```

call mpi_get_comm_id (n_size, rank)
if (n_size > 1) then
    sample_suffix = var_str ("-") // str (rank)
end if
mpi_logging = (("vamp2" == char (var_list%get_sval (var_str ("integration_method")))) &
    & .and. (n_size > 1)) &
    & .or. var_list%get_lval (var_str ("mpi_logging")))
call mpi_set_logging (mpi_logging)

```

Parameters: number of iterations

Specify number of iterations and number of calls for one integration pass.

<Commands: types>+≡

```

type, extends (command_t) :: cmd_iterations_t
private
integer :: n_pass = 0
type(parse_node_p), dimension(:), allocatable :: pn_expr_n_it
type(parse_node_p), dimension(:), allocatable :: pn_expr_n_calls
type(parse_node_p), dimension(:), allocatable :: pn_sexpr_adapt
contains
<Commands: cmd iterations: TBP>
end type cmd_iterations_t

```

Output. Display the number of passes, which is known after compilation.

(Commands: cmd iterations: TBP)≡

```
procedure :: write => cmd_iterations_write
```

(Commands: procedures)+≡

```
subroutine cmd_iterations_write (cmd, unit, indent)
  class(cmd_iterations_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  select case (cmd%n_pass)
  case (0)
    write (u, "(1x,A)") "iterations: [empty]"
  case (1)
    write (u, "(1x,A,I0,A)") "iterations: ", cmd%n_pass, " pass"
  case default
    write (u, "(1x,A,I0,A)") "iterations: ", cmd%n_pass, " passes"
  end select
end subroutine cmd_iterations_write
```

Compile. Initialize evaluation trees.

(Commands: cmd iterations: TBP)+≡

```
procedure :: compile => cmd_iterations_compile
```

(Commands: procedures)+≡

```
subroutine cmd_iterations_compile (cmd, global)
  class(cmd_iterations_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_arg, pn_n_it, pn_n_calls, pn_adapt
  type(parse_node_t), pointer :: pn_it_spec, pn_calls_spec, pn_adapt_spec
  integer :: i
  pn_arg => parse_node_get_sub_ptr (cmd%pn, 3)
  if (associated (pn_arg)) then
    cmd%n_pass = parse_node_get_n_sub (pn_arg)
    allocate (cmd%pn_expr_n_it (cmd%n_pass))
    allocate (cmd%pn_expr_n_calls (cmd%n_pass))
    allocate (cmd%pn_sexpr_adapt (cmd%n_pass))
    pn_it_spec => parse_node_get_sub_ptr (pn_arg)
    i = 1
    do while (associated (pn_it_spec))
      pn_n_it => parse_node_get_sub_ptr (pn_it_spec)
      pn_calls_spec => parse_node_get_next_ptr (pn_n_it)
      pn_n_calls => parse_node_get_sub_ptr (pn_calls_spec, 2)
      pn_adapt_spec => parse_node_get_next_ptr (pn_calls_spec)
      if (associated (pn_adapt_spec)) then
        pn_adapt => parse_node_get_sub_ptr (pn_adapt_spec, 2)
      else
        pn_adapt => null ()
      end if
      cmd%pn_expr_n_it(i)%ptr => pn_n_it
      cmd%pn_expr_n_calls(i)%ptr => pn_n_calls
      cmd%pn_sexpr_adapt(i)%ptr => pn_adapt
      i = i + 1
    end do
  end if
end subroutine cmd_iterations_compile
```

```

        pn_it_spec => parse_node_get_next_ptr (pn_it_spec)
    end do
else
    allocate (cmd%pn_expr_n_it (0))
    allocate (cmd%pn_expr_n_calls (0))
end if
end subroutine cmd_iterations_compile

```

Execute. Evaluate the trees and transfer the results to the iteration list in the runtime data set.

<Commands: cmd iterations: TBP>+≡

```

    procedure :: execute => cmd_iterations_execute

```

<Commands: procedures>+≡

```

subroutine cmd_iterations_execute (cmd, global)
    class(cmd_iterations_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(var_list_t), pointer :: var_list
    integer, dimension(cmd%n_pass) :: n_it, n_calls
    logical, dimension(cmd%n_pass) :: custom_adapt
    type(string_t), dimension(cmd%n_pass) :: adapt_code
    integer :: i
    var_list => global%get_var_list_ptr ()
    do i = 1, cmd%n_pass
        n_it(i) = eval_int (cmd%pn_expr_n_it(i)%ptr, var_list)
        n_calls(i) = &
            eval_int (cmd%pn_expr_n_calls(i)%ptr, var_list)
        if (associated (cmd%pn_sexpr_adapt(i)%ptr)) then
            adapt_code(i) = &
                eval_string (cmd%pn_sexpr_adapt(i)%ptr, &
                    var_list, is_known = custom_adapt(i))
        else
            custom_adapt(i) = .false.
        end if
    end do
    call global%it_list%init (n_it, n_calls, custom_adapt, adapt_code)
end subroutine cmd_iterations_execute

```

Range expressions

We need a special type for storing and evaluating range expressions.

<Commands: parameters>+≡

```

    integer, parameter :: STEP_NONE = 0
    integer, parameter :: STEP_ADD = 1
    integer, parameter :: STEP_SUB = 2
    integer, parameter :: STEP_MUL = 3
    integer, parameter :: STEP_DIV = 4
    integer, parameter :: STEP_COMP_ADD = 11
    integer, parameter :: STEP_COMP_MUL = 13

```

There is an abstract base type and two implementations: scan over integers and scan over reals.

<Commands: types>+≡

```

type, abstract :: range_t
  type(parse_node_t), pointer :: pn_expr => null ()
  type(parse_node_t), pointer :: pn_term => null ()
  type(parse_node_t), pointer :: pn_factor => null ()
  type(parse_node_t), pointer :: pn_value => null ()
  type(parse_node_t), pointer :: pn_literal => null ()
  type(parse_node_t), pointer :: pn_beg => null ()
  type(parse_node_t), pointer :: pn_end => null ()
  type(parse_node_t), pointer :: pn_step => null ()
  type(eval_tree_t) :: expr_beg
  type(eval_tree_t) :: expr_end
  type(eval_tree_t) :: expr_step
  integer :: step_mode = 0
  integer :: n_step = 0
contains
  <Commands: range: TBP>
end type range_t

```

These are the implementations:

```

<Commands: types>+≡
  type, extends (range_t) :: range_int_t
    integer :: i_beg = 0
    integer :: i_end = 0
    integer :: i_step = 0
  contains
    <Commands: range int: TBP>
  end type range_int_t

  type, extends (range_t) :: range_real_t
    real(default) :: r_beg = 0
    real(default) :: r_end = 0
    real(default) :: r_step = 0
    real(default) :: lr_beg = 0
    real(default) :: lr_end = 0
    real(default) :: lr_step = 0
  contains
    <Commands: range real: TBP>
  end type range_real_t

```

Finalize the allocated dummy node. The other nodes are just pointers.

```

<Commands: range: TBP>≡
  procedure :: final => range_final

<Commands: procedures>+≡
  subroutine range_final (object)
    class(range_t), intent(inout) :: object
    if (associated (object%pn_expr)) then
      call parse_node_final (object%pn_expr, recursive = .false.)
      call parse_node_final (object%pn_term, recursive = .false.)
      call parse_node_final (object%pn_factor, recursive = .false.)
      call parse_node_final (object%pn_value, recursive = .false.)
      call parse_node_final (object%pn_literal, recursive = .false.)
    deallocate (object%pn_expr)
    deallocate (object%pn_term)
  end subroutine range_final

```



```

        deallocate (object%pn_factor)
        deallocate (object%pn_value)
        deallocate (object%pn_literal)
    end if
end subroutine range_final

```

Output.

```

<Commands: range: TBP>+≡
    procedure (range_write), deferred :: write
    procedure :: base_write => range_write

<Commands: range int: TBP>≡
    procedure :: write => range_int_write

<Commands: range real: TBP>≡
    procedure :: write => range_real_write

<Commands: procedures>+≡
    subroutine range_write (object, unit)
        class(range_t), intent(in) :: object
        integer, intent(in), optional :: unit
        integer :: u
        u = given_output_unit (unit)
        write (u, "(1x,A)") "Range specification:"
        if (associated (object%pn_expr)) then
            write (u, "(1x,A)") "Dummy value:"
            call parse_node_write_rec (object%pn_expr, u)
        end if
        if (associated (object%pn_beg)) then
            write (u, "(1x,A)") "Initial value:"
            call parse_node_write_rec (object%pn_beg, u)
            call object%expr_beg%write (u)
        end if
        if (associated (object%pn_end)) then
            write (u, "(1x,A)") "Final value:"
            call parse_node_write_rec (object%pn_end, u)
            call object%expr_end%write (u)
        end if
        if (associated (object%pn_step)) then
            write (u, "(1x,A)") "Step value:"
            call parse_node_write_rec (object%pn_step, u)
            select case (object%step_mode)
            case (STEP_ADD); write (u, "(1x,A)") "Step mode: +"
            case (STEP_SUB); write (u, "(1x,A)") "Step mode: -"
            case (STEP_MUL); write (u, "(1x,A)") "Step mode: *"
            case (STEP_DIV); write (u, "(1x,A)") "Step mode: /"
            case (STEP_COMP_ADD); write (u, "(1x,A)") "Division mode: +"
            case (STEP_COMP_MUL); write (u, "(1x,A)") "Division mode: *"
            end select
        end if
    end if
end if
else
    write (u, "(1x,A)") "Expressions: [undefined]"
end if
end subroutine range_write

subroutine range_int_write (object, unit)

```

```

class(range_int_t), intent(in) :: object
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit)
call object%base_write (unit)
write (u, "(1x,A)") "Range parameters:"
write (u, "(3x,A,I0)") "i_beg = ", object%i_beg
write (u, "(3x,A,I0)") "i_end = ", object%i_end
write (u, "(3x,A,I0)") "i_step = ", object%i_step
write (u, "(3x,A,I0)") "n_step = ", object%n_step
end subroutine range_int_write

subroutine range_real_write (object, unit)
class(range_real_t), intent(in) :: object
integer, intent(in), optional :: unit
integer :: u
u = given_output_unit (unit)
call object%base_write (unit)
write (u, "(1x,A)") "Range parameters:"
write (u, "(3x,A," // FMT_19 // ")") "r_beg = ", object%r_beg
write (u, "(3x,A," // FMT_19 // ")") "r_end = ", object%r_end
write (u, "(3x,A," // FMT_19 // ")") "r_step = ", object%r_end
write (u, "(3x,A,I0)") "n_step = ", object%n_step
end subroutine range_real_write

```

Initialize, given a range expression parse node. This is common to the implementations.

<Commands: range: TBP>+≡

```
procedure :: init => range_init
```

<Commands: procedures>+≡

```

subroutine range_init (range, pn)
class(range_t), intent(out) :: range
type(parse_node_t), intent(in), target :: pn
type(parse_node_t), pointer :: pn_spec, pn_end, pn_step_spec, pn_op
select case (char (parse_node_get_rule_key (pn)))
case ("expr")
case ("range_expr")
range%pn_beg => parse_node_get_sub_ptr (pn)
pn_spec => parse_node_get_next_ptr (range%pn_beg)
if (associated (pn_spec)) then
pn_end => parse_node_get_sub_ptr (pn_spec, 2)
range%pn_end => pn_end
pn_step_spec => parse_node_get_next_ptr (pn_end)
if (associated (pn_step_spec)) then
pn_op => parse_node_get_sub_ptr (pn_step_spec)
range%pn_step => parse_node_get_next_ptr (pn_op)
select case (char (parse_node_get_rule_key (pn_op)))
case ("/+"); range%step_mode = STEP_ADD
case ("/-"); range%step_mode = STEP_SUB
case ("/*"); range%step_mode = STEP_MUL
case ("//"); range%step_mode = STEP_DIV
case ("/+/" ); range%step_mode = STEP_COMP_ADD
case ("/*/"); range%step_mode = STEP_COMP_MUL

```

```

        case default
            call range%write ()
            call msg_bug ("Range: step mode not implemented")
        end select
    else
        range%step_mode = STEP_ADD
    end if
else
    range%step_mode = STEP_NONE
end if
call range%create_value_node ()
case default
    call msg_bug ("range expression: node type '" &
        // char (parse_node_get_rule_key (pn)) &
        // "' not implemented")
end select
end subroutine range_init

```

This method manually creates a parse node (actually, a cascade of parse nodes) that hold a constant value as a literal. The idea is that this node is inserted as the right-hand side of a fake variable assignment, which is prepended to each scan iteration. Before the variable assignment is compiled and executed, we can manually reset the value of the literal and thus pretend that the loop variable is assigned this value.

<Commands: range: TBP>+≡

```
procedure :: create_value_node => range_create_value_node
```

<Commands: procedures>+≡

```

subroutine range_create_value_node (range)
    class(range_t), intent(inout) :: range
    allocate (range%pn_literal)
    allocate (range%pn_value)
    select type (range)
    type is (range_int_t)
        call parse_node_create_value (range%pn_literal, &
            syntax_get_rule_ptr (syntax_cmd_list, var_str ("integer_literal")), &
            ival = 0)
        call parse_node_create_branch (range%pn_value, &
            syntax_get_rule_ptr (syntax_cmd_list, var_str ("integer_value")))
    type is (range_real_t)
        call parse_node_create_value (range%pn_literal, &
            syntax_get_rule_ptr (syntax_cmd_list, var_str ("real_literal")), &
            rval = 0._default)
        call parse_node_create_branch (range%pn_value, &
            syntax_get_rule_ptr (syntax_cmd_list, var_str ("real_value")))
    class default
        call msg_bug ("range: create value node: type not implemented")
    end select
    call parse_node_append_sub (range%pn_value, range%pn_literal)
    call parse_node_freeze_branch (range%pn_value)
    allocate (range%pn_factor)
    call parse_node_create_branch (range%pn_factor, &
        syntax_get_rule_ptr (syntax_cmd_list, var_str ("factor")))
    call parse_node_append_sub (range%pn_factor, range%pn_value)

```

```

call parse_node_freeze_branch (range%pn_factor)
allocate (range%pn_term)
call parse_node_create_branch (range%pn_term, &
    syntax_get_rule_ptr (syntax_cmd_list, var_str ("term")))
call parse_node_append_sub (range%pn_term, range%pn_factor)
call parse_node_freeze_branch (range%pn_term)
allocate (range%pn_expr)
call parse_node_create_branch (range%pn_expr, &
    syntax_get_rule_ptr (syntax_cmd_list, var_str ("expr")))
call parse_node_append_sub (range%pn_expr, range%pn_term)
call parse_node_freeze_branch (range%pn_expr)
end subroutine range_create_value_node

```

Compile, given an environment.

```

⟨Commands: range: TBP⟩+≡
    procedure :: compile => range_compile

⟨Commands: procedures⟩+≡
    subroutine range_compile (range, global)
        class(range_t), intent(inout) :: range
        type(rt_data_t), intent(in), target :: global
        type(var_list_t), pointer :: var_list
        var_list => global%get_var_list_ptr ()
        if (associated (range%pn_beg)) then
            call range%expr_beg%init_expr (range%pn_beg, var_list)
            if (associated (range%pn_end)) then
                call range%expr_end%init_expr (range%pn_end, var_list)
                if (associated (range%pn_step)) then
                    call range%expr_step%init_expr (range%pn_step, var_list)
                end if
            end if
        end if
    end if
end subroutine range_compile

```

Evaluate: compute the actual bounds and parameters that determine the values that we can iterate.

This is implementation-specific.

```

⟨Commands: range: TBP⟩+≡
    procedure (range_evaluate), deferred :: evaluate

⟨Commands: interfaces⟩+≡
    abstract interface
        subroutine range_evaluate (range)
            import
            class(range_t), intent(inout) :: range
        end subroutine range_evaluate
    end interface

```

The version for an integer variable. If the step is subtractive, we invert the sign and treat it as an additive step. For a multiplicative step, the step must be greater than one, and the initial and final values must be of same sign and strictly ordered. Analogously for a division step.

```

⟨Commands: range int: TBP⟩+≡

```

```

procedure :: evaluate => range_int_evaluate
(Commands: procedures) +=
subroutine range_int_evaluate (range)
class(range_int_t), intent(inout) :: range
integer :: ival
if (associated (range%pn_beg)) then
call range%expr_beg%evaluate ()
if (range%expr_beg%is_known ()) then
range%i_beg = range%expr_beg%get_int ()
else
call range%write ()
call msg_fatal &
("Range expression: initial value evaluates to unknown")
end if
if (associated (range%pn_end)) then
call range%expr_end%evaluate ()
if (range%expr_end%is_known ()) then
range%i_end = range%expr_end%get_int ()
if (associated (range%pn_step)) then
call range%expr_step%evaluate ()
if (range%expr_step%is_known ()) then
range%i_step = range%expr_step%get_int ()
select case (range%step_mode)
case (STEP_SUB); range%i_step = - range%i_step
end select
else
call range%write ()
call msg_fatal &
("Range expression: step value evaluates to unknown")
end if
else
range%i_step = 1
end if
else
call range%write ()
call msg_fatal &
("Range expression: final value evaluates to unknown")
end if
else
range%i_end = range%i_beg
range%i_step = 1
end if
select case (range%step_mode)
case (STEP_NONE)
range%n_step = 1
case (STEP_ADD, STEP_SUB)
if (range%i_step /= 0) then
if (range%i_beg == range%i_end) then
range%n_step = 1
else if (sign (1, range%i_end - range%i_beg) &
== sign (1, range%i_step)) then
range%n_step = (range%i_end - range%i_beg) / range%i_step + 1
else
range%n_step = 0

```

```

        end if
    else
        call msg_fatal ("range evaluation (add): step value is zero")
    end if
case (STEP_MUL)
    if (range%i_step > 1) then
        if (range%i_beg == range%i_end) then
            range%n_step = 1
        else if (range%i_beg == 0) then
            call msg_fatal ("range evaluation (mul): initial value is zero")
        else if (sign (1, range%i_beg) == sign (1, range%i_end) &
            .and. abs (range%i_beg) < abs (range%i_end)) then
            range%n_step = 0
            ival = range%i_beg
            do while (abs (ival) <= abs (range%i_end))
                range%n_step = range%n_step + 1
                ival = ival * range%i_step
            end do
        else
            range%n_step = 0
        end if
    else
        call msg_fatal &
            ("range evaluation (mult): step value is one or less")
    end if
case (STEP_DIV)
    if (range%i_step > 1) then
        if (range%i_beg == range%i_end) then
            range%n_step = 1
        else if (sign (1, range%i_beg) == sign (1, range%i_end) &
            .and. abs (range%i_beg) > abs (range%i_end)) then
            range%n_step = 0
            ival = range%i_beg
            do while (abs (ival) >= abs (range%i_end))
                range%n_step = range%n_step + 1
                if (ival == 0) exit
                ival = ival / range%i_step
            end do
        else
            range%n_step = 0
        end if
    else
        call msg_fatal &
            ("range evaluation (div): step value is one or less")
    end if
case (STEP_COMP_ADD)
    call msg_fatal ("range evaluation: &
        &step mode /+/ not allowed for integer variable")
case (STEP_COMP_MUL)
    call msg_fatal ("range evaluation: &
        &step mode /*/ not allowed for integer variable")
case default
    call range%write ()
    call msg_bug ("range evaluation: step mode not implemented")

```



```

        range%r_step = 1
    end if
    select case (range%step_mode)
    case (STEP_NONE)
        range%n_step = 1
    case (STEP_ADD, STEP_SUB)
        if (range%r_step /= 0) then
            if (sign (1._default, range%r_end - range%r_beg) &
                == sign (1._default, range%r_step)) then
                range%n_step = &
                    nint ((range%r_end - range%r_beg) / range%r_step + 1)
            else
                range%n_step = 0
            end if
        else
            call msg_fatal ("range evaluation (add): step value is zero")
        end if
    case (STEP_MUL)
        if (range%r_step > 1) then
            if (range%r_beg == 0 .or. range%r_end == 0) then
                call msg_fatal ("range evaluation (mul): bound is zero")
            else if (sign (1._default, range%r_beg) &
                == sign (1._default, range%r_end) &
                .and. abs (range%r_beg) <= abs (range%r_end)) then
                range%lr_beg = log (abs (range%r_beg))
                range%lr_end = log (abs (range%r_end))
                range%lr_step = log (range%r_step)
                range%n_step = nint &
                    (abs ((range%lr_end - range%lr_beg) / range%lr_step) + 1)
            else
                range%n_step = 0
            end if
        else
            call msg_fatal &
                ("range evaluation (mult): step value is one or less")
        end if
    case (STEP_DIV)
        if (range%r_step > 1) then
            if (range%r_beg == 0 .or. range%r_end == 0) then
                call msg_fatal ("range evaluation (div): bound is zero")
            else if (sign (1._default, range%r_beg) &
                == sign (1._default, range%r_end) &
                .and. abs (range%r_beg) >= abs (range%r_end)) then
                range%lr_beg = log (abs (range%r_beg))
                range%lr_end = log (abs (range%r_end))
                range%lr_step = -log (range%r_step)
                range%n_step = nint &
                    (abs ((range%lr_end - range%lr_beg) / range%lr_step) + 1)
            else
                range%n_step = 0
            end if
        else
            call msg_fatal &
                ("range evaluation (mult): step value is one or less")
        end if
    end select
end if

```



```

        end if
    case (STEP_COMP_ADD)
        ! Number of steps already known
    case (STEP_COMP_MUL)
        ! Number of steps already known
        if (range%r_beg == 0 .or. range%r_end == 0) then
            call msg_fatal ("range evaluation (mul): bound is zero")
        else if (sign (1._default, range%r_beg) &
            == sign (1._default, range%r_end)) then
            range%lr_beg = log (abs (range%r_beg))
            range%lr_end = log (abs (range%r_end))
        else
            range%n_step = 0
        end if
    case default
        call range%write ()
        call msg_bug ("range evaluation: step mode not implemented")
    end select
end if
end subroutine range_real_evaluate

```

Return the number of iterations:

```

<Commands: range: TBP>+≡
    procedure :: get_n_iterations => range_get_n_iterations

<Commands: procedures>+≡
    function range_get_n_iterations (range) result (n)
        class(range_t), intent(in) :: range
        integer :: n
        n = range%n_step
    end function range_get_n_iterations

```

Compute the value for iteration i and store it in the embedded token.

```

<Commands: range: TBP>+≡
    procedure (range_set_value), deferred :: set_value

<Commands: interfaces>+≡
    abstract interface
        subroutine range_set_value (range, i)
            import
            class(range_t), intent(inout) :: range
            integer, intent(in) :: i
        end subroutine range_set_value
    end interface

```

In the integer case, we compute the value directly for additive step. For multiplicative step, we perform a loop in the same way as above, where the number of iteration was determined.

```

<Commands: range int: TBP>+≡
    procedure :: set_value => range_int_set_value

```

```

<Commands: procedures>+≡
subroutine range_int_set_value (range, i)
  class(range_int_t), intent(inout) :: range
  integer, intent(in) :: i
  integer :: k, ival
  select case (range%step_mode)
  case (STEP_NONE)
    ival = range%i_beg
  case (STEP_ADD, STEP_SUB)
    ival = range%i_beg + (i - 1) * range%i_step
  case (STEP_MUL)
    ival = range%i_beg
    do k = 1, i - 1
      ival = ival * range%i_step
    end do
  case (STEP_DIV)
    ival = range%i_beg
    do k = 1, i - 1
      ival = ival / range%i_step
    end do
  case default
    call range%write ()
    call msg_bug ("range iteration: step mode not implemented")
  end select
  call parse_node_set_value (range%pn_literal, ival = ival)
end subroutine range_int_set_value

```

In the integer case, we compute the value directly for additive step. For multiplicative step, we perform a loop in the same way as above, where the number of iteration was determined.

```

<Commands: range real: TBP>+≡
procedure :: set_value => range_real_set_value

<Commands: procedures>+≡
subroutine range_real_set_value (range, i)
  class(range_real_t), intent(inout) :: range
  integer, intent(in) :: i
  real(default) :: rval, x
  select case (range%step_mode)
  case (STEP_NONE)
    rval = range%r_beg
  case (STEP_ADD, STEP_SUB, STEP_COMP_ADD)
    if (range%n_step > 1) then
      x = real (i - 1, default) / (range%n_step - 1)
    else
      x = 1._default / 2
    end if
    rval = x * range%r_end + (1 - x) * range%r_beg
  case (STEP_MUL, STEP_DIV, STEP_COMP_MUL)
    if (range%n_step > 1) then
      x = real (i - 1, default) / (range%n_step - 1)
    else
      x = 1._default / 2
    end if

```

```

        rval = sign &
            (exp (x * range%lr_end + (1 - x) * range%lr_beg), range%r_beg)
    case default
        call range%write ()
        call msg_bug ("range iteration: step mode not implemented")
    end select
    call parse_node_set_value (range%pn_literal, rval = rval)
end subroutine range_real_set_value

```

Scan over parameters and other objects

The scan command allocates a new parse node for the variable assignment (the lhs). The rhs of this parse node is assigned from the available rhs expressions in the scan list, one at a time, so the compiled parse node can be prepended to the scan body.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_scan_t
    private
    type(string_t) :: name
    integer :: n_values = 0
    type(parse_node_p), dimension(:), allocatable :: scan_cmd
    class(range_t), dimension(:), allocatable :: range
    contains
    <Commands: cmd scan: TBP>
end type cmd_scan_t

```

Finalizer.

The auxiliary parse nodes that we have constructed have to be treated carefully: the embedded pointers all point to persistent objects somewhere else and should not be finalized, so we should not call the finalizer recursively.

```

<Commands: cmd scan: TBP>≡
    procedure :: final => cmd_scan_final

<Commands: procedures>+≡
    recursive subroutine cmd_scan_final (cmd)
    class(cmd_scan_t), intent(inout) :: cmd
    type(parse_node_t), pointer :: pn_var_single, pn_decl_single
    type(string_t) :: key
    integer :: i
    if (allocated (cmd%scan_cmd)) then
        do i = 1, size (cmd%scan_cmd)
            pn_var_single => parse_node_get_sub_ptr (cmd%scan_cmd(i)%ptr)
            key = parse_node_get_rule_key (pn_var_single)
            select case (char (key))
            case ("scan_string_decl", "scan_log_decl")
                pn_decl_single => parse_node_get_sub_ptr (pn_var_single, 2)
                call parse_node_final (pn_decl_single, recursive=.false.)
                deallocate (pn_decl_single)
            end select
            call parse_node_final (pn_var_single, recursive=.false.)
            deallocate (pn_var_single)
        end do
    end if
end subroutine cmd_scan_final

```

```

        deallocate (cmd%scan_cmd)
    end if
    if (allocated (cmd%range)) then
        do i = 1, size (cmd%range)
            call cmd%range(i)%final ()
        end do
    end if
end subroutine cmd_scan_final

```

Output.

```

⟨Commands: cmd scan: TBP⟩+≡
    procedure :: write => cmd_scan_write

⟨Commands: procedures⟩+≡
    subroutine cmd_scan_write (cmd, unit, indent)
        class(cmd_scan_t), intent(in) :: cmd
        integer, intent(in), optional :: unit, indent
        integer :: u
        u = given_output_unit (unit); if (u < 0) return
        call write_indent (u, indent)
        write (u, "(1x,A,1x,A,1x,'(',I0,')')") "scan:", char (cmd%name), &
            cmd%n_values
    end subroutine cmd_scan_write

```

Compile the scan command. We construct a new parse node that implements the variable assignment for a single element on the rhs, instead of the whole list that we get from the original parse tree. By simply copying the node, we copy all pointers and inherit the targets from the original. During execution, we should replace the rhs by the stored rhs pointers (the list elements), one by one, then (re)compile the redefined node.

```

⟨Commands: cmd scan: TBP⟩+≡
    procedure :: compile => cmd_scan_compile

⟨Commands: procedures⟩+≡
    recursive subroutine cmd_scan_compile (cmd, global)
        class(cmd_scan_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        type(parse_node_t), pointer :: pn_var, pn_body, pn_body_first
        type(parse_node_t), pointer :: pn_decl, pn_name
        type(parse_node_t), pointer :: pn_arg, pn_scan_cmd, pn_rhs
        type(parse_node_t), pointer :: pn_decl_single, pn_var_single
        type(syntax_rule_t), pointer :: var_rule_decl, var_rule
        type(string_t) :: key
        integer :: var_type
        integer :: i
        if (debug_on) call msg_debug (D_CORE, "cmd_scan_compile")
        if (debug_active (D_CORE)) call parse_node_write_rec (cmd%pn)
        pn_var => parse_node_get_sub_ptr (cmd%pn, 2)
        pn_body => parse_node_get_next_ptr (pn_var)
        if (associated (pn_body)) then
            pn_body_first => parse_node_get_sub_ptr (pn_body)
        else

```

```

        pn_body_first => null ()
    end if
    key = parse_node_get_rule_key (pn_var)
    select case (char (key))
    case ("scan_num")
        pn_name => parse_node_get_sub_ptr (pn_var)
        cmd%name = parse_node_get_string (pn_name)
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_num"))
        pn_arg => parse_node_get_next_ptr (pn_name, 2)
    case ("scan_int")
        pn_name => parse_node_get_sub_ptr (pn_var, 2)
        cmd%name = parse_node_get_string (pn_name)
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_int"))
        pn_arg => parse_node_get_next_ptr (pn_name, 2)
    case ("scan_real")
        pn_name => parse_node_get_sub_ptr (pn_var, 2)
        cmd%name = parse_node_get_string (pn_name)
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_real"))
        pn_arg => parse_node_get_next_ptr (pn_name, 2)
    case ("scan_complex")
        pn_name => parse_node_get_sub_ptr (pn_var, 2)
        cmd%name = parse_node_get_string (pn_name)
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_complex"))
        pn_arg => parse_node_get_next_ptr (pn_name, 2)
    case ("scan_alias")
        pn_name => parse_node_get_sub_ptr (pn_var, 2)
        cmd%name = parse_node_get_string (pn_name)
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, var_str ("cmd_alias"))
        pn_arg => parse_node_get_next_ptr (pn_name, 2)
    case ("scan_string_decl")
        pn_decl => parse_node_get_sub_ptr (pn_var, 2)
        pn_name => parse_node_get_sub_ptr (pn_decl, 2)
        cmd%name = parse_node_get_string (pn_name)
        var_rule_decl => syntax_get_rule_ptr (syntax_cmd_list, &
            var_str ("cmd_string"))
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
            var_str ("cmd_string_decl"))
        pn_arg => parse_node_get_next_ptr (pn_name, 2)
    case ("scan_log_decl")
        pn_decl => parse_node_get_sub_ptr (pn_var, 2)
        pn_name => parse_node_get_sub_ptr (pn_decl, 2)
        cmd%name = parse_node_get_string (pn_name)
        var_rule_decl => syntax_get_rule_ptr (syntax_cmd_list, &
            var_str ("cmd_log"))
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
            var_str ("cmd_log_decl"))
        pn_arg => parse_node_get_next_ptr (pn_name, 2)
    case ("scan_cuts")
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
            var_str ("cmd_cuts"))
        cmd%name = "cuts"
        pn_arg => parse_node_get_sub_ptr (pn_var, 3)
    case ("scan_weight")
        var_rule => syntax_get_rule_ptr (syntax_cmd_list, &

```

```

        var_str ("cmd_weight"))
    cmd%name = "weight"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_scale")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_scale"))
    cmd%name = "scale"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_ren_scale")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_ren_scale"))
    cmd%name = "renormalization_scale"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_fac_scale")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_fac_scale"))
    cmd%name = "factorization_scale"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_selection")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_selection"))
    cmd%name = "selection"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_reweight")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_reweight"))
    cmd%name = "reweight"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_analysis")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_analysis"))
    cmd%name = "analysis"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_model")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_model"))
    cmd%name = "model"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case ("scan_library")
    var_rule => syntax_get_rule_ptr (syntax_cmd_list, &
        var_str ("cmd_library"))
    cmd%name = "library"
    pn_arg => parse_node_get_sub_ptr (pn_var, 3)
case default
    call msg_bug ("scan: case ' " // char (key) // "' not implemented")
end select
if (associated (pn_arg)) then
    cmd%n_values = parse_node_get_n_sub (pn_arg)
end if
var_list => global%get_var_list_ptr ()
allocate (cmd%scan_cmd (cmd%n_values))
select case (char (key))
case ("scan_num")
    var_type = &

```

```

        var_list%get_type (cmd%name)
select case (var_type)
case (V_INT)
    allocate (range_int_t :: cmd%range (cmd%n_values))
case (V_REAL)
    allocate (range_real_t :: cmd%range (cmd%n_values))
case (V_CMPLX)
    call msg_fatal ("scan over complex variable not implemented")
case (V_NONE)
    call msg_fatal ("scan: variable '" // char (cmd%name) //" ' undefined")
case default
    call msg_bug ("scan: impossible variable type")
end select
case ("scan_int")
    allocate (range_int_t :: cmd%range (cmd%n_values))
case ("scan_real")
    allocate (range_real_t :: cmd%range (cmd%n_values))
case ("scan_complex")
    call msg_fatal ("scan over complex variable not implemented")
end select
i = 1
if (associated (pn_arg)) then
    pn_rhs => parse_node_get_sub_ptr (pn_arg)
else
    pn_rhs => null ()
end if
do while (associated (pn_rhs))
    allocate (pn_scan_cmd)
    call parse_node_create_branch (pn_scan_cmd, &
        syntax_get_rule_ptr (syntax_cmd_list, var_str ("command_list")))
    allocate (pn_var_single)
    pn_var_single = pn_var
    call parse_node_replace_rule (pn_var_single, var_rule)
    select case (char (key))
    case ("scan_num", "scan_int", "scan_real", &
        "scan_complex", "scan_alias", &
        "scan_cuts", "scan_weight", &
        "scan_scale", "scan_ren_scale", "scan_fac_scale", &
        "scan_selection", "scan_reweight", "scan_analysis", &
        "scan_model", "scan_library")
        if (allocated (cmd%range)) then
            call cmd%range(i)%init (pn_rhs)
            call parse_node_replace_last_sub &
                (pn_var_single, cmd%range(i)%pn_expr)
        else
            call parse_node_replace_last_sub (pn_var_single, pn_rhs)
        end if
    case ("scan_string_decl", "scan_log_decl")
        allocate (pn_decl_single)
        pn_decl_single = pn_decl
        call parse_node_replace_rule (pn_decl_single, var_rule_decl)
        call parse_node_replace_last_sub (pn_decl_single, pn_rhs)
        call parse_node_freeze_branch (pn_decl_single)
        call parse_node_replace_last_sub (pn_var_single, pn_decl_single)
    end select
end do

```

```

case default
  call msg_bug ("scan: case '" // char (key) &
    // "' broken")
end select
call parse_node_freeze_branch (pn_var_single)
call parse_node_append_sub (pn_scan_cmd, pn_var_single)
call parse_node_append_sub (pn_scan_cmd, pn_body_first)
call parse_node_freeze_branch (pn_scan_cmd)
cmd%scan_cmd(i)%ptr => pn_scan_cmd
i = i + 1
pn_rhs => parse_node_get_next_ptr (pn_rhs)
end do
if (debug_active (D_CORE)) then
  do i = 1, cmd%n_values
    print *, "scan command ", i
    call parse_node_write_rec (cmd%scan_cmd(i)%ptr)
    if (allocated (cmd%range)) call cmd%range(i)%write ()
  end do
  print *, "original"
  call parse_node_write_rec (cmd%pn)
end if
end subroutine cmd_scan_compile

```

Execute the loop for all values in the step list. We use the parse trees with single variable assignment that we have stored, to iteratively create a local environment, execute the stored commands, and destroy it again. When we encounter a range object, we execute the commands for each value that this object provides. Computing this value has the side effect of modifying the rhs of the variable assignment that heads the local command list, directly in the local parse tree.

(Commands: cmd scan: TBP)+≡

```
procedure :: execute => cmd_scan_execute
```

(Commands: procedures)+≡

```

recursive subroutine cmd_scan_execute (cmd, global)
  class(cmd_scan_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(rt_data_t), allocatable :: local
  integer :: i, j
  do i = 1, cmd%n_values
    if (allocated (cmd%range)) then
      call cmd%range(i)%compile (global)
      call cmd%range(i)%evaluate ()
      do j = 1, cmd%range(i)%get_n_iterations ()
        call cmd%range(i)%set_value (j)
        allocate (local)
        call build_alt_setup (local, global, cmd%scan_cmd(i)%ptr)
        call local%local_final ()
        deallocate (local)
      end do
    else
      allocate (local)
      call build_alt_setup (local, global, cmd%scan_cmd(i)%ptr)
      call local%local_final ()
    end if
  end do
end subroutine cmd_scan_execute

```



```

        deallocate (local)
    end if
end do
end subroutine cmd_scan_execute

```

Conditionals

Conditionals are implemented as a list that is compiled and evaluated recursively; this allows for a straightforward representation of `else if` constructs. A `cmd_if_t` object can hold either an `else_if` clause which is another object of this type, or an `else_body`, but not both.

If- or else-bodies are no scoping units, so all data remain global and no copy-in copy-out is needed.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_if_t
    private
        type(parse_node_t), pointer :: pn_if_lexpr => null ()
        type(command_list_t), pointer :: if_body => null ()
        type(cmd_if_t), dimension(:), pointer :: elsif_cmd => null ()
        type(command_list_t), pointer :: else_body => null ()
    contains
        ⟨Commands: cmd if: TBP⟩
    end type cmd_if_t

```

Finalizer. There are no local options, therefore we can simply override the default finalizer.

```

⟨Commands: cmd if: TBP⟩≡
    procedure :: final => cmd_if_final
⟨Commands: procedures⟩+≡
    recursive subroutine cmd_if_final (cmd)
        class(cmd_if_t), intent(inout) :: cmd
        integer :: i
        if (associated (cmd%if_body)) then
            call command_list_final (cmd%if_body)
            deallocate (cmd%if_body)
        end if
        if (associated (cmd%elsif_cmd)) then
            do i = 1, size (cmd%elsif_cmd)
                call cmd_if_final (cmd%elsif_cmd(i))
            end do
            deallocate (cmd%elsif_cmd)
        end if
        if (associated (cmd%else_body)) then
            call command_list_final (cmd%else_body)
            deallocate (cmd%else_body)
        end if
    end subroutine cmd_if_final

```

Output. Recursively write the command lists.

```

⟨Commands: cmd if: TBP⟩+≡
    procedure :: write => cmd_if_write

```

<Commands: procedures>+≡

```

subroutine cmd_if_write (cmd, unit, indent)
  class(cmd_if_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u, ind, i
  u = given_output_unit (unit); if (u < 0) return
  ind = 0; if (present (indent)) ind = indent
  call write_indent (u, indent)
  write (u, "(A)") "if <expr> then"
  if (associated (cmd%if_body)) then
    call cmd%if_body%write (unit, ind + 1)
  end if
  if (associated (cmd%elsif_cmd)) then
    do i = 1, size (cmd%elsif_cmd)
      call write_indent (u, indent)
      write (u, "(A)") "elsif <expr> then"
      if (associated (cmd%elsif_cmd(i)%if_body)) then
        call cmd%elsif_cmd(i)%if_body%write (unit, ind + 1)
      end if
    end do
  end if
  if (associated (cmd%else_body)) then
    call write_indent (u, indent)
    write (u, "(A)") "else"
    call cmd%else_body%write (unit, ind + 1)
  end if
end subroutine cmd_if_write

```

Compile the conditional.

<Commands: cmd if: TBP>+≡

```

procedure :: compile => cmd_if_compile

```

<Commands: procedures>+≡

```

recursive subroutine cmd_if_compile (cmd, global)
  class(cmd_if_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_lexpr, pn_body
  type(parse_node_t), pointer :: pn_elsif_clauses, pn_cmd_elsif
  type(parse_node_t), pointer :: pn_else_clause, pn_cmd_else
  integer :: i, n_elsif
  pn_lexpr => parse_node_get_sub_ptr (cmd%pn, 2)
  cmd%pn_if_lexpr => pn_lexpr
  pn_body => parse_node_get_next_ptr (pn_lexpr, 2)
  select case (char (parse_node_get_rule_key (pn_body)))
  case ("command_list")
    allocate (cmd%if_body)
    call cmd%if_body%compile (pn_body, global)
    pn_elsif_clauses => parse_node_get_next_ptr (pn_body)
  case default
    pn_elsif_clauses => pn_body
  end select
  select case (char (parse_node_get_rule_key (pn_elsif_clauses)))
  case ("elsif_clauses")
    n_elsif = parse_node_get_n_sub (pn_elsif_clauses)

```

```

allocate (cmd%elsif_cmd (n_elsif))
pn_cmd_elsif => parse_node_get_sub_ptr (pn_elsif_clauses)
do i = 1, n_elsif
  pn_lexpr => parse_node_get_sub_ptr (pn_cmd_elsif, 2)
  cmd%elsif_cmd(i)%pn_if_lexpr => pn_lexpr
  pn_body => parse_node_get_next_ptr (pn_lexpr, 2)
  if (associated (pn_body)) then
    allocate (cmd%elsif_cmd(i)%if_body)
    call cmd%elsif_cmd(i)%if_body%compile (pn_body, global)
  end if
  pn_cmd_elsif => parse_node_get_next_ptr (pn_cmd_elsif)
end do
pn_else_clause => parse_node_get_next_ptr (pn_elsif_clauses)
case default
  pn_else_clause => pn_elsif_clauses
end select
select case (char (parse_node_get_rule_key (pn_else_clause)))
case ("else_clause")
  pn_cmd_else => parse_node_get_sub_ptr (pn_else_clause)
  pn_body => parse_node_get_sub_ptr (pn_cmd_else, 2)
  if (associated (pn_body)) then
    allocate (cmd%else_body)
    call cmd%else_body%compile (pn_body, global)
  end if
end select
end subroutine cmd_if_compile

```

(Recursively) execute the condition. Context remains global in all cases.

<Commands: cmd if: TBP>+≡

```
procedure :: execute => cmd_if_execute
```

<Commands: procedures>+≡

```

recursive subroutine cmd_if_execute (cmd, global)
  class(cmd_if_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(var_list_t), pointer :: var_list
  logical :: lval, is_known
  integer :: i
  var_list => global%get_var_list_ptr ()
  lval = eval_log (cmd%pn_if_lexpr, var_list, is_known=is_known)
  if (is_known) then
    if (lval) then
      if (associated (cmd%if_body)) then
        call cmd%if_body%execute (global)
      end if
      return
    end if
  else
    call error_undecided ()
    return
  end if
  if (associated (cmd%elsif_cmd)) then
    SCAN_ELSEIF: do i = 1, size (cmd%elsif_cmd)
      lval = eval_log (cmd%elsif_cmd(i)%pn_if_lexpr, var_list, &

```

```

        is_known=is_known)
    if (is_known) then
        if (lval) then
            if (associated (cmd%elsif_cmd(i)%if_body)) then
                call cmd%elsif_cmd(i)%if_body%execute (global)
            end if
            return
        end if
    else
        call error_undecided ()
        return
    end if
end do SCAN_ELSIF
end if
if (associated (cmd%else_body)) then
    call cmd%else_body%execute (global)
end if
contains
    subroutine error_undecided ()
        call msg_error ("Undefined result of cmditional expression: " &
            // "neither branch will be executed")
    end subroutine error_undecided
end subroutine cmd_if_execute

```

Include another command-list file

The include command allocates a local parse tree. This must not be deleted before the command object itself is deleted, since pointers may point to subobjects of it.

```

<Commands: types>+≡
    type, extends (command_t) :: cmd_include_t
        private
        type(string_t) :: file
        type(command_list_t), pointer :: command_list => null ()
        type(parse_tree_t) :: parse_tree
    contains
        <Commands: cmd include: TBP>
    end type cmd_include_t

```

Finalizer: delete the command list. No options, so we can simply override the default finalizer.

```

<Commands: cmd include: TBP>≡
    procedure :: final => cmd_include_final

<Commands: procedures>+≡
    subroutine cmd_include_final (cmd)
        class(cmd_include_t), intent(inout) :: cmd
        call parse_tree_final (cmd%parse_tree)
        if (associated (cmd%command_list)) then
            call cmd%command_list%final ()
            deallocate (cmd%command_list)
        end if
    end subroutine cmd_include_final

```

```
end subroutine cmd_include_final
```

Write: display the command list as-is, if allocated.

(Commands: cmd include: TBP)+≡

```
procedure :: write => cmd_include_write
```

(Commands: procedures)+≡

```
subroutine cmd_include_write (cmd, unit, indent)
  class(cmd_include_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u, ind
  u = given_output_unit (unit)
  ind = 0; if (present (indent)) ind = indent
  call write_indent (u, indent)
  write (u, "(A,A,A,A)") "include ", "'", char (cmd%file), "'"
  if (associated (cmd%command_list)) then
    call cmd%command_list%write (u, ind + 1)
  end if
end subroutine cmd_include_write
```

Compile file contents: First parse the file, then immediately compile its contents.
Use the global data set.

(Commands: cmd include: TBP)+≡

```
procedure :: compile => cmd_include_compile
```

(Commands: procedures)+≡

```
subroutine cmd_include_compile (cmd, global)
  class(cmd_include_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_arg, pn_file
  type(string_t) :: file
  logical :: exist
  integer :: u
  type(stream_t), target :: stream
  type(lexer_t) :: lexer
  pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
  pn_file => parse_node_get_sub_ptr (pn_arg)
  file = parse_node_get_string (pn_file)
  inquire (file=char(file), exist=exist)
  if (exist) then
    cmd%file = file
  else
    cmd%file = global%os_data%whizard_cutspath // "/" // file
    inquire (file=char(cmd%file), exist=exist)
    if (.not. exist) then
      call msg_error ("Include file '" // char (file) // "' not found")
      return
    end if
  end if
  u = free_unit ()
  call lexer_init_cmd_list (lexer, global%lexer)
  call stream_init (stream, char (cmd%file))
  call lexer_assign_stream (lexer, stream)
  call parse_tree_init (cmd%parse_tree, syntax_cmd_list, lexer)
```

```

    call stream_final (stream)
    call lexer_final (lexer)
    close (u)
    allocate (cmd%command_list)
    call cmd%command_list%compile (cmd%parse_tree%get_root_ptr (), &
        global)
end subroutine cmd_include_compile

```

Execute file contents in the global context.

```

⟨Commands: cmd include: TBP⟩+≡
    procedure :: execute => cmd_include_execute

⟨Commands: procedures⟩+≡
    subroutine cmd_include_execute (cmd, global)
        class(cmd_include_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        if (associated (cmd%command_list)) then
            call msg_message &
                ("Including Sindarin from '" // char (cmd%file) // "'")
            call cmd%command_list%execute (global)
            call msg_message &
                ("End of included '" // char (cmd%file) // "'")
        end if
    end subroutine cmd_include_execute

```

Export values

This command exports the current values of variables or other objects to the surrounding scope. By default, a scope enclosed by braces keeps all objects local to it. The **export** command exports the values that are generated within the scope to the corresponding object in the outer scope.

The allowed set of exportable objects is, in principle, the same as the set of objects that the **show** command supports. This includes some convenience abbreviations.

TODO: The initial implementation inherits syntax from **show**, but supports only the **results** pseudo-object. The results (i.e., the process stack) is appended to the outer process stack instead of being discarded. The behavior of the **export** command for other object kinds is to be defined on a case-by-case basis. It may involve replacing the outer value or, instead, doing some sort of appending or reduction.

```

⟨Commands: types⟩+≡
    type, extends (command_t) :: cmd_export_t
        private
        type(string_t), dimension(:), allocatable :: name
    contains
        ⟨Commands: cmd export: TBP⟩
    end type cmd_export_t

```

Output: list the object names, not values.

```

⟨Commands: cmd export: TBP⟩≡
    procedure :: write => cmd_export_write

```

```

<Commands: procedures>+≡
subroutine cmd_export_write (cmd, unit, indent)
  class(cmd_export_t), intent(in) :: cmd
  integer, intent(in), optional :: unit, indent
  integer :: u, i
  u = given_output_unit (unit); if (u < 0) return
  call write_indent (u, indent)
  write (u, "(1x,A)", advance="no") "export: "
  if (allocated (cmd%name)) then
    do i = 1, size (cmd%name)
      write (u, "(1x,A)", advance="no") char (cmd%name(i))
    end do
    write (u, *)
  else
    write (u, "(5x,A)") "[undefined]"
  end if
end subroutine cmd_export_write

```

Compile. Allocate an array which is filled with the names of the variables to export.

```

<Commands: cmd export: TBP>+≡
procedure :: compile => cmd_export_compile

<Commands: procedures>+≡
subroutine cmd_export_compile (cmd, global)
  class(cmd_export_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  type(parse_node_t), pointer :: pn_arg, pn_var, pn_prefix, pn_name
  type(string_t) :: key
  integer :: i, n_args
  pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
  if (associated (pn_arg)) then
    select case (char (parse_node_get_rule_key (pn_arg)))
    case ("show_arg")
      cmd%pn_opt => parse_node_get_next_ptr (pn_arg)
    case default
      cmd%pn_opt => pn_arg
      pn_arg => null ()
    end select
  end if
  call cmd%compile_options (global)
  if (associated (pn_arg)) then
    n_args = parse_node_get_n_sub (pn_arg)
    allocate (cmd%name (n_args))
    pn_var => parse_node_get_sub_ptr (pn_arg)
    i = 0
    do while (associated (pn_var))
      i = i + 1
      select case (char (parse_node_get_rule_key (pn_var)))
      case ("model", "library", "beams", "iterations", &
        "cuts", "weight", "int", "real", "complex", &
        "scale", "factorization_scale", "renormalization_scale", &
        "selection", "reweight", "analysis", "pdg", &
        "stable", "unstable", "polarized", "unpolarized", &

```

```

        "results", "expect", "intrinsic", "string", "logical")
    cmd%name(i) = parse_node_get_key (pn_var)
case ("result_var")
    pn_prefix => parse_node_get_sub_ptr (pn_var)
    pn_name => parse_node_get_next_ptr (pn_prefix)
    if (associated (pn_name)) then
        cmd%name(i) = parse_node_get_key (pn_prefix) &
            // "(" // parse_node_get_string (pn_name) // ")"
    else
        cmd%name(i) = parse_node_get_key (pn_prefix)
    end if
case ("log_var", "string_var", "alias_var")
    pn_prefix => parse_node_get_sub_ptr (pn_var)
    pn_name => parse_node_get_next_ptr (pn_prefix)
    key = parse_node_get_key (pn_prefix)
    if (associated (pn_name)) then
        select case (char (parse_node_get_rule_key (pn_name)))
        case ("var_name")
            select case (char (key))
            case ("?", "$") ! $ sign
                cmd%name(i) = key // parse_node_get_string (pn_name)
            case ("alias")
                cmd%name(i) = parse_node_get_string (pn_name)
            end select
        case default
            call parse_node_mismatch &
                ("var_name", pn_name)
        end select
    else
        cmd%name(i) = key
    end if
case default
    cmd%name(i) = parse_node_get_string (pn_var)
end select
!!! restriction imposed by current lack of implementation
select case (char (parse_node_get_rule_key (pn_var)))
case ("results")
case default
    call msg_fatal ("export: object (type) '" &
        // char (parse_node_get_rule_key (pn_var)) &
        // "' not supported yet")
end select
pn_var => parse_node_get_next_ptr (pn_var)
end do
else
    allocate (cmd%name (0))
end if
end subroutine cmd_export_compile

```

Execute. Scan the list of objects to export.

<Commands: cmd export: TBP>+≡

procedure :: execute => cmd_export_execute

<Commands: procedures>+≡


```

subroutine cmd_export_execute (cmd, global)
  class(cmd_export_t), intent(inout) :: cmd
  type(rt_data_t), intent(inout), target :: global
  call global%append_exports (cmd%name)
end subroutine cmd_export_execute

```

Quit command execution

The code is the return code of the whole program if it is terminated by this command.

```

⟨Commands: types⟩+≡
  type, extends (command_t) :: cmd_quit_t
  private
  logical :: has_code = .false.
  type(parse_node_t), pointer :: pn_code_expr => null ()
  contains
  ⟨Commands: cmd quit: TBP⟩
end type cmd_quit_t

```

Output.

```

⟨Commands: cmd quit: TBP⟩≡
  procedure :: write => cmd_quit_write

⟨Commands: procedures⟩+≡
  subroutine cmd_quit_write (cmd, unit, indent)
    class(cmd_quit_t), intent(in) :: cmd
    integer, intent(in), optional :: unit, indent
    integer :: u
    u = given_output_unit (unit); if (u < 0) return
    call write_indent (u, indent)
    write (u, "(1x,A,L1)") "quit: has_code = ", cmd%has_code
  end subroutine cmd_quit_write

```

Compile: allocate a quit object which serves as a placeholder.

```

⟨Commands: cmd quit: TBP⟩+≡
  procedure :: compile => cmd_quit_compile

⟨Commands: procedures⟩+≡
  subroutine cmd_quit_compile (cmd, global)
    class(cmd_quit_t), intent(inout) :: cmd
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_arg
    pn_arg => parse_node_get_sub_ptr (cmd%pn, 2)
    if (associated (pn_arg)) then
      cmd%pn_code_expr => parse_node_get_sub_ptr (pn_arg)
      cmd%has_code = .true.
    end if
  end subroutine cmd_quit_compile

```

Execute: The quit command does not execute anything, it just stops command execution. This is achieved by setting quit flag and quit code in the global variable list. However, the return code, if present, is an expression which has to be evaluated.

```

<Commands: cmd quit: TBP>+≡
    procedure :: execute => cmd_quit_execute

<Commands: procedures>+≡
    subroutine cmd_quit_execute (cmd, global)
        class(cmd_quit_t), intent(inout) :: cmd
        type(rt_data_t), intent(inout), target :: global
        type(var_list_t), pointer :: var_list
        logical :: is_known
        var_list => global%get_var_list_ptr ()
        if (cmd%has_code) then
            global%quit_code = eval_int (cmd%pn_code_expr, var_list, &
                is_known=is_known)
            if (.not. is_known) then
                call msg_error ("Undefined return code of quit/exit command")
            end if
        end if
        global%quit = .true.
    end subroutine cmd_quit_execute

```

35.1.6 The command list

The command list holds a list of commands and relevant global data.

```

<Commands: public>+≡
    public :: command_list_t

<Commands: types>+≡
    type :: command_list_t
        ! not private anymore as required by the whizard-c-interface
        class(command_t), pointer :: first => null ()
        class(command_t), pointer :: last => null ()
        contains
        <Commands: command list: TBP>
    end type command_list_t

```

Output.

```

<Commands: command list: TBP>≡
    procedure :: write => command_list_write

<Commands: procedures>+≡
    recursive subroutine command_list_write (cmd_list, unit, indent)
        class(command_list_t), intent(in) :: cmd_list
        integer, intent(in), optional :: unit, indent
        class(command_t), pointer :: cmd
        cmd => cmd_list%first
        do while (associated (cmd))
            call cmd%write (unit, indent)
            cmd => cmd%next
        end do
    end subroutine command_list_write

```

```
end subroutine command_list_write
```

Append a new command to the list and free the original pointer.

```
<Commands: command list: TBP>+≡
  procedure :: append => command_list_append

<Commands: procedures>+≡
  subroutine command_list_append (cmd_list, command)
    class(command_list_t), intent(inout) :: cmd_list
    class(command_t), intent(inout), pointer :: command
    if (associated (cmd_list%last)) then
      cmd_list%last%next => command
    else
      cmd_list%first => command
    end if
    cmd_list%last => command
    command => null ()
  end subroutine command_list_append
```

Finalize.

```
<Commands: command list: TBP>+≡
  procedure :: final => command_list_final

<Commands: procedures>+≡
  recursive subroutine command_list_final (cmd_list)
    class(command_list_t), intent(inout) :: cmd_list
    class(command_t), pointer :: command
    do while (associated (cmd_list%first))
      command => cmd_list%first
      cmd_list%first => cmd_list%first%next
      call command%final ()
      deallocate (command)
    end do
    cmd_list%last => null ()
  end subroutine command_list_final
```

35.1.7 Compiling the parse tree

Transform a parse tree into a command list. Initialization is assumed to be done.

After each command, we set a breakpoint.

```
<Commands: command list: TBP>+≡
  procedure :: compile => command_list_compile

<Commands: procedures>+≡
  recursive subroutine command_list_compile (cmd_list, pn, global)
    class(command_list_t), intent(inout), target :: cmd_list
    type(parse_node_t), intent(in), target :: pn
    type(rt_data_t), intent(inout), target :: global
    type(parse_node_t), pointer :: pn_cmd
    class(command_t), pointer :: command
    integer :: i
```

```

pn_cmd => parse_node_get_sub_ptr (pn)
do i = 1, parse_node_get_n_sub (pn)
  call dispatch_command (command, pn_cmd)
  call command%compile (global)
  call cmd_list%append (command)
  call terminate_now_if_signal ()
  pn_cmd => parse_node_get_next_ptr (pn_cmd)
end do
end subroutine command_list_compile

```

35.1.8 Executing the command list

Before executing a command we should execute its options (if any). After that, reset the options, i.e., remove temporary effects from the global state.

Also here, after each command we set a breakpoint.

```

<Commands: command list: TBP>+≡
  procedure :: execute => command_list_execute

<Commands: procedures>+≡
  recursive subroutine command_list_execute (cmd_list, global)
    class(command_list_t), intent(in) :: cmd_list
    type(rt_data_t), intent(inout), target :: global
    class(command_t), pointer :: command
    command => cmd_list%first
    COMMAND_COND: do while (associated (command))
      call command%execute_options (global)
      call command%execute (global)
      call command%reset_options (global)
      call terminate_now_if_signal ()
      if (global%quit) exit COMMAND_COND
      command => command%next
    end do COMMAND_COND
  end subroutine command_list_execute

```

35.1.9 Command list syntax

```

<Commands: public>+≡
  public :: syntax_cmd_list

<Commands: variables>≡
  type(syntax_t), target, save :: syntax_cmd_list

<Commands: public>+≡
  public :: syntax_cmd_list_init

<Commands: procedures>+≡
  subroutine syntax_cmd_list_init ()
    type(ifile_t) :: ifile
    call define_cmd_list_syntax (ifile)
    call syntax_init (syntax_cmd_list, ifile)
    call ifile_final (ifile)
  end subroutine syntax_cmd_list_init

```

```

<Commands: public>+≡
    public :: syntax_cmd_list_final

<Commands: procedures>+≡
    subroutine syntax_cmd_list_final ()
        call syntax_final (syntax_cmd_list)
    end subroutine syntax_cmd_list_final

<Commands: public>+≡
    public :: syntax_cmd_list_write

<Commands: procedures>+≡
    subroutine syntax_cmd_list_write (unit)
        integer, intent(in), optional :: unit
        call syntax_write (syntax_cmd_list, unit)
    end subroutine syntax_cmd_list_write

<Commands: procedures>+≡
    subroutine define_cmd_list_syntax (ifile)
        type(ifile_t), intent(inout) :: ifile
        call ifile_append (ifile, "SEQ command_list = command*")
        call ifile_append (ifile, "ALT command = " &
            // "cmd_model | cmd_library | cmd_iterations | cmd_sample_format | " &
            // "cmd_var | cmd_slha | " &
            // "cmd_show | cmd_clear | " &
            // "cmd_expect | " &
            // "cmd_cuts | cmd_scale | cmd_fac_scale | cmd_ren_scale | " &
            // "cmd_weight | cmd_selection | cmd_reweight | " &
            // "cmd_beams | cmd_beams_pol_density | cmd_beams_pol_fraction | " &
            // "cmd_beams_momentum | cmd_beams_theta | cmd_beams_phi | " &
            // "cmd_integrate | " &
            // "cmd_observable | cmd_histogram | cmd_plot | cmd_graph | " &
            // "cmd_record | " &
            // "cmd_analysis | cmd_alt_setup | " &
            // "cmd_unstable | cmd_stable | cmd_simulate | cmd_rescan | " &
            // "cmd_process | cmd_compile | cmd_exec | " &
            // "cmd_scan | cmd_if | cmd_include | cmd_quit | " &
            // "cmd_export | " &
            // "cmd_polarized | cmd_unpolarized | " &
            // "cmd_open_out | cmd_close_out | cmd_printf | " &
            // "cmd_write_analysis | cmd_compile_analysis | cmd_nlo | cmd_components")
        call ifile_append (ifile, "GRO options = '{' local_command_list '}'")
        call ifile_append (ifile, "SEQ local_command_list = local_command*")
        call ifile_append (ifile, "ALT local_command = " &
            // "cmd_model | cmd_library | cmd_iterations | cmd_sample_format | " &
            // "cmd_var | cmd_slha | " &
            // "cmd_show | " &
            // "cmd_expect | " &
            // "cmd_cuts | cmd_scale | cmd_fac_scale | cmd_ren_scale | " &
            // "cmd_weight | cmd_selection | cmd_reweight | " &
            // "cmd_beams | cmd_beams_pol_density | cmd_beams_pol_fraction | " &
            // "cmd_beams_momentum | cmd_beams_theta | cmd_beams_phi | " &
            // "cmd_observable | cmd_histogram | cmd_plot | cmd_graph | " &
            // "cmd_clear | cmd_record | " &
            // "cmd_analysis | cmd_alt_setup | " &

```

```

// "cmd_open_out | cmd_close_out | cmd_printf | " &
// "cmd_write_analysis | cmd_compile_analysis | cmd_nlo | cmd_components")
call ifile_append (ifile, "SEQ cmd_model = model '=' model_name model_arg?")
call ifile_append (ifile, "KEY model")
call ifile_append (ifile, "ALT model_name = model_id | string_literal")
call ifile_append (ifile, "IDE model_id")
call ifile_append (ifile, "ARG model_arg = ( model_scheme? )")
call ifile_append (ifile, "ALT model_scheme = " &
// "ufo_spec | scheme_id | string_literal")
call ifile_append (ifile, "SEQ ufo_spec = ufo ufo_arg?")
call ifile_append (ifile, "KEY ufo")
call ifile_append (ifile, "ARG ufo_arg = ( string_literal )")
call ifile_append (ifile, "IDE scheme_id")
call ifile_append (ifile, "SEQ cmd_library = library '=' lib_name")
call ifile_append (ifile, "KEY library")
call ifile_append (ifile, "ALT lib_name = lib_id | string_literal")
call ifile_append (ifile, "IDE lib_id")
call ifile_append (ifile, "ALT cmd_var = " &
// "cmd_log_decl | cmd_log | " &
// "cmd_int | cmd_real | cmd_complex | cmd_num | " &
// "cmd_string_decl | cmd_string | cmd_alias | " &
// "cmd_result")
call ifile_append (ifile, "SEQ cmd_log_decl = logical cmd_log")
call ifile_append (ifile, "SEQ cmd_log = '?' var_name '=' lexpr")
call ifile_append (ifile, "SEQ cmd_int = int var_name '=' expr")
call ifile_append (ifile, "SEQ cmd_real = real var_name '=' expr")
call ifile_append (ifile, "SEQ cmd_complex = complex var_name '=' expr")
call ifile_append (ifile, "SEQ cmd_num = var_name '=' expr")
call ifile_append (ifile, "SEQ cmd_string_decl = string cmd_string")
call ifile_append (ifile, "SEQ cmd_string = " &
// "'$' var_name '=' sexpr") ! $
call ifile_append (ifile, "SEQ cmd_alias = alias var_name '=' cexpr")
call ifile_append (ifile, "SEQ cmd_result = result '=' expr")
call ifile_append (ifile, "SEQ cmd_slha = slha_action slha_arg options?")
call ifile_append (ifile, "ALT slha_action = " &
// "read_slha | write_slha")
call ifile_append (ifile, "KEY read_slha")
call ifile_append (ifile, "KEY write_slha")
call ifile_append (ifile, "ARG slha_arg = ( string_literal )")
call ifile_append (ifile, "SEQ cmd_show = show show_arg options?")
call ifile_append (ifile, "KEY show")
call ifile_append (ifile, "ARG show_arg = ( showable* )")
call ifile_append (ifile, "ALT showable = " &
// "model | library | beams | iterations | " &
// "cuts | weight | logical | string | pdg | " &
// "scale | factorization_scale | renormalization_scale | " &
// "selection | reweight | analysis | " &
// "stable | unstable | polarized | unpolarized | " &
// "expect | intrinsic | int | real | complex | " &
// "alias_var | string | results | result_var | " &
// "log_var | string_var | var_name")
call ifile_append (ifile, "KEY results")
call ifile_append (ifile, "KEY intrinsic")
call ifile_append (ifile, "SEQ alias_var = alias var_name")

```

```

call ifile_append (ifile, "SEQ result_var = result_key result_arg?")
call ifile_append (ifile, "SEQ log_var = '?' var_name")
call ifile_append (ifile, "SEQ string_var = '$' var_name") ! $
call ifile_append (ifile, "SEQ cmd_clear = clear clear_arg options?")
call ifile_append (ifile, "KEY clear")
call ifile_append (ifile, "ARG clear_arg = ( clearable* )")
call ifile_append (ifile, "ALT clearable = " &
    // "beams | iterations | " &
    // "cuts | weight | " &
    // "scale | factorization_scale | renormalization_scale | " &
// "selection | reweight | analysis | " &
    // "unstable | polarized | " &
    // "expect | " &
    // "log_var | string_var | var_name")
call ifile_append (ifile, "SEQ cmd_expect = expect expect_arg options?")
call ifile_append (ifile, "KEY expect")
call ifile_append (ifile, "ARG expect_arg = ( lexpr )")
call ifile_append (ifile, "SEQ cmd_cuts = cuts '=' lexpr")
call ifile_append (ifile, "SEQ cmd_scale = scale '=' expr")
call ifile_append (ifile, "SEQ cmd_fac_scale = " &
    // "factorization_scale '=' expr")
call ifile_append (ifile, "SEQ cmd_ren_scale = " &
    // "renormalization_scale '=' expr")
call ifile_append (ifile, "SEQ cmd_weight = weight '=' expr")
call ifile_append (ifile, "SEQ cmd_selection = selection '=' lexpr")
call ifile_append (ifile, "SEQ cmd_reweight = reweight '=' expr")
call ifile_append (ifile, "KEY cuts")
call ifile_append (ifile, "KEY scale")
call ifile_append (ifile, "KEY factorization_scale")
call ifile_append (ifile, "KEY renormalization_scale")
call ifile_append (ifile, "KEY weight")
call ifile_append (ifile, "KEY selection")
call ifile_append (ifile, "KEY reweight")
call ifile_append (ifile, "SEQ cmd_process = process process_id '=' " &
    // "process_prt '=>' prt_state_list options?")
call ifile_append (ifile, "KEY process")
call ifile_append (ifile, "KEY '=>")
call ifile_append (ifile, "LIS process_prt = cexpr+")
call ifile_append (ifile, "LIS prt_state_list = prt_state_sum+")
call ifile_append (ifile, "SEQ prt_state_sum = " &
    // "prt_state prt_state_addition*")
call ifile_append (ifile, "SEQ prt_state_addition = '+' prt_state")
call ifile_append (ifile, "ALT prt_state = grouped_prt_state_list | cexpr")
call ifile_append (ifile, "GRO grouped_prt_state_list = " &
    // "( prt_state_list )")
call ifile_append (ifile, "SEQ cmd_compile = compile_cmd options?")
call ifile_append (ifile, "SEQ compile_cmd = compile_clause compile_arg?")
call ifile_append (ifile, "SEQ compile_clause = compile_exec_name_spec?")
call ifile_append (ifile, "KEY compile")
call ifile_append (ifile, "SEQ exec_name_spec = as exec_name")
call ifile_append (ifile, "KEY as")
call ifile_append (ifile, "ALT exec_name = exec_id | string_literal")
call ifile_append (ifile, "IDE exec_id")
call ifile_append (ifile, "ARG compile_arg = ( lib_name* )")

```

```

call ifile_append (ifile, "SEQ cmd_exec = exec exec_arg")
call ifile_append (ifile, "KEY exec")
call ifile_append (ifile, "ARG exec_arg = ( sexpr )")
call ifile_append (ifile, "SEQ cmd_beams = beams '=' beam_def")
call ifile_append (ifile, "KEY beams")
call ifile_append (ifile, "SEQ beam_def = beam_spec strfun_seq*")
call ifile_append (ifile, "SEQ beam_spec = beam_list")
call ifile_append (ifile, "LIS beam_list = cexpr, cexpr?")
call ifile_append (ifile, "SEQ cmd_beams_pol_density = " &
    // "beams_pol_density '=' beams_pol_spec")
call ifile_append (ifile, "KEY beams_pol_density")
call ifile_append (ifile, "LIS beams_pol_spec = smatrix, smatrix?")
call ifile_append (ifile, "SEQ smatrix = '@' smatrix_arg")
! call ifile_append (ifile, "KEY '@'")      !!! Key already exists
call ifile_append (ifile, "ARG smatrix_arg = ( sentry* )")
call ifile_append (ifile, "SEQ sentry = expr extra_sentry*")
call ifile_append (ifile, "SEQ extra_sentry = ':' expr")
call ifile_append (ifile, "SEQ cmd_beams_pol_fraction = " &
    // "beams_pol_fraction '=' beams_par_spec")
call ifile_append (ifile, "KEY beams_pol_fraction")
call ifile_append (ifile, "SEQ cmd_beams_momentum = " &
    // "beams_momentum '=' beams_par_spec")
call ifile_append (ifile, "KEY beams_momentum")
call ifile_append (ifile, "SEQ cmd_beams_theta = " &
    // "beams_theta '=' beams_par_spec")
call ifile_append (ifile, "KEY beams_theta")
call ifile_append (ifile, "SEQ cmd_beams_phi = " &
    // "beams_phi '=' beams_par_spec")
call ifile_append (ifile, "KEY beams_phi")
call ifile_append (ifile, "LIS beams_par_spec = expr, expr?")
call ifile_append (ifile, "SEQ strfun_seq = '=>' strfun_pair")
call ifile_append (ifile, "LIS strfun_pair = strfun_def, strfun_def?")
call ifile_append (ifile, "SEQ strfun_def = strfun_id")
call ifile_append (ifile, "ALT strfun_id = " &
    // "none | lhpdf | lhpdf_photon | pdf_builtin | pdf_builtin_photon | " &
    // "isr | epa | ewa | circe1 | circe2 | energy_scan | " &
    // "gaussian | beam_events")
call ifile_append (ifile, "KEY none")
call ifile_append (ifile, "KEY lhpdf")
call ifile_append (ifile, "KEY lhpdf_photon")
call ifile_append (ifile, "KEY pdf_builtin")
call ifile_append (ifile, "KEY pdf_builtin_photon")
call ifile_append (ifile, "KEY isr")
call ifile_append (ifile, "KEY epa")
call ifile_append (ifile, "KEY ewa")
call ifile_append (ifile, "KEY circe1")
call ifile_append (ifile, "KEY circe2")
call ifile_append (ifile, "KEY energy_scan")
call ifile_append (ifile, "KEY gaussian")
call ifile_append (ifile, "KEY beam_events")
call ifile_append (ifile, "SEQ cmd_integrate = " &
    // "integrate proc_arg options?")
call ifile_append (ifile, "KEY integrate")
call ifile_append (ifile, "ARG proc_arg = ( proc_id* )")

```



```

call ifile_append (ifile, "IDE proc_id")
call ifile_append (ifile, "SEQ cmd_iterations = " &
// "iterations '=' iterations_list")
call ifile_append (ifile, "KEY iterations")
call ifile_append (ifile, "LIS iterations_list = iterations_spec+")
call ifile_append (ifile, "ALT iterations_spec = it_spec")
call ifile_append (ifile, "SEQ it_spec = expr calls_spec adapt_spec?")
call ifile_append (ifile, "SEQ calls_spec = ':' expr")
call ifile_append (ifile, "SEQ adapt_spec = ':' sexpr")
call ifile_append (ifile, "SEQ cmd_components = " &
// "active '=' component_list")
call ifile_append (ifile, "KEY active")
call ifile_append (ifile, "LIS component_list = sexpr+")
call ifile_append (ifile, "SEQ cmd_sample_format = " &
// "sample_format '=' event_format_list")
call ifile_append (ifile, "KEY sample_format")
call ifile_append (ifile, "LIS event_format_list = event_format+")
call ifile_append (ifile, "IDE event_format")
call ifile_append (ifile, "SEQ cmd_observable = " &
// "observable analysis_tag options?")
call ifile_append (ifile, "KEY observable")
call ifile_append (ifile, "SEQ cmd_histogram = " &
// "histogram analysis_tag histogram_arg " &
// "options?")
call ifile_append (ifile, "KEY histogram")
call ifile_append (ifile, "ARG histogram_arg = (expr, expr, expr?)")
call ifile_append (ifile, "SEQ cmd_plot = plot analysis_tag options?")
call ifile_append (ifile, "KEY plot")
call ifile_append (ifile, "SEQ cmd_graph = graph graph_term '=' graph_def")
call ifile_append (ifile, "KEY graph")
call ifile_append (ifile, "SEQ graph_term = analysis_tag options?")
call ifile_append (ifile, "SEQ graph_def = graph_term graph_append*")
call ifile_append (ifile, "SEQ graph_append = '&' graph_term")
call ifile_append (ifile, "SEQ cmd_analysis = analysis '=' lexpr")
call ifile_append (ifile, "KEY analysis")
call ifile_append (ifile, "SEQ cmd_alt_setup = " &
// "alt_setup '=' option_list_expr")
call ifile_append (ifile, "KEY alt_setup")
call ifile_append (ifile, "ALT option_list_expr = " &
// "grouped_option_list | option_list")
call ifile_append (ifile, "GRO grouped_option_list = ( option_list_expr )")
call ifile_append (ifile, "LIS option_list = options+")
call ifile_append (ifile, "SEQ cmd_open_out = open_out open_arg options?")
call ifile_append (ifile, "SEQ cmd_close_out = close_out open_arg options?")
call ifile_append (ifile, "KEY open_out")
call ifile_append (ifile, "KEY close_out")
call ifile_append (ifile, "ARG open_arg = (sexpr)")
call ifile_append (ifile, "SEQ cmd_printf = printf_cmd options?")
call ifile_append (ifile, "SEQ printf_cmd = printf_clause sprintf_args?")
call ifile_append (ifile, "SEQ printf_clause = printf sexpr")
call ifile_append (ifile, "KEY printf")
call ifile_append (ifile, "SEQ cmd_record = record_cmd")
call ifile_append (ifile, "SEQ cmd_unstable = " &
// "unstable cexpr unstable_arg options?")

```

```

call ifile_append (ifile, "KEY unstable")
call ifile_append (ifile, "ARG unstable_arg = ( proc_id* )")
call ifile_append (ifile, "SEQ cmd_stable = stable stable_list options?")
call ifile_append (ifile, "KEY stable")
call ifile_append (ifile, "LIS stable_list = cexpr+")
call ifile_append (ifile, "KEY polarized")
call ifile_append (ifile, "SEQ cmd_polarized = polarized polarized_list options?")
call ifile_append (ifile, "LIS polarized_list = cexpr+")
call ifile_append (ifile, "KEY unpolarized")
call ifile_append (ifile, "SEQ cmd_unpolarized = unpolarized unpolarized_list options?")
call ifile_append (ifile, "LIS unpolarized_list = cexpr+")
call ifile_append (ifile, "SEQ cmd_simulate = " &
// "simulate proc_arg options?")
call ifile_append (ifile, "KEY simulate")
call ifile_append (ifile, "SEQ cmd_rescan = " &
// "rescan sexpr proc_arg options?")
call ifile_append (ifile, "KEY rescan")
call ifile_append (ifile, "SEQ cmd_scan = scan scan_var scan_body?")
call ifile_append (ifile, "KEY scan")
call ifile_append (ifile, "ALT scan_var = " &
// "scan_log_decl | scan_log | " &
// "scan_int | scan_real | scan_complex | scan_num | " &
// "scan_string_decl | scan_string | scan_alias | " &
// "scan_cuts | scan_weight | " &
// "scan_scale | scan_ren_scale | scan_fac_scale | " &
// "scan_selection | scan_reweight | scan_analysis | " &
// "scan_model | scan_library")
call ifile_append (ifile, "SEQ scan_log_decl = logical scan_log")
call ifile_append (ifile, "SEQ scan_log = '?' var_name '=' scan_log_arg")
call ifile_append (ifile, "ARG scan_log_arg = ( lexpr* )")
call ifile_append (ifile, "SEQ scan_int = int var_name '=' scan_num_arg")
call ifile_append (ifile, "SEQ scan_real = real var_name '=' scan_num_arg")
call ifile_append (ifile, "SEQ scan_complex = " &
// "complex var_name '=' scan_num_arg")
call ifile_append (ifile, "SEQ scan_num = var_name '=' scan_num_arg")
call ifile_append (ifile, "ARG scan_num_arg = ( range* )")
call ifile_append (ifile, "ALT range = grouped_range | range_expr")
call ifile_append (ifile, "GRO grouped_range = ( range_expr )")
call ifile_append (ifile, "SEQ range_expr = expr range_spec?")
call ifile_append (ifile, "SEQ range_spec = '>' expr step_spec?")
call ifile_append (ifile, "SEQ step_spec = step_op expr")
call ifile_append (ifile, "ALT step_op = " &
// "'+' | '- ' | '* ' | '/' | '+/' | '/*'")
call ifile_append (ifile, "KEY '+'")
call ifile_append (ifile, "KEY '- '")
call ifile_append (ifile, "KEY '* '")
call ifile_append (ifile, "KEY '/'")
call ifile_append (ifile, "KEY '+/'")
call ifile_append (ifile, "KEY '/*'")
call ifile_append (ifile, "SEQ scan_string_decl = string scan_string")
call ifile_append (ifile, "SEQ scan_string = " &
// "'$' var_name '=' scan_string_arg")
call ifile_append (ifile, "ARG scan_string_arg = ( sexpr* )")
call ifile_append (ifile, "SEQ scan_alias = " &

```

```

// "alias var_name '=' scan_alias_arg")
call ifile_append (ifile, "ARG scan_alias_arg = ( cexpr* )")
call ifile_append (ifile, "SEQ scan_cuts = cuts '=' scan_lexpr_arg")
call ifile_append (ifile, "ARG scan_lexpr_arg = ( lexpr* )")
call ifile_append (ifile, "SEQ scan_scale = scale '=' scan_expr_arg")
call ifile_append (ifile, "ARG scan_expr_arg = ( expr* )")
call ifile_append (ifile, "SEQ scan_fac_scale = " &
// "factorization_scale '=' scan_expr_arg")
call ifile_append (ifile, "SEQ scan_ren_scale = " &
// "renormalization_scale '=' scan_expr_arg")
call ifile_append (ifile, "SEQ scan_weight = weight '=' scan_expr_arg")
call ifile_append (ifile, "SEQ scan_selection = selection '=' scan_lexpr_arg")
call ifile_append (ifile, "SEQ scan_reweight = reweight '=' scan_expr_arg")
call ifile_append (ifile, "SEQ scan_analysis = analysis '=' scan_lexpr_arg")
call ifile_append (ifile, "SEQ scan_model = model '=' scan_model_arg")
call ifile_append (ifile, "ARG scan_model_arg = ( model_name* )")
call ifile_append (ifile, "SEQ scan_library = library '=' scan_library_arg")
call ifile_append (ifile, "ARG scan_library_arg = ( lib_name* )")
call ifile_append (ifile, "GRO scan_body = '{' command_list '}'")
call ifile_append (ifile, "SEQ cmd_if = " &
// "if lexpr then command_list elsif_clauses else_clause endif")
call ifile_append (ifile, "SEQ elsif_clauses = cmd_elseif*")
call ifile_append (ifile, "SEQ cmd_elseif = elsif lexpr then command_list")
call ifile_append (ifile, "SEQ else_clause = cmd_else*")
call ifile_append (ifile, "SEQ cmd_else = else command_list")
call ifile_append (ifile, "SEQ cmd_include = include include_arg")
call ifile_append (ifile, "KEY include")
call ifile_append (ifile, "ARG include_arg = ( string_literal )")
call ifile_append (ifile, "SEQ cmd_quit = quit_cmd quit_arg*")
call ifile_append (ifile, "ALT quit_cmd = quit | exit")
call ifile_append (ifile, "KEY quit")
call ifile_append (ifile, "KEY exit")
call ifile_append (ifile, "ARG quit_arg = ( expr )")
call ifile_append (ifile, "SEQ cmd_export = export show_arg options*")
call ifile_append (ifile, "KEY export")
call ifile_append (ifile, "SEQ cmd_write_analysis = " &
// "write_analysis_clause options*")
call ifile_append (ifile, "SEQ cmd_compile_analysis = " &
// "compile_analysis_clause options*")
call ifile_append (ifile, "SEQ write_analysis_clause = " &
// "write_analysis write_analysis_arg*")
call ifile_append (ifile, "SEQ compile_analysis_clause = " &
// "compile_analysis write_analysis_arg*")
call ifile_append (ifile, "KEY write_analysis")
call ifile_append (ifile, "KEY compile_analysis")
call ifile_append (ifile, "ARG write_analysis_arg = ( analysis_tag* )")
call ifile_append (ifile, "SEQ cmd_nlo = " &
// "nlo_calculation '=' nlo_calculation_list")
call ifile_append (ifile, "KEY nlo_calculation")
call ifile_append (ifile, "LIS nlo_calculation_list = nlo_comp+")
call ifile_append (ifile, "ALT nlo_comp = " // &
"full | born | real | virtual | dglap | subtraction | " // &
"mismatch | GKS")
call ifile_append (ifile, "KEY full")

```

```

    call ifile_append (ifile, "KEY born")
    call ifile_append (ifile, "KEY virtual")
    call ifile_append (ifile, "KEY dglap")
    call ifile_append (ifile, "KEY subtraction")
    call ifile_append (ifile, "KEY mismatch")
    call ifile_append (ifile, "KEY GKS")
    call define_expr_syntax (ifile, particles=.true., analysis=.true.)
end subroutine define_cmd_list_syntax

```

<Commands: public>+≡

```
public :: lexer_init_cmd_list
```

<Commands: procedures>+≡

```

subroutine lexer_init_cmd_list (lexer, parent_lexer)
  type(lexer_t), intent(out) :: lexer
  type(lexer_t), intent(in), optional, target :: parent_lexer
  call lexer_init (lexer, &
    comment_chars = "#!", &
    quote_chars = "'", &
    quote_match = "'", &
    single_chars = "()[]{};,:&%?${@", &
    special_class = [ "+-*/^", "<>=~ " ], &
    keyword_list = syntax_get_keyword_list_ptr (syntax_cmd_list), &
    parent = parent_lexer)
end subroutine lexer_init_cmd_list

```

35.1.10 Unit Tests

Test module, followed by the corresponding implementation module.

<commands.ut.f90>≡

<File header>

```

module commands_ut
  use unit_tests
  use system_dependencies, only: MPOST_AVAILABLE
  use commands_uti

```

<Standard module head>

<Commands: public test>

```
contains
```

<Commands: test driver>

```
end module commands_ut
```

<commands.uti.f90>≡

<File header>

```
module commands_uti
```

<Use kinds>

```

        use kinds, only: i64
    <Use strings>
        use io_units
        use ifiles
        use parser
        use interactions, only: reset_interaction_counter
        use prclib_stacks
        use analysis
        use variables, only: var_list_t
        use models
        use slha_interface
        use rt_data
        use event_base, only: generic_event_t, event_callback_t
        use commands

    <Standard module head>

    <Commands: test declarations>

    <Commands: test auxiliary types>

contains

    <Commands: tests>

    <Commands: test auxiliary>

end module commands_util

```

API: driver for the unit tests below.

```

<Commands: public test>≡
    public :: commands_test

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

```

Prepare Sindarin code

This routine parses an internal file, prints the parse tree, and returns a parse node to the root. We use the routine in the tests below.

```

<Commands: public test auxiliary>≡
    public :: parse_ifile

<Commands: test auxiliary>≡
    subroutine parse_ifile (ifile, pn_root, u)
        use ifiles
        use lexers
        use parser
        use commands

```

```

type(ifile_t), intent(in) :: ifile
type(parse_node_t), pointer, intent(out) :: pn_root
integer, intent(in), optional :: u
type(stream_t), target :: stream
type(lexer_t), target :: lexer
type(parse_tree_t) :: parse_tree

call lexer_init_cmd_list (lexer)
call stream_init (stream, ifile)
call lexer_assign_stream (lexer, stream)

call parse_tree_init (parse_tree, syntax_cmd_list, lexer)
if (present (u)) call parse_tree_write (parse_tree, u)
pn_root => parse_tree%get_root_ptr ()

call stream_final (stream)
call lexer_final (lexer)
end subroutine parse_ifile

```

Empty command list

Compile and execute an empty command list. Should do nothing but test the integrity of the workflow.

```

<Commands: execute tests>≡
    call test (commands_1, "commands_1", &
        "empty command list", &
        u, results)

<Commands: test declarations>≡
    public :: commands_1

<Commands: tests>≡
    subroutine commands_1 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root

        write (u, "(A)")  "* Test output: commands_1"
        write (u, "(A)")  "* Purpose: compile and execute empty command list"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call global%global_init ()

        write (u, "(A)")  "* Parse empty file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)
    end subroutine commands_1

```

```

write (u, "(A)")
write (u, "(A)")  "* Compile command list"

if (associated (pn_root)) then
    call command_list%compile (pn_root, global)
end if

write (u, "(A)")
write (u, "(A)")  "* Execute command list"

call global%activate ()
call command_list%execute (global)
call global%deactivate ()

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call syntax_cmd_list_final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_1"

end subroutine commands_1

```

Read model

Execute a model assignment.

```

<Commands: execute tests>+≡
    call test (commands_2, "commands_2", &
        "model", &
        u, results)

<Commands: test declarations>+≡
    public :: commands_2

<Commands: tests>+≡
    subroutine commands_2 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root

        write (u, "(A)")  "* Test output: commands_2"
        write (u, "(A)")  "* Purpose: set model"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

```

```

call syntax_cmd_list_init ()
call syntax_model_file_init ()
call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')

call ifile_write (ifile, u)

write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_2"

end subroutine commands_2

```

Declare Process

Read a model, then declare a process. The process library is allocated explicitly. For the process definition, We take the default (*omega*) method. Since we do not compile, O'MEGA is not actually called.

```

(Commands: execute tests) +=
  call test (commands_3, "commands_3", &
    "process declaration", &

```



```

        u, results)
<Commands: test declarations>+≡
    public :: commands_3
<Commands: tests>+≡
    subroutine commands_3 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(prclib_entry_t), pointer :: lib

        write (u, "(A)")  "* Test output: commands_3"
        write (u, "(A)")  "* Purpose: define process"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call syntax_model_file_init ()
        call global%global_init ()
        call global%var_list%set_log (var_str ("?omega_openmp"), &
            .false., is_known = .true.)

        allocate (lib)
        call lib%init (var_str ("lib_cmd3"))
        call global%add_prclib (lib)

        write (u, "(A)")  "* Input file"
        write (u, "(A)")

        call ifile_append (ifile, 'model = "Test"')
        call ifile_append (ifile, 'process t3 = s, s => s, s')

        call ifile_write (ifile, u)

        write (u, "(A)")
        write (u, "(A)")  "* Parse file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)

        write (u, "(A)")
        write (u, "(A)")  "* Compile command list"
        write (u, "(A)")

        call command_list%compile (pn_root, global)
        call command_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Execute command list"
        write (u, "(A)")

```

```

call command_list%execute (global)

call global%prclib_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_3"

end subroutine commands_3

```

Compile Process

Read a model, then declare a process and compile the library. The process library is allocated explicitly. For the process definition, We take the default (`unit_test`) method. There is no external code, so compilation of the library is merely a formal status change.

```

<Commands: execute tests>+≡
  call test (commands_4, "commands_4", &
    "compilation", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_4

<Commands: tests>+≡
  subroutine commands_4 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: commands_4"
    write (u, "(A)")  "* Purpose: define process and compile library"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call syntax_model_file_init ()
    call global%global_init ()

```

```

call global%var_list%set_string (var_str ("method"), &
    var_str ("unit_test"), is_known=.true.)

allocate (lib)
call lib%init (var_str ("lib_cmd4"))
call global%add_prclib (lib)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process t4 = s, s => s, s')
call ifile_append (ifile, 'compile ("lib_cmd4")')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%prclib_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_4"

end subroutine commands_4

```

Integrate Process

Read a model, then declare a process, compile the library, and integrate over phase space. We take the default (`unit_test`) method and use the simplest methods of phase-space parameterization and integration.

```
(Commands: execute tests)+≡
    call test (commands_5, "commands_5", &
               "integration", &
               u, results)

(Commands: test declarations)+≡
    public :: commands_5

(Commands: tests)+≡
    subroutine commands_5 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(prclib_entry_t), pointer :: lib

        write (u, "(A)")  "* Test output: commands_5"
        write (u, "(A)")  "* Purpose: define process, iterations, and integrate"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call syntax_model_file_init ()
        call global%global_init ()
        call global%var_list%set_string (var_str ("method"), &
                                         var_str ("unit_test"), is_known=.true.)
        call global%var_list%set_string (var_str ("phs_method"), &
                                         var_str ("single"), is_known=.true.)
        call global%var_list%set_string (var_str ("integration_method"), &
                                         var_str ("midpoint"), is_known=.true.)
        call global%var_list%set_log (var_str ("?vis_history"), &
                                      .false., is_known=.true.)
        call global%var_list%set_log (var_str ("?integration_timer"), &
                                      .false., is_known=.true.)
        call global%var_list%set_real (var_str ("sqrts"), &
                                       1000._default, is_known=.true.)
        call global%var_list%set_int (var_str ("seed"), 0, is_known=.true.)

        allocate (lib)
        call lib%init (var_str ("lib_cmd5"))
        call global%add_prclib (lib)

        write (u, "(A)")  "* Input file"
        write (u, "(A)")

        call ifile_append (ifile, 'model = "Test"')
        call ifile_append (ifile, 'process t5 = s, s => s, s')
```

```

call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (t5)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call reset_interaction_counter ()
call command_list%execute (global)

call global%it_list%write (u)
write (u, "(A)")
call global%process_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_5"

end subroutine commands_5

```

Variables

Set intrinsic and user-defined variables.

```

(Commands: execute tests) +=
  call test (commands_6, "commands_6", &
    "variables", &
    u, results)

```

```

<Commands: test declarations>+≡
    public :: commands_6

<Commands: tests>+≡
    subroutine commands_6 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root

        write (u, "(A)")  "* Test output: commands_6"
        write (u, "(A)")  "*   Purpose: define and set variables"
        write (u, "(A)")

        write (u, "(A)")  "*   Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call global%global_init ()
        call global%write_vars (u, [ &
            var_str ("$_run_id"), &
            var_str ("?unweighted"), &
            var_str ("sqrts")] )

        write (u, "(A)")
        write (u, "(A)")  "*   Input file"
        write (u, "(A)")

        call ifile_append (ifile, '$run_id = "run1"')
        call ifile_append (ifile, '?unweighted = false')
        call ifile_append (ifile, 'sqrts = 1000')
        call ifile_append (ifile, 'int j = 10')
        call ifile_append (ifile, 'real x = 1000.')
        call ifile_append (ifile, 'complex z = 5')
        call ifile_append (ifile, 'string $text = "abcd"')
        call ifile_append (ifile, 'logical ?flag = true')

        call ifile_write (ifile, u)

        write (u, "(A)")
        write (u, "(A)")  "*   Parse file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)

        write (u, "(A)")
        write (u, "(A)")  "* Compile command list"
        write (u, "(A)")

        call command_list%compile (pn_root, global)
        call command_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Execute command list"

```

```

write (u, "(A)")

call command_list%execute (global)

call global%write_vars (u, [ &
    var_str ("$_run_id"), &
    var_str ("?unweighted"), &
    var_str ("sqrts"), &
    var_str ("j"), &
    var_str ("x"), &
    var_str ("z"), &
    var_str ("$_text"), &
    var_str ("?flag")])

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call syntax_cmd_list_final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_6"

end subroutine commands_6

```

Process library

Open process libraries explicitly.

```

<Commands: execute tests>+≡
    call test (commands_7, "commands_7", &
        "process library", &
        u, results)

<Commands: test declarations>+≡
    public :: commands_7

<Commands: tests>+≡
    subroutine commands_7 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root

        write (u, "(A)")  "* Test output: commands_7"
        write (u, "(A)")  "* Purpose: declare process libraries"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

```

```

call syntax_cmd_list_init ()
call global%global_init ()
call global%var_list%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)
global%os_data%fc = "Fortran-compiler"
global%os_data%fcflags = "Fortran-flags"
global%os_data%fclibs = "Fortran-libs"

write (u, "(A)")
write (u, "(A)")  "*  Input file"
write (u, "(A)")

call ifile_append (ifile, 'library = "lib_cmd7_1"')
call ifile_append (ifile, 'library = "lib_cmd7_2"')
call ifile_append (ifile, 'library = "lib_cmd7_1"')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "*  Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "*  Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "*  Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_libraries (u)

write (u, "(A)")
write (u, "(A)")  "*  Cleanup"

call ifile_final (ifile)

call command_list%final ()
call syntax_cmd_list_final ()
call global%final ()

write (u, "(A)")
write (u, "(A)")  "*  Test output end: commands_7"

end subroutine commands_7

```


Generate events

Read a model, then declare a process, compile the library, and generate weighted events. We take the default (`unit_test`) method and use the simplest methods of phase-space parameterization and integration.

```
(Commands: execute tests)+≡
    call test (commands_8, "commands_8", &
               "event generation", &
               u, results)

(Commands: test declarations)+≡
    public :: commands_8

(Commands: tests)+≡
    subroutine commands_8 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(prclib_entry_t), pointer :: lib

        write (u, "(A)")  "* Test output: commands_8"
        write (u, "(A)")  "* Purpose: define process, integrate, generate events"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call syntax_model_file_init ()
        call global%global_init ()
        call global%init_fallback_model &
            (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

        call global%var_list%set_string (var_str ("method"), &
            var_str ("unit_test"), is_known=.true.)
        call global%var_list%set_string (var_str ("phs_method"), &
            var_str ("single"), is_known=.true.)
        call global%var_list%set_string (var_str ("integration_method"), &
            var_str ("midpoint"), is_known=.true.)
        call global%var_list%set_log (var_str ("?vis_history"), &
            .false., is_known=.true.)
        call global%var_list%set_log (var_str ("?integration_timer"), &
            .false., is_known = .true.)
        call global%var_list%set_real (var_str ("sqrts"), &
            1000._default, is_known=.true.)

        allocate (lib)
        call lib%init (var_str ("lib_cmd8"))
        call global%add_prclib (lib)

        write (u, "(A)")  "* Input file"
        write (u, "(A)")
```

```

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_8_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (commands_8_p)')
call ifile_append (ifile, '?unweighted = false')
call ifile_append (ifile, 'n_events = 3')
call ifile_append (ifile, '?read_raw = false')
call ifile_append (ifile, 'simulate (commands_8_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"

call command_list%execute (global)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_8"

end subroutine commands_8

```

Define cuts

Declare a cut expression.

```

(Commands: execute tests) +=
  call test (commands_9, "commands_9", &
    "cuts", &
    u, results)

```

```

<Commands: test declarations>+≡
    public :: commands_9

<Commands: tests>+≡
    subroutine commands_9 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(string_t), dimension(0) :: no_vars

        write (u, "(A)")  "* Test output: commands_9"
        write (u, "(A)")  "* Purpose: define cuts"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call global%global_init ()

        write (u, "(A)")  "* Input file"
        write (u, "(A)")

        call ifile_append (ifile, 'cuts = all Pt > 0 [particle]')

        call ifile_write (ifile, u)

        write (u, "(A)")
        write (u, "(A)")  "* Parse file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)

        write (u, "(A)")
        write (u, "(A)")  "* Compile command list"
        write (u, "(A)")

        call command_list%compile (pn_root, global)
        call command_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Execute command list"
        write (u, "(A)")

        call command_list%execute (global)

        call global%write (u, vars = no_vars)

        write (u, "(A)")
        write (u, "(A)")  "* Cleanup"

        call ifile_final (ifile)

```

```

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_9"

end subroutine commands_9

```

Beams

Define beam setup.

```

<Commands: execute tests>+≡
call test (commands_10, "commands_10", &
  "beams", &
  u, results)

<Commands: test declarations>+≡
public :: commands_10

<Commands: tests>+≡
subroutine commands_10 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_10"
  write (u, "(A)")  "* Purpose: define beams"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call syntax_model_file_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, 'model = QCD')
  call ifile_append (ifile, 'sqrts = 1000')
  call ifile_append (ifile, 'beams = p, p')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

  call parse_ifile (ifile, pn_root, u)

```

```

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_beams (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_10"

end subroutine commands_10

```

Structure functions

Define beam setup with structure functions

```

<Commands: execute tests>+≡
  call test (commands_11, "commands_11", &
    "structure functions", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_11

<Commands: tests>+≡
  subroutine commands_11 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_11"
    write (u, "(A)")  "* Purpose: define beams with structure functions"
    write (u, "(A)")

```

```

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call syntax_model_file_init ()
call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = QCD')
call ifile_append (ifile, 'sqrts = 1100')
call ifile_append (ifile, 'beams = p, p => lhpdf => pdf_builtin, isr')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_beams (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_11"

end subroutine commands_11

```

Rescan events

Read a model, then declare a process, compile the library, and generate weighted events. We take the default (`unit_test`) method and use the simplest methods of phase-space parameterization and integration. Then, rescan the generated event sample.

```
(Commands: execute tests)+≡
  call test (commands_12, "commands_12", &
    "event rescanning", &
    u, results)

(Commands: test declarations)+≡
  public :: commands_12

(Commands: tests)+≡
  subroutine commands_12 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: commands_12"
    write (u, "(A)")  "* Purpose: generate events and rescan"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call syntax_model_file_init ()

    call global%global_init ()
    call global%var_list%append_log (&
      var_str ("?rebuild_phase_space"), .false., &
      intrinsic=.true.)
    call global%var_list%append_log (&
      var_str ("?rebuild_grids"), .false., &
      intrinsic=.true.)
    call global%init_fallback_model &
      (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

    call global%var_list%set_string (var_str ("$method"), &
      var_str ("unit_test"), is_known=.true.)
    call global%var_list%set_string (var_str ("$phs_method"), &
      var_str ("single"), is_known=.true.)
    call global%var_list%set_string (var_str ("$integration_method"), &
      var_str ("midpoint"), is_known=.true.)
    call global%var_list%set_log (var_str ("?vis_history"), &
      .false., is_known=.true.)
    call global%var_list%set_log (var_str ("?integration_timer"), &
      .false., is_known = .true.)
    call global%var_list%set_real (var_str ("sqrts"), &
      1000._default, is_known=.true.)
```

```

allocate (lib)
call lib%init (var_str ("lib_cmd12"))
call global%add_prclib (lib)

write (u, "(A)")  "*   Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_12_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (commands_12_p)')
call ifile_append (ifile, '?unweighted = false')
call ifile_append (ifile, 'n_events = 3')
call ifile_append (ifile, '?read_raw = false')
call ifile_append (ifile, 'simulate (commands_12_p)')
call ifile_append (ifile, '?write_raw = false')
call ifile_append (ifile, 'rescan "commands_12_p" (commands_12_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "*   Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"

call command_list%execute (global)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_12"

end subroutine commands_12

```


Event Files

Set output formats for event files.

```
(Commands: execute tests)+≡
    call test (commands_13, "commands_13", &
               "event output formats", &
               u, results)

(Commands: test declarations)+≡
    public :: commands_13

(Commands: tests)+≡
    subroutine commands_13 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        type(prclib_entry_t), pointer :: lib
        logical :: exist

        write (u, "(A)")  "* Test output: commands_13"
        write (u, "(A)")  "*   Purpose: generate events and rescan"
        write (u, "(A)")

        write (u, "(A)")  "*   Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call syntax_model_file_init ()
        call global%global_init ()
        call global%init_fallback_model &
            (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

        call global%var_list%set_string (var_str ("method"), &
            var_str ("unit_test"), is_known=.true.)
        call global%var_list%set_string (var_str ("phs_method"), &
            var_str ("single"), is_known=.true.)
        call global%var_list%set_string (var_str ("integration_method"), &
            var_str ("midpoint"), is_known=.true.)
        call global%var_list%set_real (var_str ("sqrts"), &
            1000._default, is_known=.true.)
        call global%var_list%set_log (var_str ("?vis_history"), &
            .false., is_known=.true.)
        call global%var_list%set_log (var_str ("?integration_timer"), &
            .false., is_known = .true.)

        allocate (lib)
        call lib%init (var_str ("lib_cmd13"))
        call global%add_prclib (lib)

        write (u, "(A)")  "*   Input file"
        write (u, "(A)")
```

```

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_13_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (commands_13_p)')
call ifile_append (ifile, '?unweighted = false')
call ifile_append (ifile, 'n_events = 1')
call ifile_append (ifile, '?read_raw = false')
call ifile_append (ifile, 'sample_format = weight_stream')
call ifile_append (ifile, 'simulate (commands_13_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"

call command_list%execute (global)

write (u, "(A)")
write (u, "(A)")  "* Verify output files"
write (u, "(A)")

inquire (file = "commands_13_p.evx", exist = exist)
if (exist) write (u, "(1x,A)")  "raw"

inquire (file = "commands_13_p.weights.dat", exist = exist)
if (exist) write (u, "(1x,A)")  "weight_stream"

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_13"

```

```
end subroutine commands_13
```

Compile Empty Libraries

(This is a regression test:) Declare two empty libraries and compile them.

```
<Commands: execute tests>+≡
  call test (commands_14, "commands_14", &
    "empty libraries", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_14

<Commands: tests>+≡
  subroutine commands_14 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_14"
    write (u, "(A)")  "* Purpose: define and compile empty libraries"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_model_file_init ()
    call syntax_cmd_list_init ()

    call global%global_init ()

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, 'model = "Test"')
    call ifile_append (ifile, 'library = "lib1"')
    call ifile_append (ifile, 'library = "lib2"')
    call ifile_append (ifile, 'compile ()')

    call ifile_write (ifile, u)

    write (u, "(A)")
    write (u, "(A)")  "* Parse file"
    write (u, "(A)")

    call parse_ifile (ifile, pn_root)

    write (u, "(A)")  "* Compile command list"
    write (u, "(A)")

    call command_list%compile (pn_root, global)
```

```

write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%prclib_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()

call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_14"

end subroutine commands_14

```

Compile Process

Read a model, then declare a process and compile the library. The process library is allocated explicitly. For the process definition, We take the default (`unit_test`) method. There is no external code, so compilation of the library is merely a formal status change.

```

<Commands: execute tests>+≡
  call test (commands_15, "commands_15", &
    "compilation", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_15

<Commands: tests>+≡
  subroutine commands_15 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: commands_15"
    write (u, "(A)")  "* Purpose: define process and compile library"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

```

```

call syntax_cmd_list_init ()
call syntax_model_file_init ()
call global%global_init ()
call global%var_list%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known=.true.)
call global%var_list%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known=.true.)
call global%var_list%set_string (var_str ("$integration_method"),&
    var_str ("midpoint"), is_known=.true.)
call global%var_list%set_real (var_str ("sqrts"), &
    1000._default, is_known=.true.)
call global%var_list%set_log (var_str ("?vis_history"),&
    .false., is_known=.true.)
call global%var_list%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)

allocate (lib)
call lib%init (var_str ("lib_cmd15"))
call global%add_prclib (lib)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process t15 = s, s => s, s')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (t15)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%prclib_stack%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

```

```

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_15"

end subroutine commands_15

```

Observable

Declare an observable, fill it and display.

```

<Commands: execute tests>+≡
call test (commands_16, "commands_16", &
  "observables", &
  u, results)

<Commands: test declarations>+≡
public :: commands_16

<Commands: tests>+≡
subroutine commands_16 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_16"
  write (u, "(A)")  "* Purpose: declare an observable"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, '$obs_label = "foo"')
  call ifile_append (ifile, '$obs_unit = "cm"')
  call ifile_append (ifile, '$title = "Observable foo"')
  call ifile_append (ifile, '$description = "This is observable foo"')
  call ifile_append (ifile, 'observable foo')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

```

```

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Record two data items"
write (u, "(A)")

call analysis_record_data (var_str ("foo"), 1._default)
call analysis_record_data (var_str ("foo"), 3._default)

write (u, "(A)")  "* Display analysis store"
write (u, "(A)")

call analysis_write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_16"

end subroutine commands_16

```

Histogram

Declare a histogram, fill it and display.

```

<Commands: execute tests>+≡
  call test (commands_17, "commands_17", &
    "histograms", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_17

```

```

{Commands: tests}+≡
subroutine commands_17 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root
  type(string_t), dimension(3) :: name
  integer :: i

  write (u, "(A)")  "* Test output: commands_17"
  write (u, "(A)")  "* Purpose: declare histograms"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, '$obs_label = "foo"')
  call ifile_append (ifile, '$obs_unit = "cm"')
  call ifile_append (ifile, '$title = "Histogram foo"')
  call ifile_append (ifile, '$description = "This is histogram foo"')
  call ifile_append (ifile, 'histogram foo (0,5,1)')
  call ifile_append (ifile, '$title = "Histogram bar"')
  call ifile_append (ifile, '$description = "This is histogram bar"')
  call ifile_append (ifile, 'n_bins = 2')
  call ifile_append (ifile, 'histogram bar (0,5)')
  call ifile_append (ifile, '$title = "Histogram gee"')
  call ifile_append (ifile, '$description = "This is histogram gee"')
  call ifile_append (ifile, '?normalize_bins = true')
  call ifile_append (ifile, 'histogram gee (0,5)')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

  call parse_ifile (ifile, pn_root)

  write (u, "(A)")  "* Compile command list"
  write (u, "(A)")

  call command_list%compile (pn_root, global)

  call command_list%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Execute command list"

```



```

write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Record two data items"
write (u, "(A)")

name(1) = "foo"
name(2) = "bar"
name(3) = "gee"

do i = 1, 3
  call analysis_record_data (name(i), 0.1_default, &
    weight = 0.25_default)
  call analysis_record_data (name(i), 3.1_default)
  call analysis_record_data (name(i), 4.1_default, &
    excess = 0.5_default)
  call analysis_record_data (name(i), 7.1_default)
end do

write (u, "(A)")  "* Display analysis store"
write (u, "(A)")

call analysis_write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_17"

end subroutine commands_17

```

Plot

Declare a plot, fill it and display contents.

```

<Commands: execute tests>+≡
  call test (commands_18, "commands_18", &
    "plots", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_18

<Commands: tests>+≡
  subroutine commands_18 (u)

```

```

integer, intent(in) :: u
type(ifile_t) :: ifile
type(command_list_t), target :: command_list
type(rt_data_t), target :: global
type(parse_node_t), pointer :: pn_root

write (u, "(A)")  "* Test output: commands_18"
write (u, "(A)")  "* Purpose: declare a plot"
write (u, "(A)")

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, '$obs_label = "foo"')
call ifile_append (ifile, '$obs_unit = "cm"')
call ifile_append (ifile, '$title = "Plot foo"')
call ifile_append (ifile, '$description = "This is plot foo"')
call ifile_append (ifile, '$x_label = "x axis"')
call ifile_append (ifile, '$y_label = "y axis"')
call ifile_append (ifile, '?x_log = false')
call ifile_append (ifile, '?y_log = true')
call ifile_append (ifile, 'x_min = -1')
call ifile_append (ifile, 'x_max = 1')
call ifile_append (ifile, 'y_min = 0.1')
call ifile_append (ifile, 'y_max = 1000')
call ifile_append (ifile, 'plot foo')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

```

```

write (u, "(A)")  "* Record two data items"
write (u, "(A)")

call analysis_record_data (var_str ("foo"), 0._default, 20._default, &
    xerr = 0.25_default)
call analysis_record_data (var_str ("foo"), 0.5_default, 0.2_default, &
    yerr = 0.07_default)
call analysis_record_data (var_str ("foo"), 3._default, 2._default)

write (u, "(A)")  "* Display analysis store"
write (u, "(A)")

call analysis_write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_18"

end subroutine commands_18

```

Graph

Combine two (empty) plots to a graph.

```

<Commands: execute tests>+≡
    call test (commands_19, "commands_19", &
        "graphs", &
        u, results)

<Commands: test declarations>+≡
    public :: commands_19

<Commands: tests>+≡
    subroutine commands_19 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root

        write (u, "(A)")  "* Test output: commands_19"
        write (u, "(A)")  "* Purpose: combine two plots to a graph"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"

```

```

write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'plot a')
call ifile_append (ifile, 'plot b')
call ifile_append (ifile, '$title = "Graph foo"')
call ifile_append (ifile, '$description = "This is graph foo"')
call ifile_append (ifile, 'graph foo = a & b')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis object"
write (u, "(A)")

call analysis_write (var_str ("foo"), u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_19"

```

```
end subroutine commands_19
```

Record Data

Record data in previously allocated analysis objects.

```
<Commands: execute tests>+≡
  call test (commands_20, "commands_20", &
    "record data", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_20

<Commands: tests>+≡
  subroutine commands_20 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_20"
    write (u, "(A)")  "* Purpose: record data"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization: create observable, histogram, plot"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

    call analysis_init_observable (var_str ("o"))
    call analysis_init_histogram (var_str ("h"), 0._default, 1._default, 3, &
      normalize_bins = .false.)
    call analysis_init_plot (var_str ("p"))

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, 'record o (1.234)')
    call ifile_append (ifile, 'record h (0.5)')
    call ifile_append (ifile, 'record p (1, 2)')

    call ifile_write (ifile, u)

    write (u, "(A)")
    write (u, "(A)")  "* Parse file"
    write (u, "(A)")

    call parse_ifile (ifile, pn_root)

    write (u, "(A)")  "* Compile command list"
    write (u, "(A)")
```

```

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis object"
write (u, "(A)")

call analysis_write (u, verbose = .true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_20"

end subroutine commands_20

```

Analysis

Declare an analysis expression and use it to fill an observable during event generation.

```

<Commands: execute tests>+≡
  call test (commands_21, "commands_21", &
    "analysis expression", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_21

<Commands: tests>+≡
  subroutine commands_21 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: commands_21"
  end subroutine

```

```

write (u, "(A)")  "*" Purpose: create and use analysis expression"
write (u, "(A)")

write (u, "(A)")  "*" Initialization: create observable"
write (u, "(A)")

call syntax_cmd_list_init ()
call syntax_model_file_init ()
call global%global_init ()
call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%var_list%set_string (var_str ("$method"), &
    var_str ("unit_test"), is_known=.true.)
call global%var_list%set_string (var_str ("$phs_method"), &
    var_str ("single"), is_known=.true.)
call global%var_list%set_string (var_str ("$integration_method"),&
    var_str ("midpoint"), is_known=.true.)
call global%var_list%set_log (var_str ("?vis_history"),&
    .false., is_known=.true.)
call global%var_list%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)
call global%var_list%set_real (var_str ("sqrts"), &
    1000._default, is_known=.true.)

allocate (lib)
call lib%init (var_str ("lib_cmd8"))
call global%add_prclib (lib)

call analysis_init_observable (var_str ("m"))

write (u, "(A)")  "*" Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_21_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:100')
call ifile_append (ifile, 'integrate (commands_21_p)')
call ifile_append (ifile, '?unweighted = true')
call ifile_append (ifile, 'n_events = 3')
call ifile_append (ifile, '?read_raw = false')
call ifile_append (ifile, 'observable m')
call ifile_append (ifile, 'analysis = record m (eval M [s])')
call ifile_append (ifile, 'simulate (commands_21_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "*" Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

```

```

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis object"
write (u, "(A)")

call analysis_write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_21"

end subroutine commands_21

```

Write Analysis

Write accumulated analysis data to file.

```

<Commands: execute tests>+≡
  call test (commands_22, "commands_22", &
    "write analysis", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_22

<Commands: tests>+≡
  subroutine commands_22 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    integer :: u_file, iostat
    logical :: exist

```



```

character(80) :: buffer

write (u, "(A)")  "* Test output: commands_22"
write (u, "(A)")  "* Purpose: write analysis data"
write (u, "(A)")

write (u, "(A)")  "* Initialization: create observable"
write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

call analysis_init_observable (var_str ("m"))
call analysis_record_data (var_str ("m"), 125._default)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, '$out_file = "commands_22.dat"')
call ifile_append (ifile, 'write_analysis')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis data"
write (u, "(A)")

inquire (file = "commands_22.dat", exist = exist)
if (.not. exist) then
    write (u, "(A)")  "ERROR: File commands_22.dat not found"
    return
end if

u_file = free_unit ()
open (u_file, file = "commands_22.dat", &
      action = "read", status = "old")

```

```

do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (iostat /= 0)  exit
  write (u, "(A)") trim (buffer)
end do
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_22"

end subroutine commands_22

```

Compile Analysis

Write accumulated analysis data to file and compile.

```

<Commands: execute tests>+≡
  if (MPOST_AVAILABLE) then
    call test (commands_23, "commands_23", &
      "compile analysis", &
      u, results)
  end if

<Commands: test declarations>+≡
  public :: commands_23

<Commands: tests>+≡
  subroutine commands_23 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    integer :: u_file, iostat
    character(256) :: buffer
    logical :: exist
    type(graph_options_t) :: graph_options

    write (u, "(A)")  "* Test output: commands_23"
    write (u, "(A)")  "* Purpose: write and compile analysis data"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization: create and fill histogram"
    write (u, "(A)")

```

```

call syntax_cmd_list_init ()
call global%global_init ()

call graph_options_init (graph_options)
call graph_options_set (graph_options, &
    title = var_str ("Histogram for test: commands 23"), &
    description = var_str ("This is a test."), &
    width_mm = 125, height_mm = 85)
call analysis_init_histogram (var_str ("h"), &
    0._default, 10._default, 2._default, .false., &
    graph_options = graph_options)
call analysis_record_data (var_str ("h"), 1._default)
call analysis_record_data (var_str ("h"), 1._default)
call analysis_record_data (var_str ("h"), 1._default)
call analysis_record_data (var_str ("h"), 1._default)
call analysis_record_data (var_str ("h"), 3._default)
call analysis_record_data (var_str ("h"), 3._default)
call analysis_record_data (var_str ("h"), 3._default)
call analysis_record_data (var_str ("h"), 5._default)
call analysis_record_data (var_str ("h"), 7._default)
call analysis_record_data (var_str ("h"), 7._default)
call analysis_record_data (var_str ("h"), 7._default)
call analysis_record_data (var_str ("h"), 7._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)
call analysis_record_data (var_str ("h"), 9._default)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, '$out_file = "commands_23.dat"')
call ifile_append (ifile, 'compile_analysis')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")

```

```

write (u, "(A)")  "* Delete Postscript output"
write (u, "(A)")

inquire (file = "commands_23.ps", exist = exist)
if (exist) then
    u_file = free_unit ()
    open (u_file, file = "commands_23.ps", action = "write", status = "old")
    close (u_file, status = "delete")
end if
inquire (file = "commands_23.ps", exist = exist)
write (u, "(1x,A,L1)")  "Postscript output exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* TeX file"
write (u, "(A)")

inquire (file = "commands_23.tex", exist = exist)
if (.not. exist) then
    write (u, "(A)")  "ERROR: File commands_23.tex not found"
    return
end if

u_file = free_unit ()
open (u_file, file = "commands_23.tex", &
    action = "read", status = "old")
do
    read (u_file, "(A)", iostat = iostat)  buffer
    if (iostat /= 0)  exit
    write (u, "(A)")  trim (buffer)
end do
close (u_file)
write (u, *)

inquire (file = "commands_23.ps", exist = exist)
write (u, "(1x,A,L1)")  "Postscript output exists = ", exist

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_23"

```

```
end subroutine commands_23
```

Histogram

Declare a histogram, fill it and display.

```
<Commands: execute tests>+≡
  call test (commands_24, "commands_24", &
    "drawing options", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_24

<Commands: tests>+≡
  subroutine commands_24 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_24"
    write (u, "(A)")  "* Purpose: check graph and drawing options"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, '$title = "Title"')
    call ifile_append (ifile, '$description = "Description"')
    call ifile_append (ifile, '$x_label = "X Label"')
    call ifile_append (ifile, '$y_label = "Y Label"')
    call ifile_append (ifile, 'graph_width_mm = 111')
    call ifile_append (ifile, 'graph_height_mm = 222')
    call ifile_append (ifile, 'x_min = -11')
    call ifile_append (ifile, 'x_max = 22')
    call ifile_append (ifile, 'y_min = -33')
    call ifile_append (ifile, 'y_max = 44')
    call ifile_append (ifile, '$gmlcode_bg = "GML Code BG"')
    call ifile_append (ifile, '$gmlcode_fg = "GML Code FG"')
    call ifile_append (ifile, '$fill_options = "Fill Options"')
    call ifile_append (ifile, '$draw_options = "Draw Options"')
    call ifile_append (ifile, '$err_options = "Error Options"')
    call ifile_append (ifile, '$symbol = "Symbol"')
    call ifile_append (ifile, 'histogram foo (0,1)')
    call ifile_append (ifile, 'plot bar')
```

```

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Display analysis store"
write (u, "(A)")

call analysis_write (u, verbose=.true.)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_24"

end subroutine commands_24

```

Local Environment

Declare a local environment.

```

<Commands: execute tests>+≡
  call test (commands_25, "commands_25", &
    "local process environment", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_25

```

```

<Commands: tests>+≡
subroutine commands_25 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_25"
  write (u, "(A)")  "* Purpose: declare local environment for process"
  write (u, "(A)")

  call syntax_model_file_init ()
  call syntax_cmd_list_init ()
  call global%global_init ()
  call global%var_list%set_log (var_str ("?omega_openmp"), &
    .false., is_known = .true.)

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, 'library = "commands_25_lib"')
  call ifile_append (ifile, 'model = "Test"')
  call ifile_append (ifile, 'process commands_25_p1 = g, g => g, g &
    &{ model = "QCD" }')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

  call parse_ifile (ifile, pn_root)

  write (u, "(A)")  "* Compile command list"
  write (u, "(A)")

  call command_list%compile (pn_root, global)
  call command_list%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Execute command list"
  write (u, "(A)")

  call command_list%execute (global)
  call global%write_libraries (u)

  write (u, "(A)")
  write (u, "(A)")  "* Cleanup"

  call ifile_final (ifile)

  call command_list%final ()
  call global%final ()

```

```

call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_25"

end subroutine commands_25

```

Alternative Setups

Declare a list of alternative setups.

```

<Commands: execute tests>+≡
call test (commands_26, "commands_26", &
  "alternative setups", &
  u, results)

<Commands: test declarations>+≡
public :: commands_26

<Commands: tests>+≡
subroutine commands_26 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_26"
  write (u, "(A)")  "* Purpose: declare alternative setups for simulation"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, 'int i = 0')
  call ifile_append (ifile, 'alt_setup = ({ i = 1 }, { i = 2 })')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

  call parse_ifile (ifile, pn_root)

  write (u, "(A)")  "* Compile command list"
  write (u, "(A)")

  call command_list%compile (pn_root, global)
  call command_list%write (u)

```



```

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_26"

end subroutine commands_26

```

Unstable Particle

Define decay processes and declare a particle as unstable. Also check the commands stable, polarized, unpolarized.

```

<Commands: execute tests>+≡
  call test (commands_27, "commands_27", &
    "unstable and polarized particles", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_27

<Commands: tests>+≡
  subroutine commands_27 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib

    write (u, "(A)")  "* Test output: commands_27"
    write (u, "(A)")  "* Purpose: modify particle properties"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call syntax_model_file_init ()
    call global%global_init ()
    call global%var_list%set_string (var_str ("method"), &
      var_str ("unit_test"), is_known=.true.)
    call global%var_list%set_string (var_str ("phs_method"), &

```

```

        var_str ("single"), is_known=.true.)
call global%var_list%set_string (var_str ("integration_method"),&
    var_str ("midpoint"), is_known=.true.)
call global%var_list%set_log (var_str ("?vis_history"),&
    .false., is_known=.true.)
call global%var_list%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)

allocate (lib)
call lib%init (var_str ("commands_27_lib"))
call global%add_prclib (lib)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'ff = 0.4')
call ifile_append (ifile, 'process d1 = s => f, fbar')
call ifile_append (ifile, 'unstable s (d1)')
call ifile_append (ifile, 'polarized f, fbar')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Show model"
write (u, "(A)")

call global%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extra Input"
write (u, "(A)")

call ifile_final (ifile)
call ifile_append (ifile, '?diagonal_decay = true')
call ifile_append (ifile, 'unstable s (d1)')

```

```

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%final ()
call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Show model"
write (u, "(A)")

call global%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extra Input"
write (u, "(A)")

call ifile_final (ifile)
call ifile_append (ifile, '?isotropic_decay = true')
call ifile_append (ifile, 'unstable s (d1)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%final ()
call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

```

```

write (u, "(A)")  "* Show model"
write (u, "(A)")

call global%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Extra Input"
write (u, "(A)")

call ifile_final (ifile)
call ifile_append (ifile, 'stable s')
call ifile_append (ifile, 'unpolarized f')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%final ()
call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Show model"
write (u, "(A)")

call global%model%write (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_model_file_init ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_27"

end subroutine commands_27

```

Quit the program

Quit the program.

```
(Commands: execute tests)+≡
    call test (commands_28, "commands_28", &
               "quit", &
               u, results)

(Commands: test declarations)+≡
    public :: commands_28

(Commands: tests)+≡
    subroutine commands_28 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root1, pn_root2
        type(string_t), dimension(0) :: no_vars

        write (u, "(A)")  "* Test output: commands_28"
        write (u, "(A)")  "* Purpose: quit the program"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call global%global_init ()

        write (u, "(A)")  "* Input file: quit without code"
        write (u, "(A)")

        call ifile_append (ifile, 'quit')

        call ifile_write (ifile, u)

        write (u, "(A)")
        write (u, "(A)")  "* Parse file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root1, u)

        write (u, "(A)")
        write (u, "(A)")  "* Compile command list"
        write (u, "(A)")

        call command_list%compile (pn_root1, global)
        call command_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Execute command list"
        write (u, "(A)")
```

```

call command_list%execute (global)

call global%write (u, vars = no_vars)

write (u, "(A)")
write (u, "(A)")  "* Input file: quit with code"
write (u, "(A)")

call ifile_final (ifile)
call command_list%final ()
call ifile_append (ifile, 'quit ( 3 + 4 )')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root2, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root2, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write (u, vars = no_vars)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_28"

end subroutine commands_28

```

SLHA interface

Testing commands steering the SLHA interface.

```

<Commands: execute tests>+≡
    call test (commands_29, "commands_29", &
        "SLHA interface", &
        u, results)

<Commands: test declarations>+≡
    public :: commands_29

<Commands: tests>+≡
    subroutine commands_29 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(var_list_t), pointer :: model_vars
        type(parse_node_t), pointer :: pn_root

        write (u, "(A)")  "* Test output: commands_29"
        write (u, "(A)")  "* Purpose: test SLHA interface"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call syntax_model_file_init ()
        call syntax_slha_init ()
        call global%global_init ()

        write (u, "(A)")  "* Model MSSM, read SLHA file"
        write (u, "(A)")

        call ifile_append (ifile, 'model = "MSSM"')
        call ifile_append (ifile, '?slha_read_decays = true')
        call ifile_append (ifile, 'read_slha ("sps1ap_decays.slha")')

        call ifile_write (ifile, u)

        write (u, "(A)")
        write (u, "(A)")  "* Parse file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)

        write (u, "(A)")
        write (u, "(A)")  "* Compile command list"
        write (u, "(A)")

        call command_list%compile (pn_root, global)
        call command_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Model MSSM, default values:"
        write (u, "(A)")

```

```

call global%model%write (u, verbose = .false., &
    show_vertices = .false., show_particles = .false.)

write (u, "(A)")
write (u, "(A)")  "* Selected global variables"
write (u, "(A)")

model_vars => global%model%get_var_list_ptr ()

call model_vars%write_var (var_str ("mch1"), u)
call model_vars%write_var (var_str ("wch1"), u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")  "* Model MSSM, values from SLHA file"
write (u, "(A)")

call global%model%write (u, verbose = .false., &
    show_vertices = .false., show_particles = .false.)

write (u, "(A)")
write (u, "(A)")  "* Selected global variables"
write (u, "(A)")

model_vars => global%model%get_var_list_ptr ()

call model_vars%write_var (var_str ("mch1"), u)
call model_vars%write_var (var_str ("wch1"), u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_slha_final ()
call syntax_model_file_final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_29"

end subroutine commands_29

```

Expressions for scales

Declare a scale, factorization scale or factorization scale expression.

(Commands: execute tests)+≡


```

call test (commands_30, "commands_30", &
          "scales", &
          u, results)

<Commands: test declarations>+≡
public :: commands_30

<Commands: tests>+≡
subroutine commands_30 (u)
  integer, intent(in) :: u
  type(ifile_t) :: ifile
  type(command_list_t), target :: command_list
  type(rt_data_t), target :: global
  type(parse_node_t), pointer :: pn_root

  write (u, "(A)")  "* Test output: commands_30"
  write (u, "(A)")  "* Purpose: define scales"
  write (u, "(A)")

  write (u, "(A)")  "* Initialization"
  write (u, "(A)")

  call syntax_cmd_list_init ()
  call global%global_init ()

  write (u, "(A)")  "* Input file"
  write (u, "(A)")

  call ifile_append (ifile, 'scale = 200 GeV')
  call ifile_append (ifile, &
                    'factorization_scale = eval Pt [particle]')
  call ifile_append (ifile, &
                    'renormalization_scale = eval E [particle]')

  call ifile_write (ifile, u)

  write (u, "(A)")
  write (u, "(A)")  "* Parse file"
  write (u, "(A)")

  call parse_ifile (ifile, pn_root, u)

  write (u, "(A)")
  write (u, "(A)")  "* Compile command list"
  write (u, "(A)")

  call command_list%compile (pn_root, global)
  call command_list%write (u)

  write (u, "(A)")
  write (u, "(A)")  "* Execute command list"
  write (u, "(A)")

  call command_list%execute (global)

```

```

call global%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_30"

end subroutine commands_30

```

Weight and reweight expressions

Declare an expression for event weights and reweighting.

```

<Commands: execute tests>+≡
  call test (commands_31, "commands_31", &
    "event weights/reweighting", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_31

<Commands: tests>+≡
  subroutine commands_31 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

    write (u, "(A)")  "* Test output: commands_31"
    write (u, "(A)")  "* Purpose: define weight/reweight"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization"
    write (u, "(A)")

    call syntax_cmd_list_init ()
    call global%global_init ()

    write (u, "(A)")  "* Input file"
    write (u, "(A)")

    call ifile_append (ifile, 'weight = eval Pz [particle]')
    call ifile_append (ifile, 'reweight = eval M2 [particle]')

    call ifile_write (ifile, u)

    write (u, "(A)")

```

```

write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_31"

end subroutine commands_31

```

Selecting events

Declare an expression for selecting events in an analysis.

```

<Commands: execute tests>+≡
  call test (commands_32, "commands_32", &
    "event selection", &
    u, results)

<Commands: test declarations>+≡
  public :: commands_32

<Commands: tests>+≡
  subroutine commands_32 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root

```

```

write (u, "(A)")  "* Test output: commands_32"
write (u, "(A)")  "* Purpose: define selection"
write (u, "(A)")

write (u, "(A)")  "* Initialization"
write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'selection = any PDG == 13 [particle]')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

call parse_ifile (ifile, pn_root, u)

write (u, "(A)")
write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)
call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

call global%write_expr (u)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_32"

end subroutine commands_32

```

Executing shell commands

Execute a shell command.

```
(Commands: execute tests)+≡
    call test (commands_33, "commands_33", &
        "execute shell command", &
        u, results)

(Commands: test declarations)+≡
    public :: commands_33

(Commands: tests)+≡
    subroutine commands_33 (u)
        integer, intent(in) :: u
        type(ifile_t) :: ifile
        type(command_list_t), target :: command_list
        type(rt_data_t), target :: global
        type(parse_node_t), pointer :: pn_root
        integer :: u_file, iostat
        character(3) :: buffer

        write (u, "(A)")  "* Test output: commands_33"
        write (u, "(A)")  "* Purpose: execute shell command"
        write (u, "(A)")

        write (u, "(A)")  "* Initialization"
        write (u, "(A)")

        call syntax_cmd_list_init ()
        call global%global_init ()

        write (u, "(A)")  "* Input file"
        write (u, "(A)")

        call ifile_append (ifile, 'exec ("echo foo >> bar")')

        call ifile_write (ifile, u)

        write (u, "(A)")
        write (u, "(A)")  "* Parse file"
        write (u, "(A)")

        call parse_ifile (ifile, pn_root, u)

        write (u, "(A)")
        write (u, "(A)")  "* Compile command list"
        write (u, "(A)")

        call command_list%compile (pn_root, global)
        call command_list%write (u)

        write (u, "(A)")
        write (u, "(A)")  "* Execute command list"
        write (u, "(A)")
```

```

call command_list%execute (global)
u_file = free_unit ()
open (u_file, file = "bar", &
      action = "read", status = "old")
do
  read (u_file, "(A)", iostat = iostat)  buffer
  if (iostat /= 0) exit
end do
write (u, "(A,A)")  "should be 'foo': ", trim (buffer)
close (u_file)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_33"

end subroutine commands_33

```

Callback

Instead of an explicit write, use the callback feature to write the analysis file during event generation. We generate 4 events and arrange that the callback is executed while writing the 3rd event.

```

<Commands: execute tests>+≡
  call test (commands_34, "commands_34", &
            "analysis via callback", &
            u, results)

<Commands: test declarations>+≡
  public :: commands_34

<Commands: tests>+≡
  subroutine commands_34 (u)
    integer, intent(in) :: u
    type(ifile_t) :: ifile
    type(command_list_t), target :: command_list
    type(rt_data_t), target :: global
    type(parse_node_t), pointer :: pn_root
    type(prclib_entry_t), pointer :: lib
    type(event_callback_34_t) :: event_callback

    write (u, "(A)")  "* Test output: commands_34"
    write (u, "(A)")  "* Purpose: write analysis data"
    write (u, "(A)")

    write (u, "(A)")  "* Initialization: create observable"

```

```

write (u, "(A)")

call syntax_cmd_list_init ()
call global%global_init ()

call syntax_model_file_init ()
call global%global_init ()
call global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))

call global%var_list%set_string (var_str ("method"), &
    var_str ("unit_test"), is_known=.true.)
call global%var_list%set_string (var_str ("phs_method"), &
    var_str ("single"), is_known=.true.)
call global%var_list%set_string (var_str ("integration_method"),&
    var_str ("midpoint"), is_known=.true.)
call global%var_list%set_real (var_str ("sqrts"), &
    1000._default, is_known=.true.)
call global%var_list%set_log (var_str ("?vis_history"),&
    .false., is_known=.true.)
call global%var_list%set_log (var_str ("?integration_timer"),&
    .false., is_known = .true.)
call global%var_list%set_int (var_str ("seed"), 0, is_known=.true.)

allocate (lib)
call lib%init (var_str ("lib_cmd34"))
call global%add_prclib (lib)

write (u, "(A)")  "* Prepare callback for writing analysis to I/O unit"
write (u, "(A)")

event_callback%u = u
call global%set_event_callback (event_callback)

write (u, "(A)")  "* Input file"
write (u, "(A)")

call ifile_append (ifile, 'model = "Test"')
call ifile_append (ifile, 'process commands_34_p = s, s => s, s')
call ifile_append (ifile, 'compile')
call ifile_append (ifile, 'iterations = 1:1000')
call ifile_append (ifile, 'integrate (commands_34_p)')
call ifile_append (ifile, 'observable sq')
call ifile_append (ifile, 'analysis = record sq (sqrts)')
call ifile_append (ifile, 'n_events = 4')
call ifile_append (ifile, 'event_callback_interval = 3')
call ifile_append (ifile, 'simulate (commands_34_p)')

call ifile_write (ifile, u)

write (u, "(A)")
write (u, "(A)")  "* Parse file"
write (u, "(A)")

```

```

call parse_ifile (ifile, pn_root)

write (u, "(A)")  "* Compile command list"
write (u, "(A)")

call command_list%compile (pn_root, global)

call command_list%write (u)

write (u, "(A)")
write (u, "(A)")  "* Execute command list"
write (u, "(A)")

call command_list%execute (global)

write (u, "(A)")
write (u, "(A)")  "* Cleanup"

call ifile_final (ifile)

call analysis_final ()
call command_list%final ()
call global%final ()
call syntax_cmd_list_final ()
call syntax_model_file_final ()

write (u, "(A)")
write (u, "(A)")  "* Test output end: commands_34"

end subroutine commands_34

```

For this test, we invent a callback object which simply writes the analysis file, using the standard call for this. Here we rely on the fact that the analysis data are stored as a global entity, otherwise we would have to access them via the event object.

```

<Commands: test auxiliary types>≡
type, extends (event_callback_t) :: event_callback_34_t
  private
  integer :: u = 0
contains
  procedure :: write => event_callback_34_write
  procedure :: proc => event_callback_34
end type event_callback_34_t

```

The output routine is unused. The actual callback should write the analysis data to the output unit that we have injected into the callback object.

```

<Commands: test auxiliary>+≡
subroutine event_callback_34_write (event_callback, unit)
  class(event_callback_34_t), intent(in) :: event_callback
  integer, intent(in), optional :: unit
end subroutine event_callback_34_write

```



```
subroutine event_callback_34 (event_callback, i, event)
  class(event_callback_34_t), intent(in) :: event_callback
  integer(i64), intent(in) :: i
  class(generic_event_t), intent(in) :: event
  call analysis_write (event_callback%u)
end subroutine event_callback_34
```

35.2 Toplevel module WHIZARD

```
<whizard.f90>≡  
  <File header>  
  
  module whizard  
  
    use io_units  
    <Use strings>  
    use system_defs, only: VERSION_STRING  
    use system_defs, only: EOF, BACKSLASH  
    use diagnostics  
    use os_interface  
    use ifiles  
    use lexers  
    use parser  
    use eval_trees  
    use models  
    use phs_forests  
    use prclib_stacks  
    use slha_interface  
    use blha_config  
    use rt_data  
    use commands  
  
    <Standard module head>  
  
    <WHIZARD: public>  
  
    <WHIZARD: types>  
  
    <WHIZARD: variables>  
  
    save  
  
    contains  
  
    <WHIZARD: procedures>  
  
  end module whizard
```

35.2.1 Options

Here we introduce a wrapper that holds various user options, so they can transparently be passed from the main program to the `whizard` object. Most parameters are used for initializing the `global` state.

```
<WHIZARD: public>≡  
  public :: whizard_options_t  
  
<WHIZARD: types>≡  
  type :: whizard_options_t  
    type(string_t) :: job_id  
    type(string_t), dimension(:), allocatable :: pack_args  
    type(string_t), dimension(:), allocatable :: unpack_args
```

```

    type(string_t) :: preload_model
    type(string_t) :: default_lib
    type(string_t) :: preload_libraries
    logical :: rebuild_library = .false.
    logical :: recompile_library = .false.
    logical :: rebuild_phs = .false.
    logical :: rebuild_grids = .false.
    logical :: rebuild_events = .false.
end type whizard_options_t

```

35.2.2 Parse tree stack

We collect all parse trees that we generate in the `whizard` object. To this end, we create a stack of parse trees. They must not be finalized before the `global` object is finalized, because items such as a cut definition may contain references to the parse tree from which they were generated.

```

<WHIZARD: types> +=
  type, extends (parse_tree_t) :: pt_entry_t
    type(pt_entry_t), pointer :: previous => null ()
  end type pt_entry_t

```

This is the stack. Since we always prepend, we just need the `last` pointer.

```

<WHIZARD: types> +=
  type :: pt_stack_t
    type(pt_entry_t), pointer :: last => null ()
    contains
      <WHIZARD: pt stack: TBP>
  end type pt_stack_t

```

The finalizer is called at the very end.

```

<WHIZARD: pt stack: TBP> =
  procedure :: final => pt_stack_final

<WHIZARD: procedures> =
  subroutine pt_stack_final (pt_stack)
    class(pt_stack_t), intent(inout) :: pt_stack
    type(pt_entry_t), pointer :: current
    do while (associated (pt_stack%last))
      current => pt_stack%last
      pt_stack%last => current%previous
      call parse_tree_final (current%parse_tree_t)
      deallocate (current)
    end do
  end subroutine pt_stack_final

```

Create and push a new entry, keeping the previous ones.

```

<WHIZARD: pt stack: TBP> +=
  procedure :: push => pt_stack_push

```

```

<WHIZARD: procedures>+≡
  subroutine pt_stack_push (pt_stack, parse_tree)
    class(pt_stack_t), intent(inout) :: pt_stack
    type(parse_tree_t), intent(out), pointer :: parse_tree
    type(pt_entry_t), pointer :: current
    allocate (current)
    parse_tree => current%parse_tree_t
    current%previous => pt_stack%last
    pt_stack%last => current
  end subroutine pt_stack_push

```

35.2.3 The whizard object

An object of type `whizard_t` is the top-level wrapper for a `WHIZARD` instance. The object holds various default settings and the current state of the generator, the `global` object of type `rt_data_t`. This object contains, for instance, the list of variables and the process libraries.

Since components of the `global` subobject are frequently used as targets, the `whizard` object should also consistently carry the `target` attribute.

The various self-tests do not use this object. They initialize only specific subsets of the system, according to their needs.

Note: we intend to allow several concurrent instances. In the current implementation, there are still a few obstacles to this: the model library and the syntax tables are global variables, and the error handling uses global state. This should be improved.

```

<WHIZARD: public>+≡
  public :: whizard_t

<WHIZARD: types>+≡
  type :: whizard_t
    type(whizard_options_t) :: options
    type(rt_data_t) :: global
    type(pt_stack_t) :: pt_stack
  contains
    <WHIZARD: whizard: TBP>
  end type whizard_t

```

35.2.4 Initialization and finalization

```

<WHIZARD: whizard: TBP>≡
  procedure :: init => whizard_init

<WHIZARD: procedures>+≡
  subroutine whizard_init (whizard, options, paths, logfile)
    class(whizard_t), intent(out), target :: whizard
    type(whizard_options_t), intent(in) :: options
    type(paths_t), intent(in), optional :: paths
    type(string_t), intent(in), optional :: logfile
    call init_syntax_tables ()
    whizard%options = options
    call whizard%global%global_init (paths, logfile)
  end subroutine whizard_init

```

```

call whizard%init_job_id ()
call whizard%init_rebuild_flags ()
call whizard%unpack_files ()
call whizard%preload_model ()
call whizard%preload_library ()
call whizard%global%init_fallback_model &
    (var_str ("SM_hadrons"), var_str ("SM_hadrons.mdl"))
end subroutine whizard_init

```

Apart from the global data which have been initialized above, the process and model lists need to be finalized.

```

<WHIZARD: whizard: TBP>+=
  procedure :: final => whizard_final

<WHIZARD: procedures>+=
  subroutine whizard_final (whizard)
    class(whizard_t), intent(inout), target :: whizard
    call whizard%global%final ()
    call whizard%pt_stack%final ()
    call whizard%pack_files ()
    call final_syntax_tables ()
  end subroutine whizard_final

```

Set the job ID, if nonempty. If the ID string is empty, the value remains undefined.

```

<WHIZARD: whizard: TBP>+=
  procedure :: init_job_id => whizard_init_job_id

<WHIZARD: procedures>+=
  subroutine whizard_init_job_id (whizard)
    class(whizard_t), intent(inout), target :: whizard
    associate (var_list => whizard%global%var_list, options => whizard%options)
      if (options%job_id /= "") then
        call var_list%set_string (var_str ("$_job_id"), &
          options%job_id, is_known=.true.)
      end if
    end associate
  end subroutine whizard_init_job_id

```

Set the rebuild flags. They can be specified on the command line and set the initial value for the associated logical variables.

```

<WHIZARD: whizard: TBP>+=
  procedure :: init_rebuild_flags => whizard_init_rebuild_flags

<WHIZARD: procedures>+=
  subroutine whizard_init_rebuild_flags (whizard)
    class(whizard_t), intent(inout), target :: whizard
    associate (var_list => whizard%global%var_list, options => whizard%options)
      call var_list%append_log (var_str ("?rebuild_library"), &
        options%rebuild_library, intrinsic=.true.)
      call var_list%append_log (var_str ("?recompile_library"), &
        options%recompile_library, intrinsic=.true.)
      call var_list%append_log (var_str ("?rebuild_phase_space"), &

```

```

        options%rebuild_phs, intrinsic=.true.)
    call var_list%append_log (var_str ("?rebuild_grids"), &
        options%rebuild_grids, intrinsic=.true.)
    call var_list%append_log (var_str ("?rebuild_events"), &
        options%rebuild_events, intrinsic=.true.)
end associate
end subroutine whizard_init_rebuild_flags

```

Pack/unpack files in the working directory, if requested.

```

<WHIZARD: whizard: TBP>+≡
    procedure :: pack_files => whizard_pack_files
    procedure :: unpack_files => whizard_unpack_files

<WHIZARD: procedures>+≡
    subroutine whizard_pack_files (whizard)
        class(whizard_t), intent(in), target :: whizard
        logical :: exist
        integer :: i
        type(string_t) :: file
        if (allocated (whizard%options%pack_args)) then
            do i = 1, size (whizard%options%pack_args)
                file = whizard%options%pack_args(i)
                call msg_message ("Packing file/dir '" // char (file) // "'")
                exist = os_file_exist (file) .or. os_dir_exist (file)
                if (exist) then
                    call os_pack_file (whizard%options%pack_args(i), &
                        whizard%global%os_data)
                else
                    call msg_error ("File/dir '" // char (file) // "' not found")
                end if
            end do
        end if
    end subroutine whizard_pack_files

    subroutine whizard_unpack_files (whizard)
        class(whizard_t), intent(in), target :: whizard
        logical :: exist
        integer :: i
        type(string_t) :: file
        if (allocated (whizard%options%unpack_args)) then
            do i = 1, size (whizard%options%unpack_args)
                file = whizard%options%unpack_args(i)
                call msg_message ("Unpacking file '" // char (file) // "'")
                exist = os_file_exist (file)
                if (exist) then
                    call os_unpack_file (whizard%options%unpack_args(i), &
                        whizard%global%os_data)
                else
                    call msg_error ("File '" // char (file) // "' not found")
                end if
            end do
        end if
    end subroutine whizard_unpack_files

```

This procedure preloads a model, if a model name is given.

```

<WHIZARD: whizard: TBP>+=
  procedure :: preload_model => whizard_preload_model

<WHIZARD: procedures>+=
  subroutine whizard_preload_model (whizard)
    class(whizard_t), intent(inout), target :: whizard
    type(string_t) :: model_name
    model_name = whizard%options%preload_model
    if (model_name /= "") then
      call whizard%global%read_model (model_name, whizard%global%preload_model)
      whizard%global%model => whizard%global%preload_model
      if (associated (whizard%global%model)) then
        call whizard%global%model%link_var_list (whizard%global%var_list)
        call whizard%global%var_list%set_string (var_str ("$model_name"), &
          model_name, is_known = .true.)
        call msg_message ("Preloaded model: " &
          // char (model_name))
      else
        call msg_fatal ("Preloading model " // char (model_name) &
          // " failed")
      end if
    else
      call msg_message ("No model preloaded")
    end if
  end subroutine whizard_preload_model

```

This procedure preloads a library, if a library name is given.

Note: This version just opens a new library with that name. It does not load (yet) an existing library on file, as previous WHIZARD versions would do.

```

<WHIZARD: whizard: TBP>+=
  procedure :: preload_library => whizard_preload_library

<WHIZARD: procedures>+=
  subroutine whizard_preload_library (whizard)
    class(whizard_t), intent(inout), target :: whizard
    type(string_t) :: library_name, libs
    type(string_t), dimension(:), allocatable :: libname_static
    type(prclib_entry_t), pointer :: lib_entry
    integer :: i
    call get_prclib_static (libname_static)
    do i = 1, size (libname_static)
      allocate (lib_entry)
      call lib_entry%init_static (libname_static(i))
      call whizard%global%add_prclib (lib_entry)
    end do
    libs = adjustl (whizard%options%preload_libraries)
    if (libs == "" .and. whizard%options%default_lib /= "") then
      allocate (lib_entry)
      call lib_entry%init (whizard%options%default_lib)
      call whizard%global%add_prclib (lib_entry)
      call msg_message ("Preloaded library: " // &
        char (whizard%options%default_lib))
    end if
  end subroutine whizard_preload_library

```

```

SCAN_LIBS: do while (libs /= "")
  call split (libs, library_name, " ")
  if (library_name /= "") then
    allocate (lib_entry)
    call lib_entry%init (library_name)
    call whizard%global%add_prclib (lib_entry)
    call msg_message ("Preloaded library: " // char (library_name))
  end if
end do SCAN_LIBS
end subroutine whizard_preload_library

```

35.2.5 Initialization and finalization: syntax tables

Initialize/finalize the syntax tables used by WHIZARD. These are effectively singleton objects. We introduce a module variable that tracks the initialization status.

Without syntax tables, essentially nothing will work. Any initializer has to call this.

```

{WHIZARD: variables}≡
  logical :: syntax_tables_exist = .false.

{WHIZARD: public}+≡
  public :: init_syntax_tables
  public :: final_syntax_tables

{WHIZARD: procedures}+≡
  subroutine init_syntax_tables ()
    if (.not. syntax_tables_exist) then
      call syntax_model_file_init ()
      call syntax_phs_forest_init ()
      call syntax_pexpr_init ()
      call syntax_slha_init ()
      call syntax_cmd_list_init ()
      syntax_tables_exist = .true.
    end if
  end subroutine init_syntax_tables

  subroutine final_syntax_tables ()
    if (syntax_tables_exist) then
      call syntax_model_file_final ()
      call syntax_phs_forest_final ()
      call syntax_pexpr_final ()
      call syntax_slha_final ()
      call syntax_cmd_list_final ()
      syntax_tables_exist = .false.
    end if
  end subroutine final_syntax_tables

```

Write the syntax tables to external files.

```

{WHIZARD: public}+≡
  public :: write_syntax_tables

```



```

{WHIZARD: procedures}+=
subroutine write_syntax_tables ()
  integer :: unit
  character(*), parameter :: file_model = "whizard.model_file.syntax"
  character(*), parameter :: file_phs = "whizard.phase_space_file.syntax"
  character(*), parameter :: file_pexpr = "whizard.prt_expressions.syntax"
  character(*), parameter :: file_slha = "whizard.slha.syntax"
  character(*), parameter :: file_sindarin = "whizard.sindarin.syntax"
  if (.not. syntax_tables_exist) call init_syntax_tables ()
  unit = free_unit ()
  print *, "Writing file '" // file_model // "'"
  open (unit=unit, file=file_model, status="replace", action="write")
  write (unit, "(A)")  VERSION_STRING
  write (unit, "(A)")  "Syntax definition file: " // file_model
  call syntax_model_file_write (unit)
  close (unit)
  print *, "Writing file '" // file_phs // "'"
  open (unit=unit, file=file_phs, status="replace", action="write")
  write (unit, "(A)")  VERSION_STRING
  write (unit, "(A)")  "Syntax definition file: " // file_phs
  call syntax_phs_forest_write (unit)
  close (unit)
  print *, "Writing file '" // file_pexpr // "'"
  open (unit=unit, file=file_pexpr, status="replace", action="write")
  write (unit, "(A)")  VERSION_STRING
  write (unit, "(A)")  "Syntax definition file: " // file_pexpr
  call syntax_pexpr_write (unit)
  close (unit)
  print *, "Writing file '" // file_slha // "'"
  open (unit=unit, file=file_slha, status="replace", action="write")
  write (unit, "(A)")  VERSION_STRING
  write (unit, "(A)")  "Syntax definition file: " // file_slha
  call syntax_slha_write (unit)
  close (unit)
  print *, "Writing file '" // file_sindarin // "'"
  open (unit=unit, file=file_sindarin, status="replace", action="write")
  write (unit, "(A)")  VERSION_STRING
  write (unit, "(A)")  "Syntax definition file: " // file_sindarin
  call syntax_cmd_list_write (unit)
  close (unit)
end subroutine write_syntax_tables

```

35.2.6 Execute command lists

Process commands given on the command line, stored as an ifile. The whole input is read, compiled and executed as a whole.

```

{WHIZARD: whizard: TBP}+=
  procedure :: process_ifile => whizard_process_ifile

{WHIZARD: procedures}+=
subroutine whizard_process_ifile (whizard, ifile, quit, quit_code)
  class(whizard_t), intent(inout), target :: whizard
  type(ifile_t), intent(in) :: ifile

```

```

logical, intent(out) :: quit
integer, intent(out) :: quit_code
type(lexer_t), target :: lexer
type(stream_t), target :: stream
call msg_message ("Reading commands given on the command line")
call lexer_init_cmd_list (lexer)
call stream_init (stream, ifile)
call whizard%process_stream (stream, lexer, quit, quit_code)
call stream_final (stream)
call lexer_final (lexer)
end subroutine whizard_process_ifile

```

Process standard input as a command list. The whole input is read, compiled and executed as a whole.

```

<WHIZARD: whizard: TBP>+≡
  procedure :: process_stdin => whizard_process_stdin
<WHIZARD: procedures>+≡
  subroutine whizard_process_stdin (whizard, quit, quit_code)
    class(whizard_t), intent(inout), target :: whizard
    logical, intent(out) :: quit
    integer, intent(out) :: quit_code
    type(lexer_t), target :: lexer
    type(stream_t), target :: stream
    call msg_message ("Reading commands from standard input")
    call lexer_init_cmd_list (lexer)
    call stream_init (stream, 5)
    call whizard%process_stream (stream, lexer, quit, quit_code)
    call stream_final (stream)
    call lexer_final (lexer)
  end subroutine whizard_process_stdin

```

Process a file as a command list.

```

<WHIZARD: whizard: TBP>+≡
  procedure :: process_file => whizard_process_file
<WHIZARD: procedures>+≡
  subroutine whizard_process_file (whizard, file, quit, quit_code)
    class(whizard_t), intent(inout), target :: whizard
    type(string_t), intent(in) :: file
    logical, intent(out) :: quit
    integer, intent(out) :: quit_code
    type(lexer_t), target :: lexer
    type(stream_t), target :: stream
    logical :: exist
    call msg_message ("Reading commands from file '" // char (file) // "'")
    inquire (file=char(file), exist=exist)
    if (exist) then
      call lexer_init_cmd_list (lexer)
      call stream_init (stream, char (file))
      call whizard%process_stream (stream, lexer, quit, quit_code)
      call stream_final (stream)
      call lexer_final (lexer)
    else

```

```

        call msg_error ("File '" // char (file) // "' not found")
    end if
end subroutine whizard_process_file

```

```

<WHIZARD: whizard: TBP>+≡
    procedure :: process_stream => whizard_process_stream

<WHIZARD: procedures>+≡
    subroutine whizard_process_stream (whizard, stream, lexer, quit, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        type(stream_t), intent(inout), target :: stream
        type(lexer_t), intent(inout), target :: lexer
        logical, intent(out) :: quit
        integer, intent(out) :: quit_code
        type(parse_tree_t), pointer :: parse_tree
        type(command_list_t), target :: command_list
        call lexer_assign_stream (lexer, stream)
        call whizard%pt_stack%push (parse_tree)
        call parse_tree_init (parse_tree, syntax_cmd_list, lexer)
        if (associated (parse_tree%get_root_ptr ())) then
            whizard%global%lexer => lexer
            call command_list%compile (parse_tree%get_root_ptr (), &
                whizard%global)
        end if
        call whizard%global%activate ()
        call command_list%execute (whizard%global)
        call command_list%final ()
        quit = whizard%global%quit
        quit_code = whizard%global%quit_code
    end subroutine whizard_process_stream

```

35.2.7 The WHIZARD shell

This procedure implements interactive mode. One line is processed at a time.

```

<WHIZARD: whizard: TBP>+≡
    procedure :: shell => whizard_shell

<WHIZARD: procedures>+≡
    subroutine whizard_shell (whizard, quit_code)
        class(whizard_t), intent(inout), target :: whizard
        integer, intent(out) :: quit_code
        type(lexer_t), target :: lexer
        type(stream_t), target :: stream
        type(string_t) :: prompt1
        type(string_t) :: prompt2
        type(string_t) :: input
        type(string_t) :: extra
        integer :: last
        integer :: iostat
        logical :: mask_tmp
        logical :: quit
        call msg_message ("Launching interactive shell")
        call lexer_init_cmd_list (lexer)

```

```

prompt1 = "whish? "
prompt2 = "      > "
COMMAND_LOOP: do
  call put (6, prompt1)
  call get (5, input, iostat=iostat)
  if (iostat > 0 .or. iostat == EOF) exit COMMAND_LOOP
CONTINUE_INPUT: do
  last = len_trim (input)
  if (extract (input, last, last) /= BACKSLASH) exit CONTINUE_INPUT
  call put (6, prompt2)
  call get (5, extra, iostat=iostat)
  if (iostat > 0) exit COMMAND_LOOP
  input = replace (input, last, extra)
end do CONTINUE_INPUT
call stream_init (stream, input)
mask_tmp = mask_fatal_errors
mask_fatal_errors = .true.
call whizard%process_stream (stream, lexer, quit, quit_code)
msg_count = 0
mask_fatal_errors = mask_tmp
call stream_final (stream)
if (quit) exit COMMAND_LOOP
end do COMMAND_LOOP
print *
call lexer_final (lexer)
end subroutine whizard_shell

```

35.3 Query Feature Support

This module accesses the various optional features (modules) that WHIZARD can support and reports on their availability.

```
<features.f90>≡
  module features

    use string_utils, only: lower_case
    use system_dependencies, only: WHIZARD_VERSION
    <Features: dependencies>

    <Standard module head>

    <Features: public>

    contains

    <Features: procedures>

  end module features
```

35.3.1 Output

```
<Features: public>≡
  public :: print_features

<Features: procedures>≡
  subroutine print_features ()
    print "(A)", "WHIZARD " // WHIZARD_VERSION
    print "(A)", "Build configuration:"
    <Features: config>
    print "(A)", "Optional features available in this build:"
    <Features: print>
  end subroutine print_features
```

35.3.2 Query function

```
<Features: procedures>+≡
  subroutine check (feature, recognized, result, help)
    character(*), intent(in) :: feature
    logical, intent(out) :: recognized
    character(*), intent(out) :: result, help
    recognized = .true.
    result = "no"
    select case (lower_case (trim (feature)))
    <Features: cases>
    case default
      recognized = .false.
    end select
  end subroutine check
```

Print this result:

```
<Features: procedures>+≡
  subroutine print_check (feature)
    character(*), intent(in) :: feature
    character(16) :: f
    logical :: recognized
    character(10) :: result
    character(48) :: help
    call check (feature, recognized, result, help)
    if (.not. recognized) then
      result = "unknown"
      help = ""
    end if
    f = feature
    print "(2x,A,1x,A,'(',A,')')", f, result, trim (help)
  end subroutine print_check
```

35.3.3 Basic configuration

```
<Features: config>≡
  call print_check ("precision")
<Features: dependencies>≡
  use kinds, only: default
<Features: cases>≡
  case ("precision")
    write (result, "(IO)") precision (1._default)
    help = "significant decimals of real/complex numbers"
```

35.3.4 Optional features case by case

```
<Features: print>≡
  call print_check ("OpenMP")
<Features: dependencies>+≡
  use system_dependencies, only: openmp_is_active
<Features: cases>+≡
  case ("openmp")
    if (openmp_is_active ()) then
      result = "yes"
    end if
    help = "OpenMP parallel execution"
<Features: print>+≡
  call print_check ("GoSam")
<Features: dependencies>+≡
  use system_dependencies, only: GOSAM_AVAILABLE
<Features: cases>+≡
  case ("gosam")
    if (GOSAM_AVAILABLE) then
      result = "yes"
    end if
    help = "external NLO matrix element provider"
```

```

<Features: print>+≡
    call print_check ("OpenLoops")

<Features: dependencies>+≡
    use system_dependencies, only: OPENLOOPS_AVAILABLE

<Features: cases>+≡
    case ("openloops")
        if (OPENLOOPS_AVAILABLE) then
            result = "yes"
        end if
        help = "external NLO matrix element provider"

<Features: print>+≡
    call print_check ("Recola")

<Features: dependencies>+≡
    use system_dependencies, only: RECOLA_AVAILABLE

<Features: cases>+≡
    case ("recola")
        if (RECOLA_AVAILABLE) then
            result = "yes"
        end if
        help = "external NLO matrix element provider"

<Features: print>+≡
    call print_check ("LHAPDF")

<Features: dependencies>+≡
    use system_dependencies, only: LHAPDF5_AVAILABLE
    use system_dependencies, only: LHAPDF6_AVAILABLE

<Features: cases>+≡
    case ("lhpdf")
        if (LHAPDF5_AVAILABLE) then
            result = "v5"
        else if (LHAPDF6_AVAILABLE) then
            result = "v6"
        end if
        help = "PDF library"

<Features: print>+≡
    call print_check ("HOPPET")

<Features: dependencies>+≡
    use system_dependencies, only: HOPPET_AVAILABLE

<Features: cases>+≡
    case ("hoppet")
        if (HOPPET_AVAILABLE) then
            result = "yes"
        end if
        help = "PDF evolution package"

<Features: print>+≡
    call print_check ("fastjet")

<Features: dependencies>+≡
    use jets, only: fastjet_available

```

```

<Features: cases>+=
  case ("fastjet")
    if (fastjet_available ()) then
      result = "yes"
    end if
    help = "jet-clustering package"

<Features: print>+=
  call print_check ("Pythia6")

<Features: dependencies>+=
  use system_dependencies, only: PYTHIA6_AVAILABLE

<Features: cases>+=
  case ("pythia6")
    if (PYTHIA6_AVAILABLE) then
      result = "yes"
    end if
    help = "direct access for shower/hadronization"

<Features: print>+=
  call print_check ("Pythia8")

<Features: dependencies>+=
  use system_dependencies, only: PYTHIA8_AVAILABLE

<Features: cases>+=
  case ("pythia8")
    if (PYTHIA8_AVAILABLE) then
      result = "yes"
    end if
    help = "direct access for shower/hadronization"

<Features: print>+=
  call print_check ("StdHEP")

<Features: cases>+=
  case ("stdhep")
    result = "yes"
    help = "event I/O format"

<Features: print>+=
  call print_check ("HepMC")

<Features: dependencies>+=
  use hepmc_interface, only: hepmc_is_available

<Features: cases>+=
  case ("hepmc")
    if (hepmc_is_available ()) then
      result = "yes"
    end if
    help = "event I/O format"

<Features: print>+=
  call print_check ("LCIO")

<Features: dependencies>+=
  use lcio_interface, only: lcio_is_available

```



```

<Features: cases>+≡
  case ("lcio")
    if (lcio_is_available ()) then
      result = "yes"
    end if
    help = "event I/O format"

<Features: print>+≡
  call print_check ("MetaPost")

<Features: dependencies>+≡
  use system_dependencies, only: EVENT_ANALYSIS

<Features: cases>+≡
  case ("metapost")
    result = EVENT_ANALYSIS
    help = "graphical event analysis via LaTeX/MetaPost"

```

Chapter 36

Cross References

36.1 Identifiers

36.2 Chunks